



# Full wwPDB NMR Structure Validation Report ⓘ

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BMRB ID : 17481  
Title : Solution NMR Structure of Q5HLI9 from Staphylococcus epidermidis, Northeast Structural Genomics Consortium Target SeR147  
Authors : Mills, J.L.; Eletsky, A.; Lee, H.; Lee, D.; Ciccocanti, C.; Sapin, A.; Mao, L.; Nair, R.; Rost, B.; Acton, T.B.; Xiao, R.; Everett, J.K.; Prestegard, J.H.; Montelione, G.T.; Szyperski, T.; Northeast Structural Genomics Consortium (NESG)  
Deposited on : 2011-02-22

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| wwPDB-RCI                      | : | v_1n_11_5_13_A (Berjanski et al., 2005)                          |
| PANAV                          | : | Wang et al. (2010)                                               |
| wwPDB-ShiftChecker             | : | v1.2                                                             |
| BMRB Restraints Analysis       | : | v1.2                                                             |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

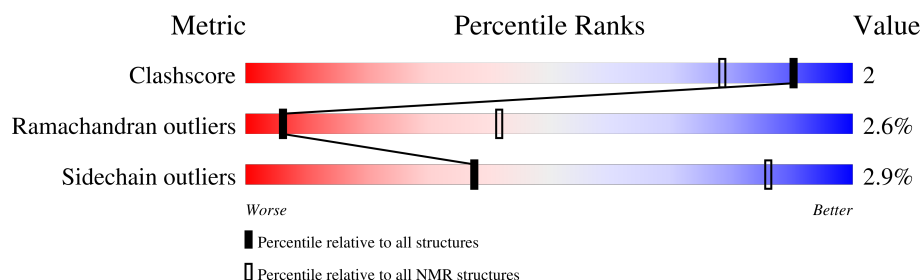
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 89%.

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     | 164    |                  |

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:3-A:110, A:114-A:155<br>(150) | 0.84              | 1            |

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 5 clusters and 4 single-model clusters were found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2608 atoms, of which 1286 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Uncharacterized protein.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|-------|
| 1   | A     | 164      | Total | C   | H    | N   | O   | S | 0     |
|     |       |          | 2608  | 845 | 1286 | 216 | 255 | 6 |       |

There are 10 discrepancies between the modelled and reference sequences:

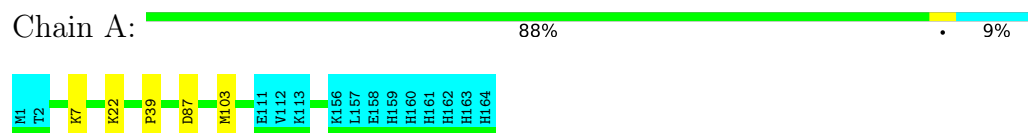
| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 56      | SER      | ASN    | variant        | UNP Q5HLI9 |
| A     | 67      | ILE      | THR    | variant        | UNP Q5HLI9 |
| A     | 157     | LEU      | -      | expression tag | UNP Q5HLI9 |
| A     | 158     | GLU      | -      | expression tag | UNP Q5HLI9 |
| A     | 159     | HIS      | -      | expression tag | UNP Q5HLI9 |
| A     | 160     | HIS      | -      | expression tag | UNP Q5HLI9 |
| A     | 161     | HIS      | -      | expression tag | UNP Q5HLI9 |
| A     | 162     | HIS      | -      | expression tag | UNP Q5HLI9 |
| A     | 163     | HIS      | -      | expression tag | UNP Q5HLI9 |
| A     | 164     | HIS      | -      | expression tag | UNP Q5HLI9 |

## 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: Uncharacterized protein

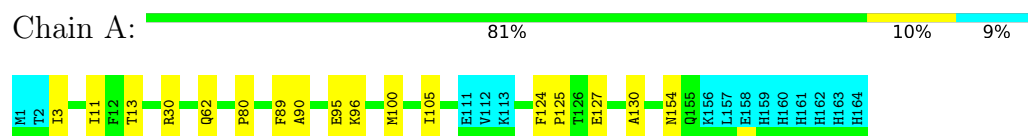


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

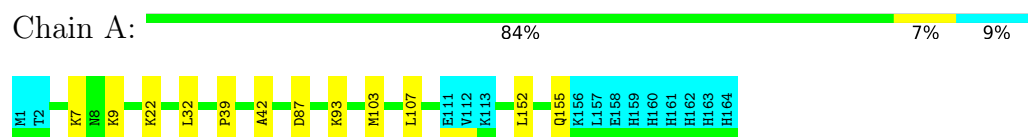
#### 4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Uncharacterized protein



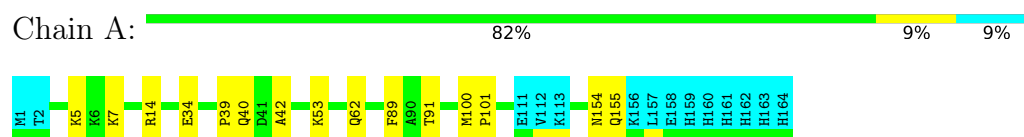
#### 4.2.2 Score per residue for model 2

- Molecule 1: Uncharacterized protein



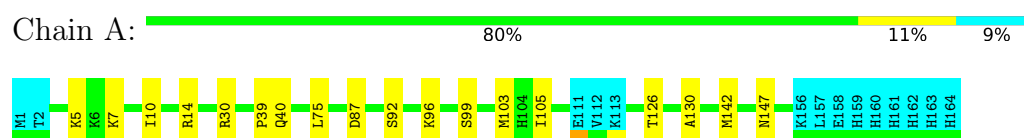
### 4.2.3 Score per residue for model 3

- Molecule 1: Uncharacterized protein



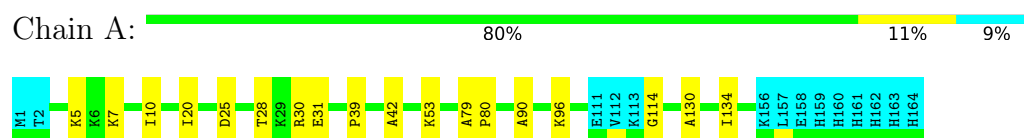
### 4.2.4 Score per residue for model 4

- Molecule 1: Uncharacterized protein



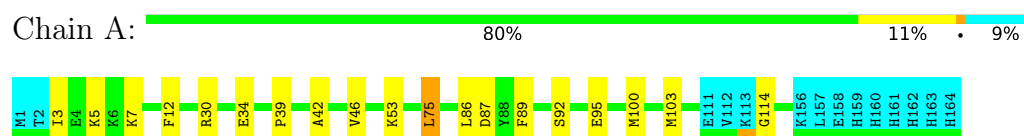
### 4.2.5 Score per residue for model 5

- Molecule 1: Uncharacterized protein



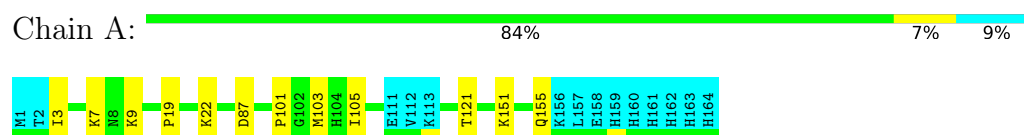
### 4.2.6 Score per residue for model 6

- Molecule 1: Uncharacterized protein



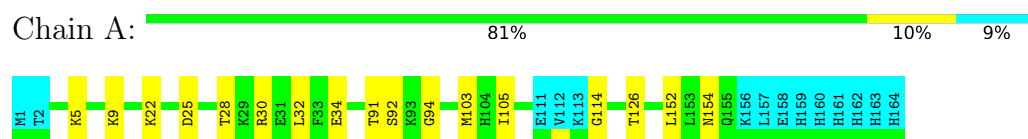
### 4.2.7 Score per residue for model 7

- Molecule 1: Uncharacterized protein



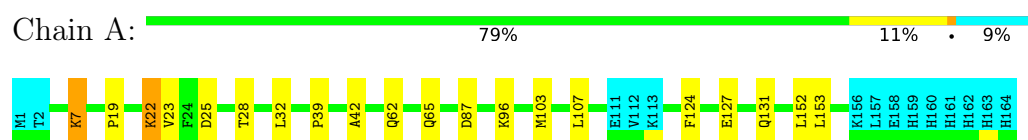
### 4.2.8 Score per residue for model 8

- Molecule 1: Uncharacterized protein



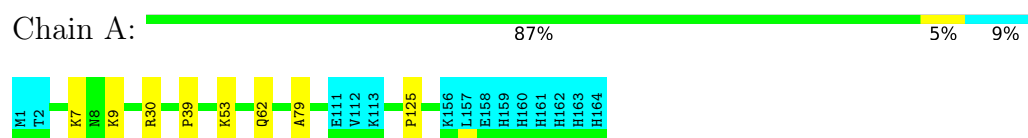
### 4.2.9 Score per residue for model 9

- Molecule 1: Uncharacterized protein



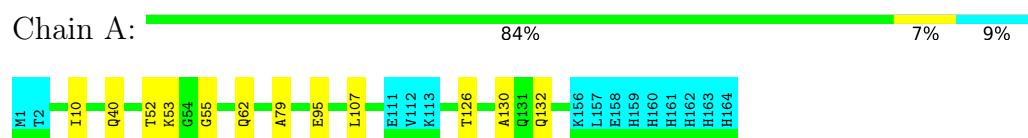
### 4.2.10 Score per residue for model 10

- Molecule 1: Uncharacterized protein



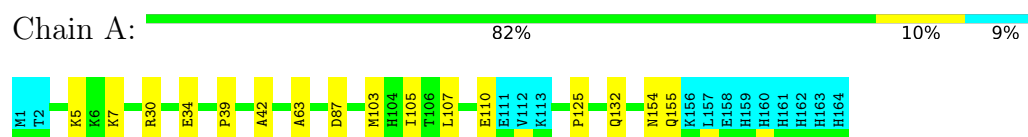
### 4.2.11 Score per residue for model 11

- Molecule 1: Uncharacterized protein



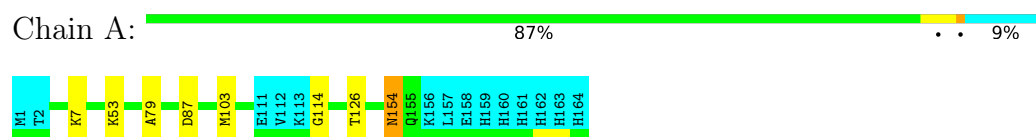
### 4.2.12 Score per residue for model 12

- Molecule 1: Uncharacterized protein



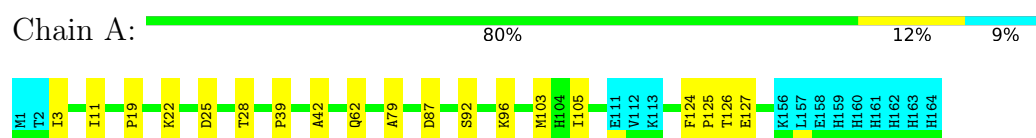
### 4.2.13 Score per residue for model 13

- Molecule 1: Uncharacterized protein



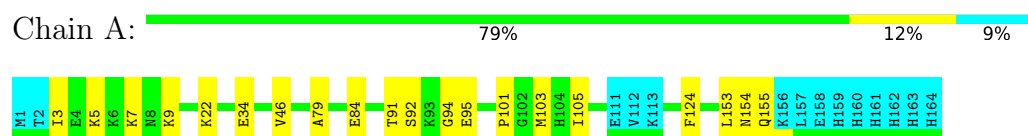
### 4.2.14 Score per residue for model 14

- Molecule 1: Uncharacterized protein



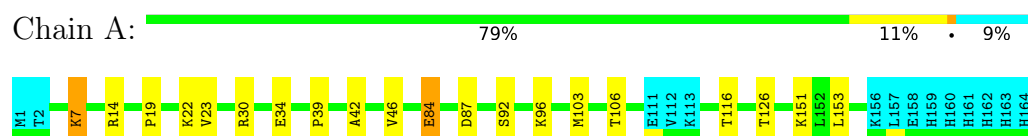
### 4.2.15 Score per residue for model 15

- Molecule 1: Uncharacterized protein



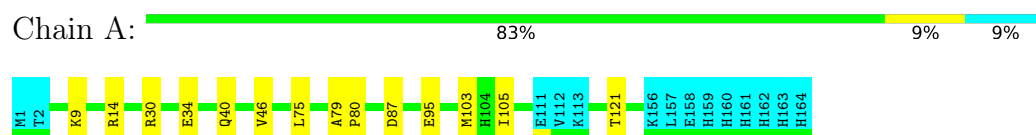
### 4.2.16 Score per residue for model 16

- Molecule 1: Uncharacterized protein



### 4.2.17 Score per residue for model 17

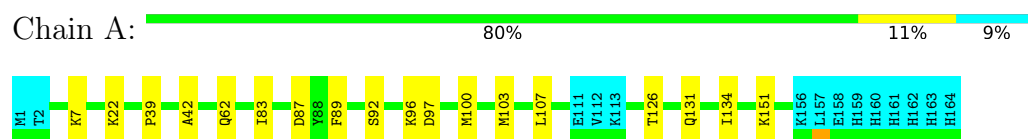
- Molecule 1: Uncharacterized protein





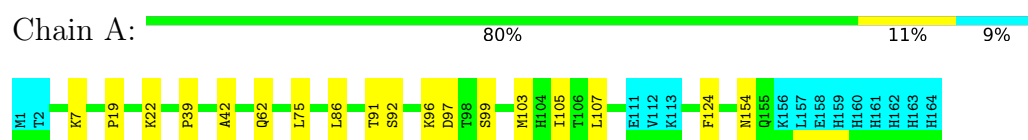
### 4.2.18 Score per residue for model 18

- Molecule 1: Uncharacterized protein



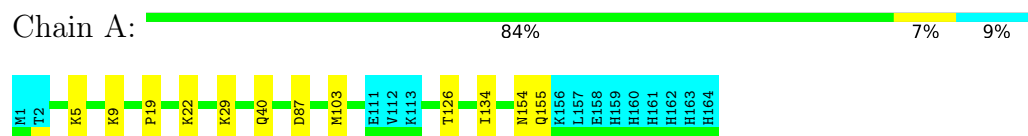
### 4.2.19 Score per residue for model 19

- Molecule 1: Uncharacterized protein



### 4.2.20 Score per residue for model 20

- Molecule 1: Uncharacterized protein



## 5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

| Software name | Classification        | Version |
|---------------|-----------------------|---------|
| TALOS+        | geometry optimization |         |
| CNS           | refinement            |         |

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

|                                              |                |
|----------------------------------------------|----------------|
| Chemical shift file(s)                       | working_cs.cif |
| Number of chemical shift lists               | 1              |
| Total number of shifts                       | 1840           |
| Number of shifts mapped to atoms             | 1840           |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 89%            |

## 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     | 1.43±0.01    | 0±1/1225 ( 0.0± 0.1%) | 0.90±0.01   | 0±0/1662 ( 0.0± 0.0%) |
| All | All   | 1.43         | 9/24500 ( 0.0%)       | 0.90        | 0/33240 ( 0.0%)       |

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     | 105 | ILE  | CA-CB | 5.43 | 1.60        | 1.54     | 8      | 5     |
| 1   | A     | 52  | THR  | CA-CB | 5.35 | 1.58        | 1.53     | 11     | 1     |
| 1   | A     | 95  | GLU  | CA-C  | 5.22 | 1.55        | 1.52     | 6      | 1     |
| 1   | A     | 63  | ALA  | C-N   | 5.19 | 1.39        | 1.34     | 12     | 1     |
| 1   | A     | 55  | GLY  | N-CA  | 5.09 | 1.48        | 1.44     | 11     | 1     |

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1   | A     | 1196  | 1162     | 1160     | 4±2     |
| All | All   | 23920 | 23240    | 23200    | 82      |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

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

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:89:PHE:HB2   | 1:A:100:MET:SD   | 0.61     | 2.35        | 3      | 2     |
| 1:A:75:LEU:HD21  | 1:A:86:LEU:HG    | 0.57     | 1.76        | 6      | 2     |
| 1:A:34:GLU:HB3   | 1:A:46:VAL:HG23  | 0.56     | 1.78        | 15     | 4     |
| 1:A:39:PRO:HG2   | 1:A:42:ALA:HB3   | 0.55     | 1.77        | 6      | 10    |
| 1:A:84:GLU:HG2   | 1:A:106:THR:HG22 | 0.55     | 1.79        | 16     | 1     |
| 1:A:87:ASP:HB3   | 1:A:103:MET:HB3  | 0.54     | 1.80        | 7      | 12    |
| 1:A:103:MET:SD   | 1:A:124:PHE:HA   | 0.52     | 2.44        | 19     | 4     |
| 1:A:90:ALA:HA    | 1:A:96:LYS:HA    | 0.51     | 1.82        | 5      | 2     |
| 1:A:89:PHE:HB3   | 1:A:100:MET:SD   | 0.49     | 2.47        | 18     | 2     |
| 1:A:23:VAL:HG22  | 1:A:153:LEU:HD13 | 0.48     | 1.84        | 16     | 2     |
| 1:A:10:ILE:HG13  | 1:A:130:ALA:HB1  | 0.48     | 1.85        | 5      | 3     |
| 1:A:19:PRO:HG2   | 1:A:22:LYS:HB3   | 0.48     | 1.86        | 9      | 1     |
| 1:A:30:ARG:O     | 1:A:34:GLU:HG2   | 0.47     | 2.09        | 6      | 5     |
| 1:A:53:LYS:H     | 1:A:53:LYS:HD3   | 0.47     | 1.68        | 13     | 2     |
| 1:A:19:PRO:HG2   | 1:A:22:LYS:HG2   | 0.47     | 1.86        | 14     | 4     |
| 1:A:20:ILE:HG13  | 1:A:80:PRO:HB2   | 0.46     | 1.86        | 5      | 1     |
| 1:A:9:LYS:HE3    | 1:A:121:THR:HG23 | 0.46     | 1.86        | 7      | 1     |
| 1:A:3:ILE:HG22   | 1:A:13:THR:HG22  | 0.45     | 1.88        | 1      | 1     |
| 1:A:30:ARG:HD2   | 1:A:31:GLU:N     | 0.45     | 2.26        | 5      | 1     |
| 1:A:83:ILE:HB    | 1:A:107:LEU:HD13 | 0.45     | 1.89        | 18     | 1     |
| 1:A:25:ASP:HA    | 1:A:28:THR:OG1   | 0.44     | 2.13        | 14     | 4     |
| 1:A:3:ILE:HB     | 1:A:11:ILE:O     | 0.44     | 2.13        | 1      | 2     |
| 1:A:32:LEU:HB3   | 1:A:152:LEU:HD21 | 0.43     | 1.91        | 2      | 2     |
| 1:A:19:PRO:HG2   | 1:A:22:LYS:HG3   | 0.42     | 1.91        | 20     | 1     |
| 1:A:14:ARG:HH12  | 1:A:147:ASN:ND2  | 0.42     | 2.13        | 4      | 1     |
| 1:A:131:GLN:HA   | 1:A:134:ILE:HD12 | 0.42     | 1.91        | 18     | 1     |
| 1:A:22:LYS:HB3   | 1:A:153:LEU:HD22 | 0.42     | 1.90        | 15     | 1     |
| 1:A:5:LYS:HG2    | 1:A:134:ILE:HG13 | 0.41     | 1.91        | 20     | 2     |
| 1:A:3:ILE:HD13   | 1:A:12:PHE:HD1   | 0.41     | 1.75        | 6      | 1     |
| 1:A:32:LEU:HD22  | 1:A:152:LEU:HD11 | 0.41     | 1.93        | 8      | 1     |
| 1:A:154:ASN:HD22 | 1:A:154:ASN:N    | 0.41     | 2.13        | 13     | 1     |
| 1:A:10:ILE:HG21  | 1:A:142:MET:HE1  | 0.40     | 1.92        | 4      | 1     |
| 1:A:124:PHE:HB2  | 1:A:130:ALA:HB2  | 0.40     | 1.94        | 1      | 1     |
| 1:A:91:THR:HB    | 1:A:97:ASP:HA    | 0.40     | 1.93        | 19     | 1     |
| 1:A:9:LYS:HD3    | 1:A:121:THR:HG23 | 0.40     | 1.93        | 17     | 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     | 150/164 (91%)   | 135±3 (90±2%) | 12±2 (8±1%) | 4±1 (3±1%) | 6           | 42 |
| All | All   | 3000/3280 (91%) | 2691 (90%)    | 230 (8%)    | 79 (3%)    | 6           | 42 |

All 19 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 7   | LYS  | 14             |
| 1   | A     | 92  | SER  | 8              |
| 1   | A     | 126 | THR  | 8              |
| 1   | A     | 79  | ALA  | 7              |
| 1   | A     | 155 | GLN  | 6              |
| 1   | A     | 95  | GLU  | 4              |
| 1   | A     | 125 | PRO  | 4              |
| 1   | A     | 40  | GLN  | 4              |
| 1   | A     | 53  | LYS  | 4              |
| 1   | A     | 114 | GLY  | 4              |
| 1   | A     | 101 | PRO  | 3              |
| 1   | A     | 80  | PRO  | 2              |
| 1   | A     | 127 | GLU  | 2              |
| 1   | A     | 39  | PRO  | 2              |
| 1   | A     | 99  | SER  | 2              |
| 1   | A     | 94  | GLY  | 2              |
| 1   | A     | 3   | ILE  | 1              |
| 1   | A     | 103 | MET  | 1              |
| 1   | A     | 97  | ASP  | 1              |

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

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

| Mol | Chain | Analysed        | Rotameric     | Outliers   | Percentiles |    |
|-----|-------|-----------------|---------------|------------|-------------|----|
| 1   | A     | 130/144 (90%)   | 126±2 (97±1%) | 4±2 (3±1%) | 38          | 86 |
| All | All   | 2600/2880 (90%) | 2525 (97%)    | 75 (3%)    | 38          | 86 |

All 25 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     | 62  | GLN  | 8              |
| 1   | A     | 154 | ASN  | 8              |
| 1   | A     | 5   | LYS  | 6              |
| 1   | A     | 96  | LYS  | 6              |
| 1   | A     | 9   | LYS  | 5              |
| 1   | A     | 107 | LEU  | 5              |
| 1   | A     | 105 | ILE  | 4              |
| 1   | A     | 22  | LYS  | 4              |
| 1   | A     | 30  | ARG  | 3              |
| 1   | A     | 14  | ARG  | 3              |
| 1   | A     | 91  | THR  | 3              |
| 1   | A     | 75  | LEU  | 3              |
| 1   | A     | 151 | LYS  | 2              |
| 1   | A     | 7   | LYS  | 2              |
| 1   | A     | 132 | GLN  | 2              |
| 1   | A     | 84  | GLU  | 2              |
| 1   | A     | 93  | LYS  | 1              |
| 1   | A     | 34  | GLU  | 1              |
| 1   | A     | 65  | GLN  | 1              |
| 1   | A     | 127 | GLU  | 1              |
| 1   | A     | 131 | GLN  | 1              |
| 1   | A     | 110 | GLU  | 1              |
| 1   | A     | 3   | ILE  | 1              |
| 1   | A     | 40  | GLN  | 1              |
| 1   | A     | 29  | LYS  | 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 89% for the well-defined parts and 82% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

Chemical shift list name: *DEPOSIT3.str*

#### 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                  | 1840 |
| Number of shifts mapped to atoms        | 1840 |
| Number of unparsed shifts               | 0    |
| Number of shifts with mapping errors    | 0    |
| Number of shifts with mapping warnings  | 0    |
| Number of shift outliers (ShiftChecker) | 5    |

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 152      | $-0.24 \pm 0.11$                | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}_\beta$  | 145      | $-0.17 \pm 0.15$                | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}'$       | 136      | $0.17 \pm 0.16$                 | None needed ( $< 0.5$ ppm) |
| $^{15}\text{N}$        | 138      | $-1.05 \pm 0.22$                | Should be applied          |

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 89%, i.e. 1787 atoms were assigned a chemical shift out of a possible 2018. 0 out of 14 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total          | $^1\text{H}$  | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|----------------|---------------|-----------------|-----------------|
| Backbone  | 701/745 (94%)  | 288/301 (96%) | 279/300 (93%)   | 134/144 (93%)   |
| Sidechain | 971/1064 (91%) | 661/692 (96%) | 294/339 (87%)   | 16/33 (48%)     |

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|          | <b>Total</b>    | <b><sup>1</sup>H</b> | <b><sup>13</sup>C</b> | <b><sup>15</sup>N</b> |
|----------|-----------------|----------------------|-----------------------|-----------------------|
| Aromatic | 115/209 (55%)   | 73/100 (73%)         | 41/104 (39%)          | 1/5 (20%)             |
| Overall  | 1787/2018 (89%) | 1022/1093 (94%)      | 614/743 (83%)         | 151/182 (83%)         |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 82%, i.e. 1840 atoms were assigned a chemical shift out of a possible 2233. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | <b>Total</b>    | <b><sup>1</sup>H</b> | <b><sup>13</sup>C</b> | <b><sup>15</sup>N</b> |
|-----------|-----------------|----------------------|-----------------------|-----------------------|
| Backbone  | 722/815 (89%)   | 296/329 (90%)        | 288/328 (88%)         | 138/158 (87%)         |
| Sidechain | 1003/1161 (86%) | 680/755 (90%)        | 307/371 (83%)         | 16/35 (46%)           |
| Aromatic  | 115/257 (45%)   | 73/124 (59%)         | 41/116 (35%)          | 1/17 (6%)             |
| Overall   | 1840/2233 (82%) | 1049/1208 (87%)      | 636/815 (78%)         | 155/210 (74%)         |

#### 7.1.4 Statistically unusual chemical shifts ⓘ

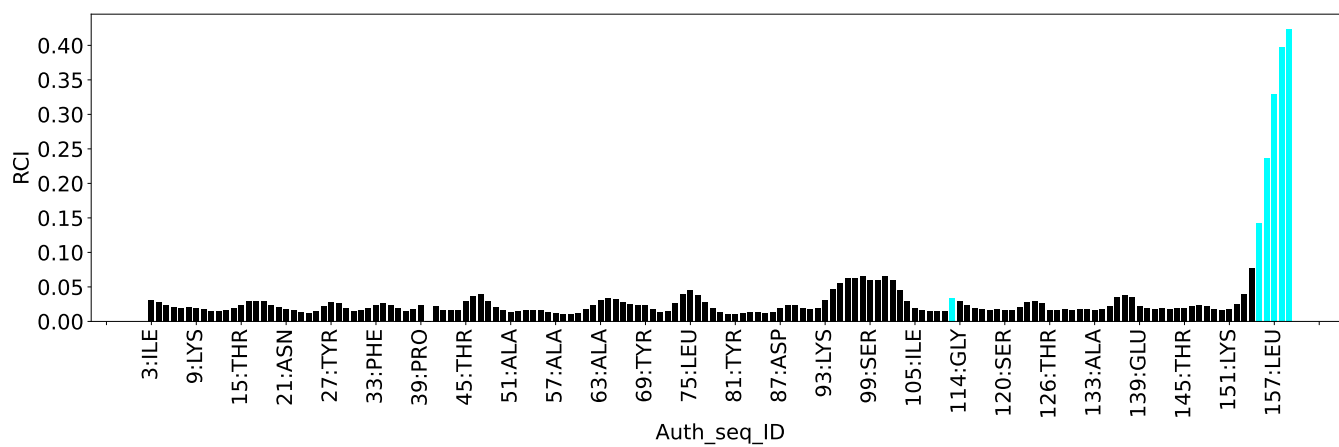
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

| List Id | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|---------|-------|-----|------|------|------------|---------------------|---------|
| 1       | A     | 37  | PHE  | HB3  | -0.21      | 1.03 – 4.85         | -8.3    |
| 1       | A     | 80  | PRO  | HA   | 2.02       | 2.78 – 6.00         | -7.3    |
| 1       | A     | 105 | ILE  | HB   | 0.14       | 0.35 – 3.22         | -5.7    |
| 1       | A     | 149 | LEU  | HG   | -0.30      | -0.13 – 3.16        | -5.5    |
| 1       | A     | 70  | THR  | HB   | 2.55       | 2.57 – 5.77         | -5.0    |

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

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

Random coil index (RCI) for chain A:



## 8 NMR restraints analysis

### 8.1 Conformationally restricting restraints

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

| Description                                              | Value |
|----------------------------------------------------------|-------|
| Total distance restraints                                | 5380  |
| Intra-residue ( $ i-j =0$ )                              | 2122  |
| Sequential ( $ i-j =1$ )                                 | 1199  |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 663   |
| Long range ( $ i-j \geq 5$ )                             | 1396  |
| Inter-chain                                              | 0     |
| Hydrogen bond restraints                                 | 0     |
| Disulfide bond restraints                                | 0     |
| Total dihedral-angle restraints                          | 202   |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 34.0  |
| Number of long range restraints per residue <sup>1</sup> | 8.5   |

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

### 8.2 Residual restraint violations

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

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

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

| Bins (Å)         | Average number of violations per model | Max (Å) |
|------------------|----------------------------------------|---------|
| 0.1-0.2 (Small)  | 23.4                                   | 0.2     |
| 0.2-0.5 (Medium) | 11.4                                   | 0.43    |
| >0.5 (Large)     | None                                   | None    |

### 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)   | 25.2                                   | 8.15    |
| 10.0-20.0 (Medium) | None                                   | None    |
| >20.0 (Large)      | None                                   | None    |

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

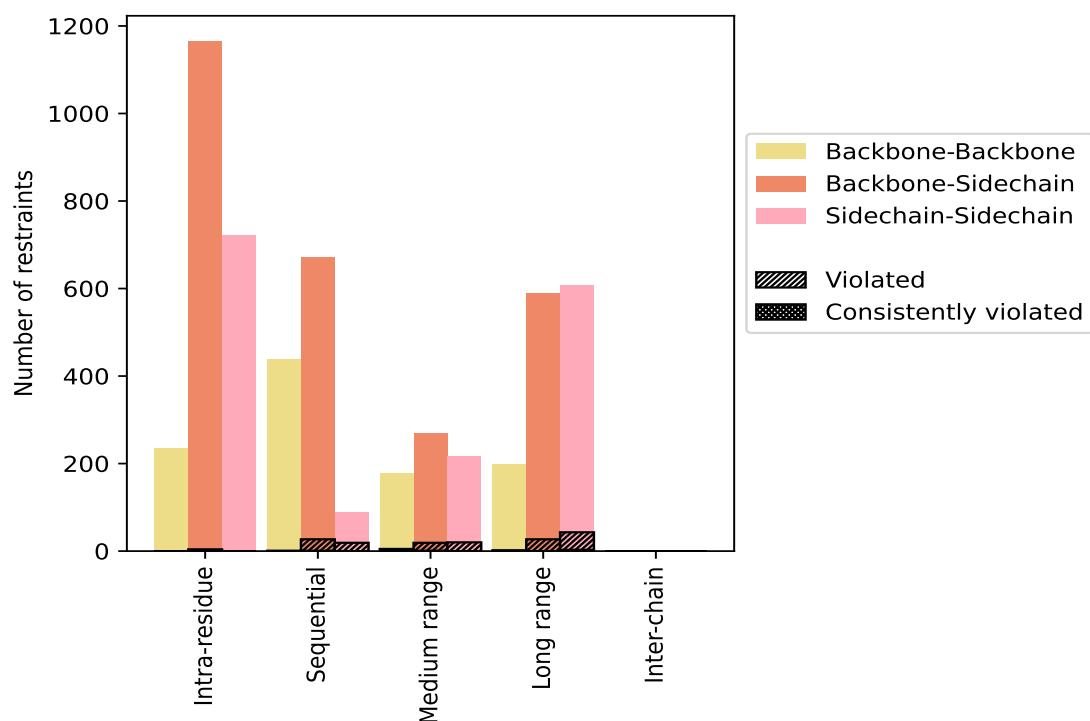
### 9.1 Summary of distance violations [i](#)

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

| Restrains type                                             | Count                | % <sup>1</sup>        | Violated <sup>3</sup> |                     |                     | Consistently Violated <sup>4</sup> |                     |                     |
|------------------------------------------------------------|----------------------|-----------------------|-----------------------|---------------------|---------------------|------------------------------------|---------------------|---------------------|
|                                                            |                      |                       | Count                 | % <sup>2</sup>      | % <sup>1</sup>      | Count                              | % <sup>2</sup>      | % <sup>1</sup>      |
| <a href="#">Intra-residue ( i-j =0)</a>                    | <a href="#">2122</a> | <a href="#">39.4</a>  | <a href="#">4</a>     | <a href="#">0.2</a> | <a href="#">0.1</a> | <a href="#">0</a>                  | <a href="#">0.0</a> | <a href="#">0.0</a> |
| Backbone-Backbone                                          | 235                  | 4.4                   | 0                     | 0.0                 | 0.0                 | 0                                  | 0.0                 | 0.0                 |
| Backbone-Sidechain                                         | 1165                 | 21.7                  | 4                     | 0.3                 | 0.1                 | 0                                  | 0.0                 | 0.0                 |
| Sidechain-Sidechain                                        | 722                  | 13.4                  | 0                     | 0.0                 | 0.0                 | 0                                  | 0.0                 | 0.0                 |
| <a href="#">Sequential ( i-j =1)</a>                       | <a href="#">1199</a> | <a href="#">22.3</a>  | <a href="#">47</a>    | <a href="#">3.9</a> | <a href="#">0.9</a> | <a href="#">1</a>                  | <a href="#">0.1</a> | <a href="#">0.0</a> |
| Backbone-Backbone                                          | 439                  | 8.2                   | 1                     | 0.2                 | 0.0                 | 0                                  | 0.0                 | 0.0                 |
| Backbone-Sidechain                                         | 671                  | 12.5                  | 27                    | 4.0                 | 0.5                 | 1                                  | 0.1                 | 0.0                 |
| Sidechain-Sidechain                                        | 89                   | 1.7                   | 19                    | 21.3                | 0.4                 | 0                                  | 0.0                 | 0.0                 |
| <a href="#">Medium range ( i-j &gt;1 &amp;  i-j &lt;5)</a> | <a href="#">663</a>  | <a href="#">12.3</a>  | <a href="#">44</a>    | <a href="#">6.6</a> | <a href="#">0.8</a> | <a href="#">1</a>                  | <a href="#">0.2</a> | <a href="#">0.0</a> |
| Backbone-Backbone                                          | 177                  | 3.3                   | 5                     | 2.8                 | 0.1                 | 0                                  | 0.0                 | 0.0                 |
| Backbone-Sidechain                                         | 269                  | 5.0                   | 19                    | 7.1                 | 0.4                 | 1                                  | 0.4                 | 0.0                 |
| Sidechain-Sidechain                                        | 217                  | 4.0                   | 20                    | 9.2                 | 0.4                 | 0                                  | 0.0                 | 0.0                 |
| <a href="#">Long range ( i-j ≥5)</a>                       | <a href="#">1396</a> | <a href="#">25.9</a>  | <a href="#">72</a>    | <a href="#">5.2</a> | <a href="#">1.3</a> | <a href="#">3</a>                  | <a href="#">0.2</a> | <a href="#">0.1</a> |
| Backbone-Backbone                                          | 198                  | 3.7                   | 2                     | 1.0                 | 0.0                 | 0                                  | 0.0                 | 0.0                 |
| Backbone-Sidechain                                         | 590                  | 11.0                  | 27                    | 4.6                 | 0.5                 | 0                                  | 0.0                 | 0.0                 |
| Sidechain-Sidechain                                        | 608                  | 11.3                  | 43                    | 7.1                 | 0.8                 | 3                                  | 0.5                 | 0.1                 |
| <a href="#">Inter-chain</a>                                | <a href="#">0</a>    | <a href="#">0.0</a>   | <a href="#">0</a>     | <a href="#">0.0</a> | <a href="#">0.0</a> | <a href="#">0</a>                  | <a href="#">0.0</a> | <a href="#">0.0</a> |
| 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                 |
| <a href="#">Hydrogen bond</a>                              | <a href="#">0</a>    | <a href="#">0.0</a>   | <a href="#">0</a>     | <a href="#">0.0</a> | <a href="#">0.0</a> | <a href="#">0</a>                  | <a href="#">0.0</a> | <a href="#">0.0</a> |
| <a href="#">Disulfide bond</a>                             | <a href="#">0</a>    | <a href="#">0.0</a>   | <a href="#">0</a>     | <a href="#">0.0</a> | <a href="#">0.0</a> | <a href="#">0</a>                  | <a href="#">0.0</a> | <a href="#">0.0</a> |
| <a href="#">Total</a>                                      | <a href="#">5380</a> | <a href="#">100.0</a> | <a href="#">167</a>   | <a href="#">3.1</a> | <a href="#">3.1</a> | <a href="#">5</a>                  | <a href="#">0.1</a> | <a href="#">0.1</a> |
| Backbone-Backbone                                          | 1049                 | 19.5                  | 8                     | 0.8                 | 0.1                 | 0                                  | 0.0                 | 0.0                 |
| Backbone-Sidechain                                         | 2695                 | 50.1                  | 77                    | 2.9                 | 1.4                 | 2                                  | 0.1                 | 0.0                 |
| Sidechain-Sidechain                                        | 1636                 | 30.4                  | 82                    | 5.0                 | 1.5                 | 3                                  | 0.2                 | 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 disulfied bonds are counted in their appropriate category on the x-axis

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

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

| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 1        | 1                    | 13              | 7               | 12              | 0               | 33    | 0.2      | 0.4     | 0.08                | 0.18       |
| 2        | 1                    | 7               | 11              | 16              | 0               | 35    | 0.2      | 0.42    | 0.07                | 0.18       |
| 3        | 0                    | 12              | 12              | 12              | 0               | 36    | 0.17     | 0.4     | 0.06                | 0.16       |
| 4        | 1                    | 9               | 11              | 12              | 0               | 33    | 0.18     | 0.34    | 0.06                | 0.17       |
| 5        | 1                    | 11              | 9               | 15              | 0               | 36    | 0.19     | 0.38    | 0.07                | 0.18       |
| 6        | 1                    | 10              | 10              | 18              | 0               | 39    | 0.17     | 0.36    | 0.06                | 0.15       |
| 7        | 1                    | 10              | 9               | 14              | 0               | 34    | 0.17     | 0.32    | 0.05                | 0.17       |
| 8        | 1                    | 11              | 7               | 16              | 0               | 35    | 0.18     | 0.38    | 0.07                | 0.16       |
| 9        | 0                    | 11              | 7               | 18              | 0               | 36    | 0.18     | 0.42    | 0.08                | 0.16       |
| 10       | 1                    | 12              | 13              | 18              | 0               | 44    | 0.17     | 0.37    | 0.07                | 0.16       |

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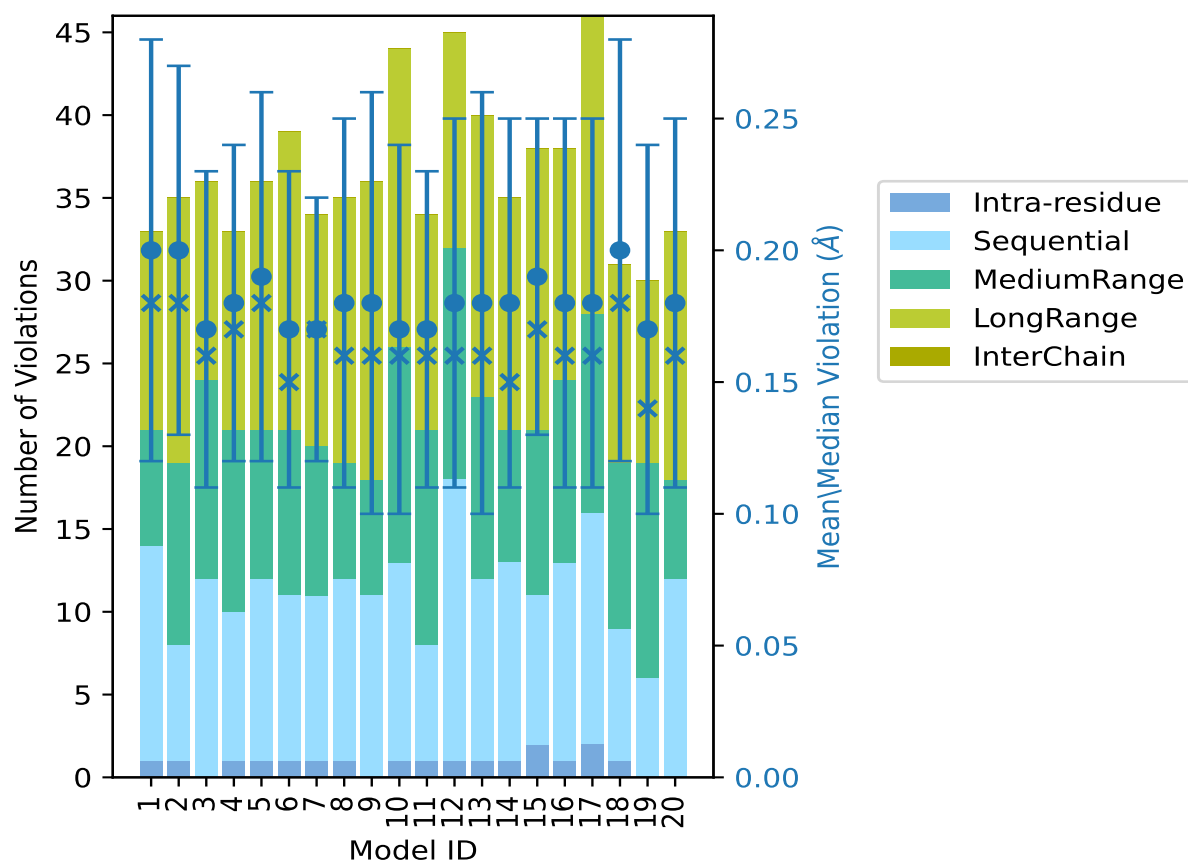
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| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 11       | 1                    | 7               | 13              | 13              | 0               | 34    | 0.17     | 0.33    | 0.06                | 0.16       |
| 12       | 1                    | 17              | 14              | 13              | 0               | 45    | 0.18     | 0.4     | 0.07                | 0.16       |
| 13       | 1                    | 11              | 11              | 17              | 0               | 40    | 0.18     | 0.43    | 0.08                | 0.16       |
| 14       | 1                    | 12              | 8               | 14              | 0               | 35    | 0.18     | 0.38    | 0.07                | 0.15       |
| 15       | 2                    | 9               | 10              | 17              | 0               | 38    | 0.19     | 0.39    | 0.06                | 0.17       |
| 16       | 1                    | 12              | 11              | 14              | 0               | 38    | 0.18     | 0.36    | 0.07                | 0.16       |
| 17       | 2                    | 14              | 12              | 18              | 0               | 46    | 0.18     | 0.37    | 0.07                | 0.16       |
| 18       | 1                    | 8               | 10              | 12              | 0               | 31    | 0.2      | 0.37    | 0.08                | 0.18       |
| 19       | 0                    | 6               | 13              | 11              | 0               | 30    | 0.17     | 0.36    | 0.07                | 0.14       |
| 20       | 0                    | 12              | 6               | 15              | 0               | 33    | 0.18     | 0.34    | 0.07                | 0.16       |

<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, 5213(IR:2118, SQ:1152, MR:619, LR:1324, IC:0) restraints are not violated in the ensemble.

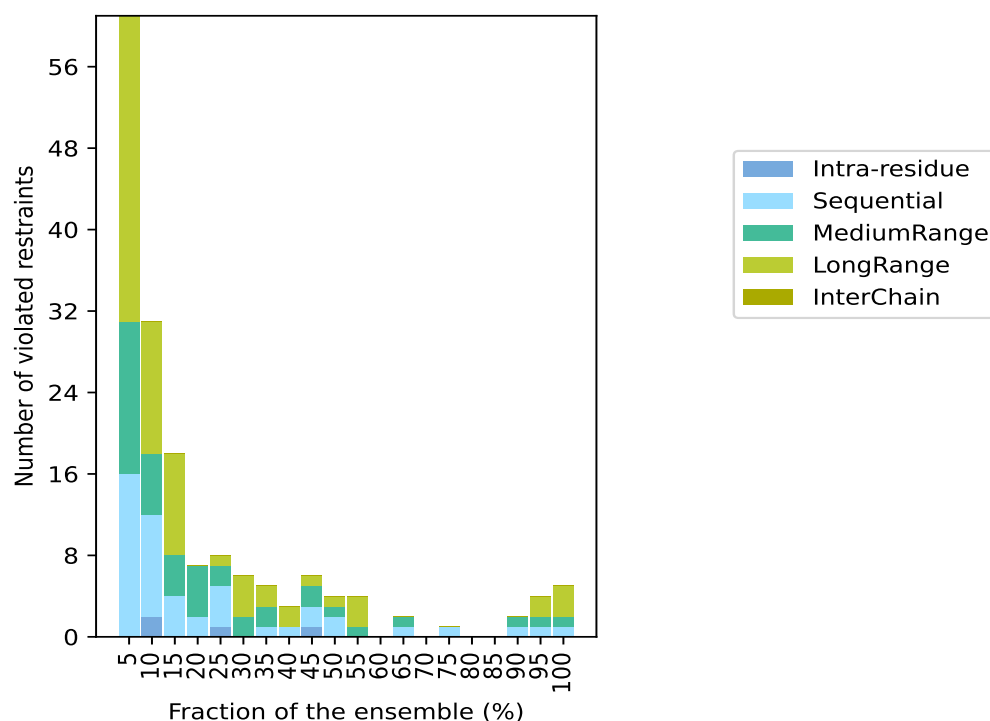
| Number of violated restraints |                 |                 |                 |                 |       | Fraction of the ensemble |       |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|-------|
| IR <sup>1</sup>               | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total | Count <sup>6</sup>       | %     |
| 0                             | 16              | 15              | 30              | 0               | 61    | 1                        | 5.0   |
| 2                             | 10              | 6               | 13              | 0               | 31    | 2                        | 10.0  |
| 0                             | 4               | 4               | 10              | 0               | 18    | 3                        | 15.0  |
| 0                             | 2               | 5               | 0               | 0               | 7     | 4                        | 20.0  |
| 1                             | 4               | 2               | 1               | 0               | 8     | 5                        | 25.0  |
| 0                             | 0               | 2               | 4               | 0               | 6     | 6                        | 30.0  |
| 0                             | 1               | 2               | 2               | 0               | 5     | 7                        | 35.0  |
| 0                             | 1               | 0               | 2               | 0               | 3     | 8                        | 40.0  |
| 1                             | 2               | 2               | 1               | 0               | 6     | 9                        | 45.0  |
| 0                             | 2               | 1               | 1               | 0               | 4     | 10                       | 50.0  |
| 0                             | 0               | 1               | 3               | 0               | 4     | 11                       | 55.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 12                       | 60.0  |
| 0                             | 1               | 1               | 0               | 0               | 2     | 13                       | 65.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 14                       | 70.0  |
| 0                             | 1               | 0               | 0               | 0               | 1     | 15                       | 75.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 16                       | 80.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 17                       | 85.0  |
| 0                             | 1               | 1               | 0               | 0               | 2     | 18                       | 90.0  |
| 0                             | 1               | 1               | 2               | 0               | 4     | 19                       | 95.0  |
| 0                             | 1               | 1               | 3               | 0               | 5     | 20                       | 100.0 |

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

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



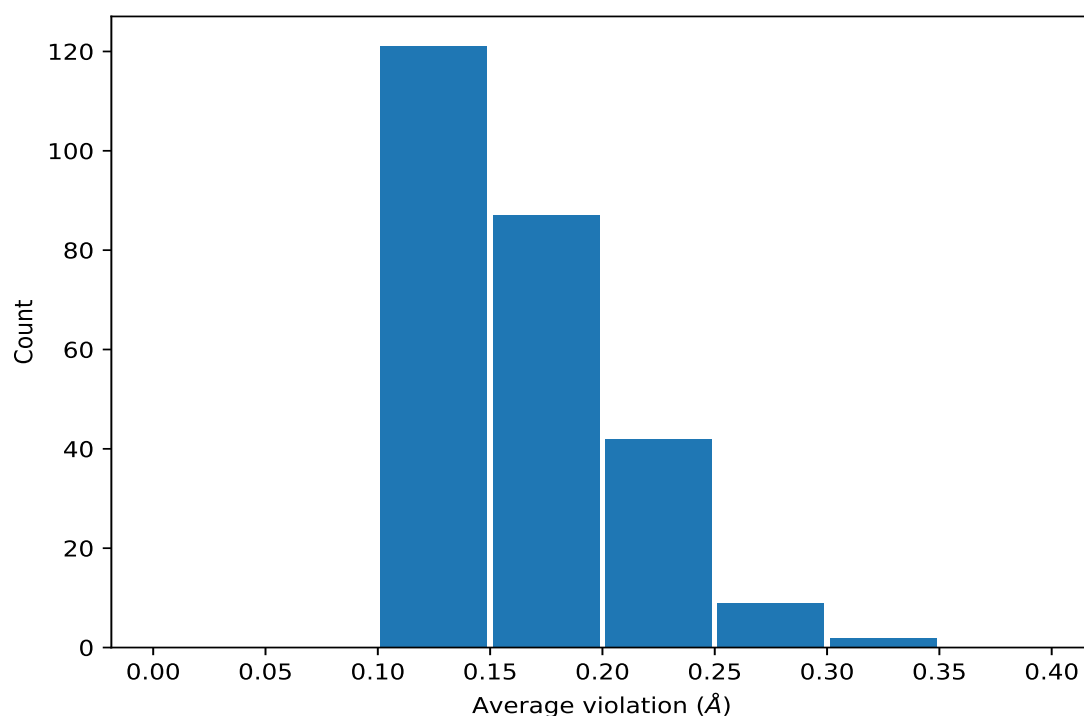
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

| Key      | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,2535) | 1:125:A:PRO:HD2 | 1:130:A:ALA:HB1  | 20                  | 0.3      | 0.06                | 0.29       |
| (1,2535) | 1:125:A:PRO:HD2 | 1:130:A:ALA:HB2  | 20                  | 0.3      | 0.06                | 0.29       |
| (1,2535) | 1:125:A:PRO:HD2 | 1:130:A:ALA:HB3  | 20                  | 0.3      | 0.06                | 0.29       |
| (2,661)  | 1:30:A:ARG:HA   | 1:32:A:LEU:HD11  | 20                  | 0.24     | 0.05                | 0.22       |
| (2,661)  | 1:30:A:ARG:HA   | 1:32:A:LEU:HD12  | 20                  | 0.24     | 0.05                | 0.22       |
| (2,661)  | 1:30:A:ARG:HA   | 1:32:A:LEU:HD13  | 20                  | 0.24     | 0.05                | 0.22       |
| (1,3277) | 1:12:A:PHE:HB2  | 1:120:A:SER:HB3  | 20                  | 0.23     | 0.04                | 0.24       |
| (1,3391) | 1:131:A:GLN:HG2 | 1:132:A:GLN:HA   | 20                  | 0.23     | 0.05                | 0.24       |
| (1,3155) | 1:83:A:ILE:HG21 | 1:106:A:THR:HG21 | 20                  | 0.18     | 0.05                | 0.18       |
| (1,3155) | 1:83:A:ILE:HG21 | 1:106:A:THR:HG22 | 20                  | 0.18     | 0.05                | 0.18       |
| (1,3155) | 1:83:A:ILE:HG21 | 1:106:A:THR:HG23 | 20                  | 0.18     | 0.05                | 0.18       |
| (1,3155) | 1:83:A:ILE:HG22 | 1:106:A:THR:HG21 | 20                  | 0.18     | 0.05                | 0.18       |
| (1,3155) | 1:83:A:ILE:HG22 | 1:106:A:THR:HG22 | 20                  | 0.18     | 0.05                | 0.18       |
| (1,3155) | 1:83:A:ILE:HG22 | 1:106:A:THR:HG23 | 20                  | 0.18     | 0.05                | 0.18       |
| (1,3155) | 1:83:A:ILE:HG23 | 1:106:A:THR:HG21 | 20                  | 0.18     | 0.05                | 0.18       |
| (1,3155) | 1:83:A:ILE:HG23 | 1:106:A:THR:HG22 | 20                  | 0.18     | 0.05                | 0.18       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,3155) | 1:83:A:ILE:HG23  | 1:106:A:THR:HG23 | 20                  | 0.18     | 0.05                | 0.18       |
| (1,3141) | 1:105:A:ILE:HG13 | 1:107:A:LEU:HG   | 19                  | 0.3      | 0.09                | 0.33       |
| (1,2410) | 1:12:A:PHE:HE1   | 1:146:A:LEU:HD21 | 19                  | 0.24     | 0.06                | 0.23       |
| (1,2410) | 1:12:A:PHE:HE1   | 1:146:A:LEU:HD22 | 19                  | 0.24     | 0.06                | 0.23       |
| (1,2410) | 1:12:A:PHE:HE1   | 1:146:A:LEU:HD23 | 19                  | 0.24     | 0.06                | 0.23       |
| (1,2410) | 1:12:A:PHE:HE2   | 1:146:A:LEU:HD21 | 19                  | 0.24     | 0.06                | 0.23       |
| (1,2410) | 1:12:A:PHE:HE2   | 1:146:A:LEU:HD22 | 19                  | 0.24     | 0.06                | 0.23       |
| (1,2410) | 1:12:A:PHE:HE2   | 1:146:A:LEU:HD23 | 19                  | 0.24     | 0.06                | 0.23       |
| (1,4229) | 1:152:A:LEU:HD11 | 1:153:A:LEU:HD11 | 19                  | 0.2      | 0.05                | 0.2        |
| (1,4229) | 1:152:A:LEU:HD11 | 1:153:A:LEU:HD12 | 19                  | 0.2      | 0.05                | 0.2        |
| (1,4229) | 1:152:A:LEU:HD11 | 1:153:A:LEU:HD13 | 19                  | 0.2      | 0.05                | 0.2        |
| (1,4229) | 1:152:A:LEU:HD12 | 1:153:A:LEU:HD11 | 19                  | 0.2      | 0.05                | 0.2        |
| (1,4229) | 1:152:A:LEU:HD12 | 1:153:A:LEU:HD12 | 19                  | 0.2      | 0.05                | 0.2        |
| (1,4229) | 1:152:A:LEU:HD12 | 1:153:A:LEU:HD13 | 19                  | 0.2      | 0.05                | 0.2        |
| (1,4229) | 1:152:A:LEU:HD13 | 1:153:A:LEU:HD11 | 19                  | 0.2      | 0.05                | 0.2        |
| (1,4229) | 1:152:A:LEU:HD13 | 1:153:A:LEU:HD12 | 19                  | 0.2      | 0.05                | 0.2        |
| (1,4229) | 1:152:A:LEU:HD13 | 1:153:A:LEU:HD13 | 19                  | 0.2      | 0.05                | 0.2        |
| (2,22)   | 1:32:A:LEU:H     | 1:49:A:PHE:HE1   | 19                  | 0.19     | 0.03                | 0.2        |
| (2,22)   | 1:32:A:LEU:H     | 1:49:A:PHE:HE2   | 19                  | 0.19     | 0.03                | 0.2        |
| (1,4362) | 1:68:A:SER:HA    | 1:69:A:TYR:HE1   | 18                  | 0.16     | 0.04                | 0.16       |
| (1,4362) | 1:68:A:SER:HA    | 1:69:A:TYR:HE2   | 18                  | 0.16     | 0.04                | 0.16       |
| (1,1163) | 1:149:A:LEU:H    | 1:153:A:LEU:HD11 | 18                  | 0.14     | 0.03                | 0.14       |
| (1,1163) | 1:149:A:LEU:H    | 1:153:A:LEU:HD12 | 18                  | 0.14     | 0.03                | 0.14       |
| (1,1163) | 1:149:A:LEU:H    | 1:153:A:LEU:HD13 | 18                  | 0.14     | 0.03                | 0.14       |
| (1,937)  | 1:117:A:THR:H    | 1:118:A:VAL:HB   | 15                  | 0.17     | 0.06                | 0.13       |
| (2,684)  | 1:30:A:ARG:HG2   | 1:34:A:GLU:HG3   | 13                  | 0.26     | 0.08                | 0.27       |
| (1,2134) | 1:36:A:TRP:HH2   | 1:37:A:PHE:HA    | 13                  | 0.15     | 0.04                | 0.15       |
| (1,4021) | 1:19:A:PRO:HG2   | 1:22:A:LYS:HG3   | 11                  | 0.27     | 0.06                | 0.27       |
| (1,1019) | 1:124:A:PHE:HB2  | 1:131:A:GLN:H    | 11                  | 0.16     | 0.04                | 0.15       |
| (1,2930) | 1:71:A:ILE:HD11  | 1:91:A:THR:HG21  | 11                  | 0.16     | 0.06                | 0.13       |
| (1,2930) | 1:71:A:ILE:HD11  | 1:91:A:THR:HG22  | 11                  | 0.16     | 0.06                | 0.13       |
| (1,2930) | 1:71:A:ILE:HD11  | 1:91:A:THR:HG23  | 11                  | 0.16     | 0.06                | 0.13       |
| (1,2930) | 1:71:A:ILE:HD12  | 1:91:A:THR:HG21  | 11                  | 0.16     | 0.06                | 0.13       |
| (1,2930) | 1:71:A:ILE:HD12  | 1:91:A:THR:HG22  | 11                  | 0.16     | 0.06                | 0.13       |
| (1,2930) | 1:71:A:ILE:HD12  | 1:91:A:THR:HG23  | 11                  | 0.16     | 0.06                | 0.13       |
| (1,2930) | 1:71:A:ILE:HD13  | 1:91:A:THR:HG21  | 11                  | 0.16     | 0.06                | 0.13       |
| (1,2930) | 1:71:A:ILE:HD13  | 1:91:A:THR:HG22  | 11                  | 0.16     | 0.06                | 0.13       |
| (1,2930) | 1:71:A:ILE:HD13  | 1:91:A:THR:HG23  | 11                  | 0.16     | 0.06                | 0.13       |
| (1,2889) | 1:87:A:ASP:HB2   | 1:103:A:MET:HB2  | 11                  | 0.15     | 0.04                | 0.15       |
| (1,1988) | 1:27:A:TYR:HB3   | 1:28:A:THR:HG21  | 10                  | 0.23     | 0.03                | 0.24       |
| (1,1988) | 1:27:A:TYR:HB3   | 1:28:A:THR:HG22  | 10                  | 0.23     | 0.03                | 0.24       |
| (1,1988) | 1:27:A:TYR:HB3   | 1:28:A:THR:HG23  | 10                  | 0.23     | 0.03                | 0.24       |

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| Key      | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,226)  | 1:27:A:TYR:H    | 1:28:A:THR:HG21  | 10                  | 0.16     | 0.03                | 0.16       |
| (1,226)  | 1:27:A:TYR:H    | 1:28:A:THR:HG22  | 10                  | 0.16     | 0.03                | 0.16       |
| (1,226)  | 1:27:A:TYR:H    | 1:28:A:THR:HG23  | 10                  | 0.16     | 0.03                | 0.16       |
| (2,676)  | 1:32:A:LEU:HD11 | 1:149:A:LEU:HD21 | 10                  | 0.15     | 0.04                | 0.14       |
| (2,676)  | 1:32:A:LEU:HD11 | 1:149:A:LEU:HD22 | 10                  | 0.15     | 0.04                | 0.14       |
| (2,676)  | 1:32:A:LEU:HD11 | 1:149:A:LEU:HD23 | 10                  | 0.15     | 0.04                | 0.14       |
| (2,676)  | 1:32:A:LEU:HD12 | 1:149:A:LEU:HD21 | 10                  | 0.15     | 0.04                | 0.14       |
| (2,676)  | 1:32:A:LEU:HD12 | 1:149:A:LEU:HD22 | 10                  | 0.15     | 0.04                | 0.14       |
| (2,676)  | 1:32:A:LEU:HD12 | 1:149:A:LEU:HD23 | 10                  | 0.15     | 0.04                | 0.14       |
| (2,676)  | 1:32:A:LEU:HD13 | 1:149:A:LEU:HD21 | 10                  | 0.15     | 0.04                | 0.14       |
| (2,676)  | 1:32:A:LEU:HD13 | 1:149:A:LEU:HD22 | 10                  | 0.15     | 0.04                | 0.14       |
| (2,676)  | 1:32:A:LEU:HD13 | 1:149:A:LEU:HD23 | 10                  | 0.15     | 0.04                | 0.14       |
| (1,150)  | 1:21:A:ASN:H    | 1:23:A:VAL:HB    | 10                  | 0.14     | 0.05                | 0.13       |
| (1,1850) | 1:28:A:THR:HB   | 1:29:A:LYS:HB2   | 9                   | 0.34     | 0.02                | 0.33       |
| (1,1850) | 1:28:A:THR:HB   | 1:29:A:LYS:HB3   | 9                   | 0.34     | 0.02                | 0.33       |
| (1,1546) | 1:22:A:LYS:HG3  | 1:23:A:VAL:HB    | 9                   | 0.19     | 0.05                | 0.19       |
| (1,320)  | 1:154:A:ASN:HA  | 1:154:A:ASN:HD22 | 9                   | 0.19     | 0.04                | 0.18       |
| (1,999)  | 1:126:A:THR:HA  | 1:130:A:ALA:H    | 9                   | 0.18     | 0.06                | 0.17       |
| (1,4020) | 1:19:A:PRO:HG2  | 1:22:A:LYS:HG2   | 9                   | 0.15     | 0.02                | 0.16       |
| (1,1832) | 1:35:A:GLN:HB3  | 1:152:A:LEU:HA   | 9                   | 0.15     | 0.02                | 0.14       |
| (1,3026) | 1:91:A:THR:HG21 | 1:97:A:ASP:HB3   | 8                   | 0.21     | 0.08                | 0.2        |
| (1,3026) | 1:91:A:THR:HG22 | 1:97:A:ASP:HB3   | 8                   | 0.21     | 0.08                | 0.2        |
| (1,3026) | 1:91:A:THR:HG23 | 1:97:A:ASP:HB3   | 8                   | 0.21     | 0.08                | 0.2        |
| (1,195)  | 1:108:A:ASN:H   | 1:118:A:VAL:HG21 | 8                   | 0.16     | 0.03                | 0.16       |
| (1,195)  | 1:108:A:ASN:H   | 1:118:A:VAL:HG22 | 8                   | 0.16     | 0.03                | 0.16       |
| (1,195)  | 1:108:A:ASN:H   | 1:118:A:VAL:HG23 | 8                   | 0.16     | 0.03                | 0.16       |
| (1,1394) | 1:3:A:ILE:HG21  | 1:4:A:GLU:HA     | 8                   | 0.13     | 0.01                | 0.12       |
| (1,1394) | 1:3:A:ILE:HG22  | 1:4:A:GLU:HA     | 8                   | 0.13     | 0.01                | 0.12       |
| (1,1394) | 1:3:A:ILE:HG23  | 1:4:A:GLU:HA     | 8                   | 0.13     | 0.01                | 0.12       |
| (1,1247) | 1:128:A:SER:HA  | 1:132:A:GLN:H    | 7                   | 0.16     | 0.04                | 0.16       |
| (1,2911) | 1:89:A:PHE:HB2  | 1:97:A:ASP:HB2   | 7                   | 0.14     | 0.03                | 0.14       |
| (1,1542) | 1:6:A:LYS:HG2   | 1:9:A:LYS:HE2    | 7                   | 0.14     | 0.02                | 0.14       |
| (1,1542) | 1:6:A:LYS:HG2   | 1:9:A:LYS:HE3    | 7                   | 0.14     | 0.02                | 0.14       |
| (1,1542) | 1:6:A:LYS:HG3   | 1:9:A:LYS:HE2    | 7                   | 0.14     | 0.02                | 0.14       |
| (1,1542) | 1:6:A:LYS:HG3   | 1:9:A:LYS:HE3    | 7                   | 0.14     | 0.02                | 0.14       |
| (1,3797) | 1:34:A:GLU:HG2  | 1:35:A:GLN:HA    | 7                   | 0.13     | 0.02                | 0.13       |
| (1,3272) | 1:107:A:LEU:HB3 | 1:120:A:SER:HB2  | 7                   | 0.12     | 0.01                | 0.12       |
| (1,3296) | 1:9:A:LYS:HA    | 1:122:A:SER:HB3  | 6                   | 0.23     | 0.1                 | 0.22       |
| (1,4016) | 1:20:A:ILE:HD11 | 1:23:A:VAL:HB    | 6                   | 0.2      | 0.05                | 0.19       |
| (1,4016) | 1:20:A:ILE:HD12 | 1:23:A:VAL:HB    | 6                   | 0.2      | 0.05                | 0.19       |
| (1,4016) | 1:20:A:ILE:HD13 | 1:23:A:VAL:HB    | 6                   | 0.2      | 0.05                | 0.19       |
| (1,3897) | 1:89:A:PHE:HD1  | 1:100:A:MET:HB2  | 6                   | 0.18     | 0.04                | 0.17       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,3897) | 1:89:A:PHE:HD2   | 1:100:A:MET:HB2  | 6                   | 0.18     | 0.04                | 0.17       |
| (1,1675) | 1:53:A:LYS:HD2   | 1:77:A:VAL:HG11  | 6                   | 0.16     | 0.04                | 0.15       |
| (1,1675) | 1:53:A:LYS:HD2   | 1:77:A:VAL:HG12  | 6                   | 0.16     | 0.04                | 0.15       |
| (1,1675) | 1:53:A:LYS:HD2   | 1:77:A:VAL:HG13  | 6                   | 0.16     | 0.04                | 0.15       |
| (1,1675) | 1:53:A:LYS:HD3   | 1:77:A:VAL:HG11  | 6                   | 0.16     | 0.04                | 0.15       |
| (1,1675) | 1:53:A:LYS:HD3   | 1:77:A:VAL:HG12  | 6                   | 0.16     | 0.04                | 0.15       |
| (1,1675) | 1:53:A:LYS:HD3   | 1:77:A:VAL:HG13  | 6                   | 0.16     | 0.04                | 0.15       |
| (1,3246) | 1:24:A:PHE:HD1   | 1:118:A:VAL:HG11 | 6                   | 0.14     | 0.02                | 0.14       |
| (1,3246) | 1:24:A:PHE:HD1   | 1:118:A:VAL:HG12 | 6                   | 0.14     | 0.02                | 0.14       |
| (1,3246) | 1:24:A:PHE:HD1   | 1:118:A:VAL:HG13 | 6                   | 0.14     | 0.02                | 0.14       |
| (1,3246) | 1:24:A:PHE:HD2   | 1:118:A:VAL:HG11 | 6                   | 0.14     | 0.02                | 0.14       |
| (1,3246) | 1:24:A:PHE:HD2   | 1:118:A:VAL:HG12 | 6                   | 0.14     | 0.02                | 0.14       |
| (1,3246) | 1:24:A:PHE:HD2   | 1:118:A:VAL:HG13 | 6                   | 0.14     | 0.02                | 0.14       |
| (2,449)  | 1:154:A:ASN:HA   | 1:157:A:LEU:HG   | 6                   | 0.13     | 0.02                | 0.12       |
| (1,572)  | 1:62:A:GLN:HA    | 1:62:A:GLN:HE22  | 5                   | 0.29     | 0.03                | 0.28       |
| (2,801)  | 1:96:A:LYS:HD3   | 1:97:A:ASP:HA    | 5                   | 0.18     | 0.08                | 0.13       |
| (2,641)  | 1:20:A:ILE:HG21  | 1:21:A:ASN:HD22  | 5                   | 0.18     | 0.04                | 0.15       |
| (2,641)  | 1:20:A:ILE:HG22  | 1:21:A:ASN:HD22  | 5                   | 0.18     | 0.04                | 0.15       |
| (2,641)  | 1:20:A:ILE:HG23  | 1:21:A:ASN:HD22  | 5                   | 0.18     | 0.04                | 0.15       |
| (1,3008) | 1:95:A:GLU:HB2   | 1:96:A:LYS:HB2   | 5                   | 0.15     | 0.05                | 0.13       |
| (1,3008) | 1:95:A:GLU:HB2   | 1:96:A:LYS:HB3   | 5                   | 0.15     | 0.05                | 0.13       |
| (1,1772) | 1:18:A:ALA:HB1   | 1:22:A:LYS:HB3   | 5                   | 0.15     | 0.03                | 0.15       |
| (1,1772) | 1:18:A:ALA:HB2   | 1:22:A:LYS:HB3   | 5                   | 0.15     | 0.03                | 0.15       |
| (1,1772) | 1:18:A:ALA:HB3   | 1:22:A:LYS:HB3   | 5                   | 0.15     | 0.03                | 0.15       |
| (1,703)  | 1:79:A:ALA:HA    | 1:81:A:TYR:H     | 5                   | 0.13     | 0.01                | 0.13       |
| (1,2667) | 1:70:A:THR:H     | 1:71:A:ILE:HD11  | 5                   | 0.13     | 0.02                | 0.12       |
| (1,2667) | 1:70:A:THR:H     | 1:71:A:ILE:HD12  | 5                   | 0.13     | 0.02                | 0.12       |
| (1,2667) | 1:70:A:THR:H     | 1:71:A:ILE:HD13  | 5                   | 0.13     | 0.02                | 0.12       |
| (1,289)  | 1:34:A:GLU:H     | 1:49:A:PHE:HE1   | 5                   | 0.12     | 0.02                | 0.11       |
| (1,289)  | 1:34:A:GLU:H     | 1:49:A:PHE:HE2   | 5                   | 0.12     | 0.02                | 0.11       |
| (1,3249) | 1:118:A:VAL:HG11 | 1:119:A:THR:HB   | 4                   | 0.19     | 0.06                | 0.2        |
| (1,3249) | 1:118:A:VAL:HG12 | 1:119:A:THR:HB   | 4                   | 0.19     | 0.06                | 0.2        |
| (1,3249) | 1:118:A:VAL:HG13 | 1:119:A:THR:HB   | 4                   | 0.19     | 0.06                | 0.2        |
| (1,3143) | 1:103:A:MET:HG3  | 1:105:A:ILE:HG12 | 4                   | 0.18     | 0.02                | 0.18       |
| (1,1136) | 1:144:A:SER:HA   | 1:147:A:ASN:HD22 | 4                   | 0.16     | 0.04                | 0.15       |
| (1,3740) | 1:154:A:ASN:HA   | 1:157:A:LEU:HB3  | 4                   | 0.15     | 0.04                | 0.13       |
| (1,4410) | 1:79:A:ALA:HA    | 1:81:A:TYR:HD1   | 4                   | 0.13     | 0.02                | 0.12       |
| (1,4410) | 1:79:A:ALA:HA    | 1:81:A:TYR:HD2   | 4                   | 0.13     | 0.02                | 0.12       |
| (1,1382) | 1:117:A:THR:HG21 | 1:119:A:THR:H    | 4                   | 0.13     | 0.03                | 0.12       |
| (1,1382) | 1:117:A:THR:HG22 | 1:119:A:THR:H    | 4                   | 0.13     | 0.03                | 0.12       |
| (1,1382) | 1:117:A:THR:HG23 | 1:119:A:THR:H    | 4                   | 0.13     | 0.03                | 0.12       |
| (1,4202) | 1:125:A:PRO:HB3  | 1:126:A:THR:HG21 | 4                   | 0.12     | 0.02                | 0.12       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,4202) | 1:125:A:PRO:HB3  | 1:126:A:THR:HG22 | 4                   | 0.12     | 0.02                | 0.12       |
| (1,4202) | 1:125:A:PRO:HB3  | 1:126:A:THR:HG23 | 4                   | 0.12     | 0.02                | 0.12       |
| (1,4206) | 1:126:A:THR:HG21 | 1:129:A:ALA:HB1  | 3                   | 0.24     | 0.1                 | 0.23       |
| (1,4206) | 1:126:A:THR:HG21 | 1:129:A:ALA:HB2  | 3                   | 0.24     | 0.1                 | 0.23       |
| (1,4206) | 1:126:A:THR:HG21 | 1:129:A:ALA:HB3  | 3                   | 0.24     | 0.1                 | 0.23       |
| (1,4206) | 1:126:A:THR:HG22 | 1:129:A:ALA:HB1  | 3                   | 0.24     | 0.1                 | 0.23       |
| (1,4206) | 1:126:A:THR:HG22 | 1:129:A:ALA:HB2  | 3                   | 0.24     | 0.1                 | 0.23       |
| (1,4206) | 1:126:A:THR:HG22 | 1:129:A:ALA:HB3  | 3                   | 0.24     | 0.1                 | 0.23       |
| (1,4206) | 1:126:A:THR:HG23 | 1:129:A:ALA:HB1  | 3                   | 0.24     | 0.1                 | 0.23       |
| (1,4206) | 1:126:A:THR:HG23 | 1:129:A:ALA:HB2  | 3                   | 0.24     | 0.1                 | 0.23       |
| (1,4206) | 1:126:A:THR:HG23 | 1:129:A:ALA:HB3  | 3                   | 0.24     | 0.1                 | 0.23       |
| (1,1739) | 1:15:A:THR:HB    | 1:115:A:LYS:HE2  | 3                   | 0.22     | 0.06                | 0.2        |
| (1,1739) | 1:15:A:THR:HB    | 1:115:A:LYS:HE3  | 3                   | 0.22     | 0.06                | 0.2        |
| (1,486)  | 1:53:A:LYS:HD2   | 1:54:A:GLY:H     | 3                   | 0.18     | 0.06                | 0.19       |
| (1,486)  | 1:53:A:LYS:HD3   | 1:54:A:GLY:H     | 3                   | 0.18     | 0.06                | 0.19       |
| (1,2929) | 1:91:A:THR:HG21  | 1:96:A:LYS:HD2   | 3                   | 0.18     | 0.04                | 0.16       |
| (1,2929) | 1:91:A:THR:HG22  | 1:96:A:LYS:HD2   | 3                   | 0.18     | 0.04                | 0.16       |
| (1,2929) | 1:91:A:THR:HG23  | 1:96:A:LYS:HD2   | 3                   | 0.18     | 0.04                | 0.16       |
| (1,1676) | 1:13:A:THR:HG21  | 1:14:A:ARG:HB2   | 3                   | 0.15     | 0.04                | 0.13       |
| (1,1676) | 1:13:A:THR:HG22  | 1:14:A:ARG:HB2   | 3                   | 0.15     | 0.04                | 0.13       |
| (1,1676) | 1:13:A:THR:HG23  | 1:14:A:ARG:HB2   | 3                   | 0.15     | 0.04                | 0.13       |
| (1,4401) | 1:82:A:TYR:HE1   | 1:108:A:ASN:HB2  | 3                   | 0.14     | 0.02                | 0.15       |
| (1,4401) | 1:82:A:TYR:HE2   | 1:108:A:ASN:HB2  | 3                   | 0.14     | 0.02                | 0.15       |
| (1,270)  | 1:31:A:GLU:HG3   | 1:32:A:LEU:H     | 3                   | 0.14     | 0.03                | 0.15       |
| (1,3659) | 1:151:A:LYS:HB2  | 1:157:A:LEU:HB3  | 3                   | 0.14     | 0.02                | 0.15       |
| (1,3659) | 1:151:A:LYS:HB3  | 1:157:A:LEU:HB3  | 3                   | 0.14     | 0.02                | 0.15       |
| (1,1399) | 1:20:A:ILE:HD11  | 1:81:A:TYR:HD1   | 3                   | 0.14     | 0.04                | 0.12       |
| (1,1399) | 1:20:A:ILE:HD11  | 1:81:A:TYR:HD2   | 3                   | 0.14     | 0.04                | 0.12       |
| (1,1399) | 1:20:A:ILE:HD12  | 1:81:A:TYR:HD1   | 3                   | 0.14     | 0.04                | 0.12       |
| (1,1399) | 1:20:A:ILE:HD12  | 1:81:A:TYR:HD2   | 3                   | 0.14     | 0.04                | 0.12       |
| (1,1399) | 1:20:A:ILE:HD13  | 1:81:A:TYR:HD1   | 3                   | 0.14     | 0.04                | 0.12       |
| (1,1399) | 1:20:A:ILE:HD13  | 1:81:A:TYR:HD2   | 3                   | 0.14     | 0.04                | 0.12       |
| (1,4196) | 1:8:A:ASN:HB2    | 1:125:A:PRO:HD2  | 3                   | 0.14     | 0.02                | 0.14       |
| (1,980)  | 1:9:A:LYS:HB2    | 1:122:A:SER:H    | 3                   | 0.13     | 0.01                | 0.14       |
| (1,4136) | 1:73:A:GLU:HA    | 1:86:A:LEU:HD11  | 3                   | 0.13     | 0.02                | 0.12       |
| (1,4136) | 1:73:A:GLU:HA    | 1:86:A:LEU:HD12  | 3                   | 0.13     | 0.02                | 0.12       |
| (1,4136) | 1:73:A:GLU:HA    | 1:86:A:LEU:HD13  | 3                   | 0.13     | 0.02                | 0.12       |
| (1,1402) | 1:3:A:ILE:HG12   | 1:139:A:GLU:HA   | 3                   | 0.13     | 0.03                | 0.12       |
| (1,2036) | 1:4:A:GLU:HG2    | 1:6:A:LYS:HG2    | 3                   | 0.13     | 0.0                 | 0.13       |
| (1,2036) | 1:4:A:GLU:HG2    | 1:6:A:LYS:HG3    | 3                   | 0.13     | 0.0                 | 0.13       |
| (1,2529) | 1:100:A:MET:HG3  | 1:101:A:PRO:HD3  | 3                   | 0.12     | 0.01                | 0.12       |
| (1,3433) | 1:5:A:LYS:HB2    | 1:134:A:ILE:HD11 | 3                   | 0.12     | 0.01                | 0.11       |

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| Key      | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,3433) | 1:5:A:LYS:HB2   | 1:134:A:ILE:HD12 | 3                   | 0.12     | 0.01                | 0.11       |
| (1,3433) | 1:5:A:LYS:HB2   | 1:134:A:ILE:HD13 | 3                   | 0.12     | 0.01                | 0.11       |
| (1,1554) | 1:6:A:LYS:HE2   | 1:9:A:LYS:HD3    | 3                   | 0.12     | 0.0                 | 0.12       |
| (1,1554) | 1:6:A:LYS:HE3   | 1:9:A:LYS:HD3    | 3                   | 0.12     | 0.0                 | 0.12       |
| (1,1804) | 1:20:A:ILE:HG21 | 1:23:A:VAL:H     | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,1804) | 1:20:A:ILE:HG22 | 1:23:A:VAL:H     | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,1804) | 1:20:A:ILE:HG23 | 1:23:A:VAL:H     | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,3380) | 1:5:A:LYS:HE2   | 1:131:A:GLN:HA   | 2                   | 0.25     | 0.13                | 0.25       |
| (1,3380) | 1:5:A:LYS:HE3   | 1:131:A:GLN:HA   | 2                   | 0.25     | 0.13                | 0.25       |
| (1,2835) | 1:93:A:LYS:HB3  | 1:95:A:GLU:HG2   | 2                   | 0.22     | 0.04                | 0.22       |
| (1,9)    | 1:4:A:GLU:H     | 1:13:A:THR:HG21  | 2                   | 0.18     | 0.05                | 0.18       |
| (1,9)    | 1:4:A:GLU:H     | 1:13:A:THR:HG22  | 2                   | 0.18     | 0.05                | 0.18       |
| (1,9)    | 1:4:A:GLU:H     | 1:13:A:THR:HG23  | 2                   | 0.18     | 0.05                | 0.18       |
| (1,2552) | 1:100:A:MET:HB2 | 1:101:A:PRO:HD2  | 2                   | 0.18     | 0.03                | 0.18       |
| (1,3176) | 1:108:A:ASN:HA  | 1:109:A:PHE:HD1  | 2                   | 0.18     | 0.03                | 0.18       |
| (1,3176) | 1:108:A:ASN:HA  | 1:109:A:PHE:HD2  | 2                   | 0.18     | 0.03                | 0.18       |
| (1,811)  | 1:91:A:THR:H    | 1:95:A:GLU:H     | 2                   | 0.17     | 0.0                 | 0.17       |
| (1,4104) | 1:66:A:MET:HA   | 1:66:A:MET:HE1   | 2                   | 0.16     | 0.01                | 0.16       |
| (1,4104) | 1:66:A:MET:HA   | 1:66:A:MET:HE2   | 2                   | 0.16     | 0.01                | 0.16       |
| (1,4104) | 1:66:A:MET:HA   | 1:66:A:MET:HE3   | 2                   | 0.16     | 0.01                | 0.16       |
| (1,786)  | 1:91:A:THR:H    | 1:95:A:GLU:H     | 2                   | 0.16     | 0.0                 | 0.16       |
| (1,2591) | 1:61:A:ILE:HG21 | 1:66:A:MET:HE1   | 2                   | 0.16     | 0.02                | 0.16       |
| (1,2591) | 1:61:A:ILE:HG21 | 1:66:A:MET:HE2   | 2                   | 0.16     | 0.02                | 0.16       |
| (1,2591) | 1:61:A:ILE:HG21 | 1:66:A:MET:HE3   | 2                   | 0.16     | 0.02                | 0.16       |
| (1,2591) | 1:61:A:ILE:HG22 | 1:66:A:MET:HE1   | 2                   | 0.16     | 0.02                | 0.16       |
| (1,2591) | 1:61:A:ILE:HG22 | 1:66:A:MET:HE2   | 2                   | 0.16     | 0.02                | 0.16       |
| (1,2591) | 1:61:A:ILE:HG22 | 1:66:A:MET:HE3   | 2                   | 0.16     | 0.02                | 0.16       |
| (1,2591) | 1:61:A:ILE:HG23 | 1:66:A:MET:HE1   | 2                   | 0.16     | 0.02                | 0.16       |
| (1,2591) | 1:61:A:ILE:HG23 | 1:66:A:MET:HE2   | 2                   | 0.16     | 0.02                | 0.16       |
| (1,2591) | 1:61:A:ILE:HG23 | 1:66:A:MET:HE3   | 2                   | 0.16     | 0.02                | 0.16       |
| (1,4203) | 1:128:A:SER:HB3 | 1:131:A:GLN:HG2  | 2                   | 0.16     | 0.02                | 0.16       |
| (1,3524) | 1:133:A:ALA:HB1 | 1:142:A:MET:HE1  | 2                   | 0.16     | 0.01                | 0.16       |
| (1,3524) | 1:133:A:ALA:HB1 | 1:142:A:MET:HE2  | 2                   | 0.16     | 0.01                | 0.16       |
| (1,3524) | 1:133:A:ALA:HB1 | 1:142:A:MET:HE3  | 2                   | 0.16     | 0.01                | 0.16       |
| (1,3524) | 1:133:A:ALA:HB2 | 1:142:A:MET:HE1  | 2                   | 0.16     | 0.01                | 0.16       |
| (1,3524) | 1:133:A:ALA:HB2 | 1:142:A:MET:HE2  | 2                   | 0.16     | 0.01                | 0.16       |
| (1,3524) | 1:133:A:ALA:HB2 | 1:142:A:MET:HE3  | 2                   | 0.16     | 0.01                | 0.16       |
| (1,3524) | 1:133:A:ALA:HB3 | 1:142:A:MET:HE1  | 2                   | 0.16     | 0.01                | 0.16       |
| (1,3524) | 1:133:A:ALA:HB3 | 1:142:A:MET:HE2  | 2                   | 0.16     | 0.01                | 0.16       |
| (1,3524) | 1:133:A:ALA:HB3 | 1:142:A:MET:HE3  | 2                   | 0.16     | 0.01                | 0.16       |
| (1,4052) | 1:34:A:GLU:HG2  | 1:35:A:GLN:HG3   | 2                   | 0.16     | 0.02                | 0.16       |
| (1,2566) | 1:129:A:ALA:HA  | 1:132:A:GLN:HG2  | 2                   | 0.15     | 0.0                 | 0.15       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1291) | 1:91:A:THR:HB   | 1:92:A:SER:H    | 2                   | 0.15     | 0.0                 | 0.15       |
| (1,395)  | 1:53:A:LYS:HB2  | 1:77:A:VAL:H    | 2                   | 0.14     | 0.04                | 0.14       |
| (1,4014) | 1:20:A:ILE:HD11 | 1:80:A:PRO:HB2  | 2                   | 0.14     | 0.01                | 0.14       |
| (1,4014) | 1:20:A:ILE:HD12 | 1:80:A:PRO:HB2  | 2                   | 0.14     | 0.01                | 0.14       |
| (1,4014) | 1:20:A:ILE:HD13 | 1:80:A:PRO:HB2  | 2                   | 0.14     | 0.01                | 0.14       |
| (1,2739) | 1:53:A:LYS:HD2  | 1:76:A:GLN:HG3  | 2                   | 0.14     | 0.04                | 0.14       |
| (1,2739) | 1:53:A:LYS:HD3  | 1:76:A:GLN:HG3  | 2                   | 0.14     | 0.04                | 0.14       |
| (1,2042) | 1:31:A:GLU:HG3  | 1:32:A:LEU:HA   | 2                   | 0.13     | 0.02                | 0.13       |
| (1,3236) | 1:108:A:ASN:HB2 | 1:119:A:THR:HB  | 2                   | 0.13     | 0.01                | 0.13       |
| (1,4412) | 1:20:A:ILE:HG21 | 1:81:A:TYR:HD1  | 2                   | 0.13     | 0.01                | 0.13       |
| (1,4412) | 1:20:A:ILE:HG21 | 1:81:A:TYR:HD2  | 2                   | 0.13     | 0.01                | 0.13       |
| (1,4412) | 1:20:A:ILE:HG22 | 1:81:A:TYR:HD1  | 2                   | 0.13     | 0.01                | 0.13       |
| (1,4412) | 1:20:A:ILE:HG22 | 1:81:A:TYR:HD2  | 2                   | 0.13     | 0.01                | 0.13       |
| (1,4412) | 1:20:A:ILE:HG23 | 1:81:A:TYR:HD1  | 2                   | 0.13     | 0.01                | 0.13       |
| (1,4412) | 1:20:A:ILE:HG23 | 1:81:A:TYR:HD2  | 2                   | 0.13     | 0.01                | 0.13       |
| (1,124)  | 1:14:A:ARG:HG3  | 1:15:A:THR:H    | 2                   | 0.12     | 0.02                | 0.12       |
| (1,830)  | 1:99:A:SER:H    | 1:100:A:MET:HG2 | 2                   | 0.12     | 0.01                | 0.12       |
| (2,764)  | 1:73:A:GLU:HG2  | 1:88:A:TYR:HB3  | 2                   | 0.12     | 0.01                | 0.12       |
| (1,1264) | 1:8:A:ASN:HD22  | 1:124:A:PHE:H   | 2                   | 0.12     | 0.02                | 0.12       |
| (1,3047) | 1:142:A:MET:HA  | 1:142:A:MET:HE1 | 2                   | 0.12     | 0.01                | 0.12       |
| (1,3047) | 1:142:A:MET:HA  | 1:142:A:MET:HE2 | 2                   | 0.12     | 0.01                | 0.12       |
| (1,3047) | 1:142:A:MET:HA  | 1:142:A:MET:HE3 | 2                   | 0.12     | 0.01                | 0.12       |
| (1,4098) | 1:62:A:GLN:HB2  | 1:67:A:ILE:HD11 | 2                   | 0.12     | 0.01                | 0.12       |
| (1,4098) | 1:62:A:GLN:HB2  | 1:67:A:ILE:HD12 | 2                   | 0.12     | 0.01                | 0.12       |
| (1,4098) | 1:62:A:GLN:HB2  | 1:67:A:ILE:HD13 | 2                   | 0.12     | 0.01                | 0.12       |
| (1,378)  | 1:39:A:PRO:HG2  | 1:43:A:SER:H    | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,378)  | 1:39:A:PRO:HG3  | 1:43:A:SER:H    | 2                   | 0.12     | 0.0                 | 0.12       |
| (2,612)  | 1:7:A:LYS:HB2   | 1:8:A:ASN:HD21  | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,4300) | 1:38:A:HIS:HD2  | 1:44:A:VAL:HG21 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,4300) | 1:38:A:HIS:HD2  | 1:44:A:VAL:HG22 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,4300) | 1:38:A:HIS:HD2  | 1:44:A:VAL:HG23 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1972) | 1:27:A:TYR:HB3  | 1:28:A:THR:HG21 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1972) | 1:27:A:TYR:HB3  | 1:28:A:THR:HG22 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1972) | 1:27:A:TYR:HB3  | 1:28:A:THR:HG23 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,4112) | 1:67:A:ILE:H    | 1:68:A:SER:HA   | 2                   | 0.11     | 0.0                 | 0.11       |

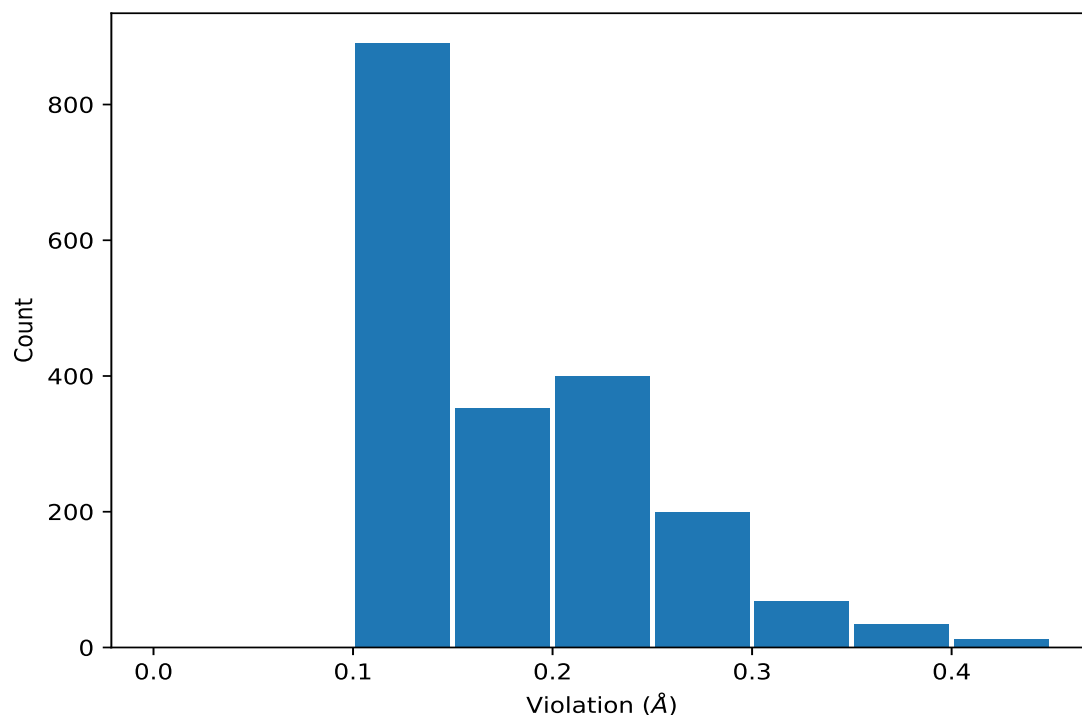
<sup>1</sup>Number of violated models, <sup>2</sup>Standard deviation



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

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

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



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

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

| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2535) | 1:125:A:PRO:HD2  | 1:130:A:ALA:HB1 | 13       | 0.43          |
| (1,2535) | 1:125:A:PRO:HD2  | 1:130:A:ALA:HB2 | 13       | 0.43          |
| (1,2535) | 1:125:A:PRO:HD2  | 1:130:A:ALA:HB3 | 13       | 0.43          |
| (1,4021) | 1:19:A:PRO:HG2   | 1:22:A:LYS:HG3  | 9        | 0.42          |
| (1,3296) | 1:9:A:LYS:HA     | 1:122:A:SER:HB3 | 2        | 0.42          |
| (1,3141) | 1:105:A:ILE:HG13 | 1:107:A:LEU:HG  | 1        | 0.4           |
| (1,3141) | 1:105:A:ILE:HG13 | 1:107:A:LEU:HG  | 9        | 0.4           |
| (1,3026) | 1:91:A:THR:HG21  | 1:97:A:ASP:HB3  | 3        | 0.4           |
| (1,3026) | 1:91:A:THR:HG22  | 1:97:A:ASP:HB3  | 3        | 0.4           |
| (1,3026) | 1:91:A:THR:HG23  | 1:97:A:ASP:HB3  | 3        | 0.4           |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2535) | 1:125:A:PRO:HD2  | 1:130:A:ALA:HB1 | 12       | 0.4           |
| (1,2535) | 1:125:A:PRO:HD2  | 1:130:A:ALA:HB2 | 12       | 0.4           |
| (1,2535) | 1:125:A:PRO:HD2  | 1:130:A:ALA:HB3 | 12       | 0.4           |
| (1,3141) | 1:105:A:ILE:HG13 | 1:107:A:LEU:HG  | 15       | 0.39          |
| (2,684)  | 1:30:A:ARG:HG2   | 1:34:A:GLU:HG3  | 8        | 0.38          |
| (1,3380) | 1:5:A:LYS:HE2    | 1:131:A:GLN:HA  | 1        | 0.38          |
| (1,3380) | 1:5:A:LYS:HE3    | 1:131:A:GLN:HA  | 1        | 0.38          |
| (1,3141) | 1:105:A:ILE:HG13 | 1:107:A:LEU:HG  | 5        | 0.38          |
| (1,3141) | 1:105:A:ILE:HG13 | 1:107:A:LEU:HG  | 13       | 0.38          |
| (1,3141) | 1:105:A:ILE:HG13 | 1:107:A:LEU:HG  | 14       | 0.38          |
| (1,2535) | 1:125:A:PRO:HD2  | 1:130:A:ALA:HB1 | 18       | 0.37          |
| (1,2535) | 1:125:A:PRO:HD2  | 1:130:A:ALA:HB2 | 18       | 0.37          |
| (1,2535) | 1:125:A:PRO:HD2  | 1:130:A:ALA:HB3 | 18       | 0.37          |
| (1,1850) | 1:28:A:THR:HB    | 1:29:A:LYS:HB2  | 10       | 0.37          |
| (1,1850) | 1:28:A:THR:HB    | 1:29:A:LYS:HB3  | 10       | 0.37          |
| (1,8)    | 1:4:A:GLU:H      | 1:5:A:LYS:HD2   | 17       | 0.37          |
| (1,8)    | 1:4:A:GLU:H      | 1:5:A:LYS:HD3   | 17       | 0.37          |
| (1,4206) | 1:126:A:THR:HG21 | 1:129:A:ALA:HB1 | 6        | 0.36          |
| (1,4206) | 1:126:A:THR:HG21 | 1:129:A:ALA:HB2 | 6        | 0.36          |
| (1,4206) | 1:126:A:THR:HG21 | 1:129:A:ALA:HB3 | 6        | 0.36          |
| (1,4206) | 1:126:A:THR:HG22 | 1:129:A:ALA:HB1 | 6        | 0.36          |
| (1,4206) | 1:126:A:THR:HG22 | 1:129:A:ALA:HB2 | 6        | 0.36          |
| (1,4206) | 1:126:A:THR:HG22 | 1:129:A:ALA:HB3 | 6        | 0.36          |
| (1,4206) | 1:126:A:THR:HG23 | 1:129:A:ALA:HB1 | 6        | 0.36          |
| (1,4206) | 1:126:A:THR:HG23 | 1:129:A:ALA:HB2 | 6        | 0.36          |
| (1,4206) | 1:126:A:THR:HG23 | 1:129:A:ALA:HB3 | 6        | 0.36          |
| (1,3141) | 1:105:A:ILE:HG13 | 1:107:A:LEU:HG  | 18       | 0.36          |
| (1,3141) | 1:105:A:ILE:HG13 | 1:107:A:LEU:HG  | 19       | 0.36          |
| (1,2535) | 1:125:A:PRO:HD2  | 1:130:A:ALA:HB1 | 16       | 0.36          |
| (1,2535) | 1:125:A:PRO:HD2  | 1:130:A:ALA:HB2 | 16       | 0.36          |
| (1,2535) | 1:125:A:PRO:HD2  | 1:130:A:ALA:HB3 | 16       | 0.36          |
| (1,1850) | 1:28:A:THR:HB    | 1:29:A:LYS:HB2  | 13       | 0.36          |
| (1,1850) | 1:28:A:THR:HB    | 1:29:A:LYS:HB3  | 13       | 0.36          |
| (1,1850) | 1:28:A:THR:HB    | 1:29:A:LYS:HB2  | 14       | 0.36          |
| (1,1850) | 1:28:A:THR:HB    | 1:29:A:LYS:HB3  | 14       | 0.36          |
| (1,1850) | 1:28:A:THR:HB    | 1:29:A:LYS:HB2  | 18       | 0.36          |
| (1,1850) | 1:28:A:THR:HB    | 1:29:A:LYS:HB3  | 18       | 0.36          |
| (2,684)  | 1:30:A:ARG:HG2   | 1:34:A:GLU:HG3  | 5        | 0.34          |
| (2,684)  | 1:30:A:ARG:HG2   | 1:34:A:GLU:HG3  | 16       | 0.34          |
| (1,3141) | 1:105:A:ILE:HG13 | 1:107:A:LEU:HG  | 2        | 0.34          |
| (1,2535) | 1:125:A:PRO:HD2  | 1:130:A:ALA:HB1 | 4        | 0.34          |
| (1,2535) | 1:125:A:PRO:HD2  | 1:130:A:ALA:HB2 | 4        | 0.34          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2535) | 1:125:A:PRO:HD2  | 1:130:A:ALA:HB3  | 4        | 0.34          |
| (1,2535) | 1:125:A:PRO:HD2  | 1:130:A:ALA:HB1  | 10       | 0.34          |
| (1,2535) | 1:125:A:PRO:HD2  | 1:130:A:ALA:HB2  | 10       | 0.34          |
| (1,2535) | 1:125:A:PRO:HD2  | 1:130:A:ALA:HB3  | 10       | 0.34          |
| (1,2535) | 1:125:A:PRO:HD2  | 1:130:A:ALA:HB1  | 20       | 0.34          |
| (1,2535) | 1:125:A:PRO:HD2  | 1:130:A:ALA:HB2  | 20       | 0.34          |
| (1,2535) | 1:125:A:PRO:HD2  | 1:130:A:ALA:HB3  | 20       | 0.34          |
| (2,661)  | 1:30:A:ARG:HA    | 1:32:A:LEU:HD11  | 20       | 0.33          |
| (2,661)  | 1:30:A:ARG:HA    | 1:32:A:LEU:HD12  | 20       | 0.33          |
| (2,661)  | 1:30:A:ARG:HA    | 1:32:A:LEU:HD13  | 20       | 0.33          |
| (1,3141) | 1:105:A:ILE:HG13 | 1:107:A:LEU:HG   | 20       | 0.33          |
| (1,2535) | 1:125:A:PRO:HD2  | 1:130:A:ALA:HB1  | 8        | 0.33          |
| (1,2535) | 1:125:A:PRO:HD2  | 1:130:A:ALA:HB2  | 8        | 0.33          |
| (1,2535) | 1:125:A:PRO:HD2  | 1:130:A:ALA:HB3  | 8        | 0.33          |
| (1,2535) | 1:125:A:PRO:HD2  | 1:130:A:ALA:HB1  | 19       | 0.33          |
| (1,2535) | 1:125:A:PRO:HD2  | 1:130:A:ALA:HB2  | 19       | 0.33          |
| (1,2535) | 1:125:A:PRO:HD2  | 1:130:A:ALA:HB3  | 19       | 0.33          |
| (1,1850) | 1:28:A:THR:HB    | 1:29:A:LYS:HB2   | 8        | 0.33          |
| (1,1850) | 1:28:A:THR:HB    | 1:29:A:LYS:HB3   | 8        | 0.33          |
| (1,1850) | 1:28:A:THR:HB    | 1:29:A:LYS:HB2   | 9        | 0.33          |
| (1,1850) | 1:28:A:THR:HB    | 1:29:A:LYS:HB3   | 9        | 0.33          |
| (1,1850) | 1:28:A:THR:HB    | 1:29:A:LYS:HB2   | 11       | 0.33          |
| (1,1850) | 1:28:A:THR:HB    | 1:29:A:LYS:HB3   | 11       | 0.33          |
| (1,937)  | 1:117:A:THR:H    | 1:118:A:VAL:HB   | 10       | 0.33          |
| (1,572)  | 1:62:A:GLN:HA    | 1:62:A:GLN:HE22  | 13       | 0.33          |
| (2,684)  | 1:30:A:ARG:HG2   | 1:34:A:GLU:HG3   | 18       | 0.32          |
| (2,661)  | 1:30:A:ARG:HA    | 1:32:A:LEU:HD11  | 7        | 0.32          |
| (2,661)  | 1:30:A:ARG:HA    | 1:32:A:LEU:HD12  | 7        | 0.32          |
| (2,661)  | 1:30:A:ARG:HA    | 1:32:A:LEU:HD13  | 7        | 0.32          |
| (1,3141) | 1:105:A:ILE:HG13 | 1:107:A:LEU:HG   | 6        | 0.32          |
| (1,2410) | 1:12:A:PHE:HE1   | 1:146:A:LEU:HD21 | 14       | 0.32          |
| (1,2410) | 1:12:A:PHE:HE1   | 1:146:A:LEU:HD22 | 14       | 0.32          |
| (1,2410) | 1:12:A:PHE:HE1   | 1:146:A:LEU:HD23 | 14       | 0.32          |
| (1,2410) | 1:12:A:PHE:HE2   | 1:146:A:LEU:HD21 | 14       | 0.32          |
| (1,2410) | 1:12:A:PHE:HE2   | 1:146:A:LEU:HD22 | 14       | 0.32          |
| (1,2410) | 1:12:A:PHE:HE2   | 1:146:A:LEU:HD23 | 14       | 0.32          |
| (1,2410) | 1:12:A:PHE:HE1   | 1:146:A:LEU:HD21 | 16       | 0.32          |
| (1,2410) | 1:12:A:PHE:HE1   | 1:146:A:LEU:HD22 | 16       | 0.32          |
| (1,2410) | 1:12:A:PHE:HE1   | 1:146:A:LEU:HD23 | 16       | 0.32          |
| (1,2410) | 1:12:A:PHE:HE2   | 1:146:A:LEU:HD21 | 16       | 0.32          |
| (1,2410) | 1:12:A:PHE:HE2   | 1:146:A:LEU:HD22 | 16       | 0.32          |
| (1,2410) | 1:12:A:PHE:HE2   | 1:146:A:LEU:HD23 | 16       | 0.32          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2410) | 1:12:A:PHE:HE1   | 1:146:A:LEU:HD21 | 18       | 0.32          |
| (1,2410) | 1:12:A:PHE:HE1   | 1:146:A:LEU:HD22 | 18       | 0.32          |
| (1,2410) | 1:12:A:PHE:HE1   | 1:146:A:LEU:HD23 | 18       | 0.32          |
| (1,2410) | 1:12:A:PHE:HE2   | 1:146:A:LEU:HD21 | 18       | 0.32          |
| (1,2410) | 1:12:A:PHE:HE2   | 1:146:A:LEU:HD22 | 18       | 0.32          |
| (1,2410) | 1:12:A:PHE:HE2   | 1:146:A:LEU:HD23 | 18       | 0.32          |
| (1,1850) | 1:28:A:THR:HB    | 1:29:A:LYS:HB2   | 5        | 0.32          |
| (1,1850) | 1:28:A:THR:HB    | 1:29:A:LYS:HB3   | 5        | 0.32          |
| (1,572)  | 1:62:A:GLN:HA    | 1:62:A:GLN:HE22  | 15       | 0.32          |
| (1,3141) | 1:105:A:ILE:HG13 | 1:107:A:LEU:HG   | 17       | 0.31          |
| (1,2535) | 1:125:A:PRO:HD2  | 1:130:A:ALA:HB1  | 2        | 0.31          |
| (1,2535) | 1:125:A:PRO:HD2  | 1:130:A:ALA:HB2  | 2        | 0.31          |
| (1,2535) | 1:125:A:PRO:HD2  | 1:130:A:ALA:HB3  | 2        | 0.31          |
| (1,2410) | 1:12:A:PHE:HE1   | 1:146:A:LEU:HD21 | 2        | 0.31          |
| (1,2410) | 1:12:A:PHE:HE1   | 1:146:A:LEU:HD22 | 2        | 0.31          |
| (1,2410) | 1:12:A:PHE:HE1   | 1:146:A:LEU:HD23 | 2        | 0.31          |
| (1,2410) | 1:12:A:PHE:HE2   | 1:146:A:LEU:HD21 | 2        | 0.31          |
| (1,2410) | 1:12:A:PHE:HE2   | 1:146:A:LEU:HD22 | 2        | 0.31          |
| (1,2410) | 1:12:A:PHE:HE2   | 1:146:A:LEU:HD23 | 2        | 0.31          |
| (1,1739) | 1:15:A:THR:HB    | 1:115:A:LYS:HE2  | 17       | 0.31          |
| (1,1739) | 1:15:A:THR:HB    | 1:115:A:LYS:HE3  | 17       | 0.31          |
| (2,684)  | 1:30:A:ARG:HG2   | 1:34:A:GLU:HG3   | 6        | 0.3           |
| (2,661)  | 1:30:A:ARG:HA    | 1:32:A:LEU:HD11  | 9        | 0.3           |
| (2,661)  | 1:30:A:ARG:HA    | 1:32:A:LEU:HD12  | 9        | 0.3           |
| (2,661)  | 1:30:A:ARG:HA    | 1:32:A:LEU:HD13  | 9        | 0.3           |
| (1,4229) | 1:152:A:LEU:HD11 | 1:153:A:LEU:HD11 | 10       | 0.3           |
| (1,4229) | 1:152:A:LEU:HD11 | 1:153:A:LEU:HD12 | 10       | 0.3           |
| (1,4229) | 1:152:A:LEU:HD11 | 1:153:A:LEU:HD13 | 10       | 0.3           |
| (1,4229) | 1:152:A:LEU:HD12 | 1:153:A:LEU:HD11 | 10       | 0.3           |
| (1,4229) | 1:152:A:LEU:HD12 | 1:153:A:LEU:HD12 | 10       | 0.3           |
| (1,4229) | 1:152:A:LEU:HD12 | 1:153:A:LEU:HD13 | 10       | 0.3           |
| (1,4229) | 1:152:A:LEU:HD13 | 1:153:A:LEU:HD11 | 10       | 0.3           |
| (1,4229) | 1:152:A:LEU:HD13 | 1:153:A:LEU:HD12 | 10       | 0.3           |
| (1,4229) | 1:152:A:LEU:HD13 | 1:153:A:LEU:HD13 | 10       | 0.3           |
| (1,4016) | 1:20:A:ILE:HD11  | 1:23:A:VAL:HB    | 12       | 0.3           |
| (1,4016) | 1:20:A:ILE:HD12  | 1:23:A:VAL:HB    | 12       | 0.3           |
| (1,4016) | 1:20:A:ILE:HD13  | 1:23:A:VAL:HB    | 12       | 0.3           |
| (1,2410) | 1:12:A:PHE:HE1   | 1:146:A:LEU:HD21 | 4        | 0.3           |
| (1,2410) | 1:12:A:PHE:HE1   | 1:146:A:LEU:HD22 | 4        | 0.3           |
| (1,2410) | 1:12:A:PHE:HE1   | 1:146:A:LEU:HD23 | 4        | 0.3           |
| (1,2410) | 1:12:A:PHE:HE2   | 1:146:A:LEU:HD21 | 4        | 0.3           |
| (1,2410) | 1:12:A:PHE:HE2   | 1:146:A:LEU:HD22 | 4        | 0.3           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2410) | 1:12:A:PHE:HE2   | 1:146:A:LEU:HD23 | 4        | 0.3           |
| (2,661)  | 1:30:A:ARG:HA    | 1:32:A:LEU:HD11  | 2        | 0.29          |
| (2,661)  | 1:30:A:ARG:HA    | 1:32:A:LEU:HD12  | 2        | 0.29          |
| (2,661)  | 1:30:A:ARG:HA    | 1:32:A:LEU:HD13  | 2        | 0.29          |
| (1,4021) | 1:19:A:PRO:HG2   | 1:22:A:LYS:HG3   | 12       | 0.29          |
| (1,4021) | 1:19:A:PRO:HG2   | 1:22:A:LYS:HG3   | 16       | 0.29          |
| (1,3505) | 1:140:A:THR:HG21 | 1:141:A:GLY:HA3  | 18       | 0.29          |
| (1,3505) | 1:140:A:THR:HG22 | 1:141:A:GLY:HA3  | 18       | 0.29          |
| (1,3505) | 1:140:A:THR:HG23 | 1:141:A:GLY:HA3  | 18       | 0.29          |
| (1,3391) | 1:131:A:GLN:HG2  | 1:132:A:GLN:HA   | 1        | 0.29          |
| (1,3277) | 1:12:A:PHE:HB2   | 1:120:A:SER:HB3  | 4        | 0.29          |
| (1,2930) | 1:71:A:ILE:HD11  | 1:91:A:THR:HG21  | 15       | 0.29          |
| (1,2930) | 1:71:A:ILE:HD11  | 1:91:A:THR:HG22  | 15       | 0.29          |
| (1,2930) | 1:71:A:ILE:HD11  | 1:91:A:THR:HG23  | 15       | 0.29          |
| (1,2930) | 1:71:A:ILE:HD12  | 1:91:A:THR:HG21  | 15       | 0.29          |
| (1,2930) | 1:71:A:ILE:HD12  | 1:91:A:THR:HG22  | 15       | 0.29          |
| (1,2930) | 1:71:A:ILE:HD12  | 1:91:A:THR:HG23  | 15       | 0.29          |
| (1,2930) | 1:71:A:ILE:HD13  | 1:91:A:THR:HG21  | 15       | 0.29          |
| (1,2930) | 1:71:A:ILE:HD13  | 1:91:A:THR:HG22  | 15       | 0.29          |
| (1,2930) | 1:71:A:ILE:HD13  | 1:91:A:THR:HG23  | 15       | 0.29          |
| (1,1850) | 1:28:A:THR:HB    | 1:29:A:LYS:HB2   | 16       | 0.29          |
| (1,1850) | 1:28:A:THR:HB    | 1:29:A:LYS:HB3   | 16       | 0.29          |
| (1,1546) | 1:22:A:LYS:HG3   | 1:23:A:VAL:HB    | 3        | 0.29          |
| (2,801)  | 1:96:A:LYS:HD3   | 1:97:A:ASP:HA    | 1        | 0.28          |
| (2,684)  | 1:30:A:ARG:HG2   | 1:34:A:GLU:HG3   | 4        | 0.28          |
| (2,359)  | 1:82:A:TYR:HA    | 1:109:A:PHE:HD1  | 5        | 0.28          |
| (2,359)  | 1:82:A:TYR:HA    | 1:109:A:PHE:HD2  | 5        | 0.28          |
| (1,4362) | 1:68:A:SER:HA    | 1:69:A:TYR:HE1   | 9        | 0.28          |
| (1,4362) | 1:68:A:SER:HA    | 1:69:A:TYR:HE2   | 9        | 0.28          |
| (1,4229) | 1:152:A:LEU:HD11 | 1:153:A:LEU:HD11 | 7        | 0.28          |
| (1,4229) | 1:152:A:LEU:HD11 | 1:153:A:LEU:HD12 | 7        | 0.28          |
| (1,4229) | 1:152:A:LEU:HD11 | 1:153:A:LEU:HD13 | 7        | 0.28          |
| (1,4229) | 1:152:A:LEU:HD12 | 1:153:A:LEU:HD11 | 7        | 0.28          |
| (1,4229) | 1:152:A:LEU:HD12 | 1:153:A:LEU:HD12 | 7        | 0.28          |
| (1,4229) | 1:152:A:LEU:HD12 | 1:153:A:LEU:HD13 | 7        | 0.28          |
| (1,4229) | 1:152:A:LEU:HD13 | 1:153:A:LEU:HD11 | 7        | 0.28          |
| (1,4229) | 1:152:A:LEU:HD13 | 1:153:A:LEU:HD12 | 7        | 0.28          |
| (1,4229) | 1:152:A:LEU:HD13 | 1:153:A:LEU:HD13 | 7        | 0.28          |
| (1,4229) | 1:152:A:LEU:HD11 | 1:153:A:LEU:HD11 | 12       | 0.28          |
| (1,4229) | 1:152:A:LEU:HD11 | 1:153:A:LEU:HD12 | 12       | 0.28          |
| (1,4229) | 1:152:A:LEU:HD11 | 1:153:A:LEU:HD13 | 12       | 0.28          |
| (1,4229) | 1:152:A:LEU:HD12 | 1:153:A:LEU:HD11 | 12       | 0.28          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,4229) | 1:152:A:LEU:HD12 | 1:153:A:LEU:HD12 | 12       | 0.28          |
| (1,4229) | 1:152:A:LEU:HD12 | 1:153:A:LEU:HD13 | 12       | 0.28          |
| (1,4229) | 1:152:A:LEU:HD13 | 1:153:A:LEU:HD11 | 12       | 0.28          |
| (1,4229) | 1:152:A:LEU:HD13 | 1:153:A:LEU:HD12 | 12       | 0.28          |
| (1,4229) | 1:152:A:LEU:HD13 | 1:153:A:LEU:HD13 | 12       | 0.28          |
| (1,3391) | 1:131:A:GLN:HG2  | 1:132:A:GLN:HA   | 2        | 0.28          |
| (1,3391) | 1:131:A:GLN:HG2  | 1:132:A:GLN:HA   | 11       | 0.28          |
| (1,3391) | 1:131:A:GLN:HG2  | 1:132:A:GLN:HA   | 12       | 0.28          |
| (1,3391) | 1:131:A:GLN:HG2  | 1:132:A:GLN:HA   | 18       | 0.28          |
| (1,3277) | 1:12:A:PHE:HB2   | 1:120:A:SER:HB3  | 5        | 0.28          |
| (1,3277) | 1:12:A:PHE:HB2   | 1:120:A:SER:HB3  | 14       | 0.28          |
| (1,3277) | 1:12:A:PHE:HB2   | 1:120:A:SER:HB3  | 17       | 0.28          |
| (1,3141) | 1:105:A:ILE:HG13 | 1:107:A:LEU:HG   | 11       | 0.28          |
| (1,2410) | 1:12:A:PHE:HE1   | 1:146:A:LEU:HD21 | 11       | 0.28          |
| (1,2410) | 1:12:A:PHE:HE1   | 1:146:A:LEU:HD22 | 11       | 0.28          |
| (1,2410) | 1:12:A:PHE:HE1   | 1:146:A:LEU:HD23 | 11       | 0.28          |
| (1,2410) | 1:12:A:PHE:HE2   | 1:146:A:LEU:HD21 | 11       | 0.28          |
| (1,2410) | 1:12:A:PHE:HE2   | 1:146:A:LEU:HD22 | 11       | 0.28          |
| (1,2410) | 1:12:A:PHE:HE2   | 1:146:A:LEU:HD23 | 11       | 0.28          |
| (1,2410) | 1:12:A:PHE:HE1   | 1:146:A:LEU:HD21 | 17       | 0.28          |
| (1,2410) | 1:12:A:PHE:HE1   | 1:146:A:LEU:HD22 | 17       | 0.28          |
| (1,2410) | 1:12:A:PHE:HE1   | 1:146:A:LEU:HD23 | 17       | 0.28          |
| (1,2410) | 1:12:A:PHE:HE2   | 1:146:A:LEU:HD21 | 17       | 0.28          |
| (1,2410) | 1:12:A:PHE:HE2   | 1:146:A:LEU:HD22 | 17       | 0.28          |
| (1,2410) | 1:12:A:PHE:HE2   | 1:146:A:LEU:HD23 | 17       | 0.28          |
| (1,572)  | 1:62:A:GLN:HA    | 1:62:A:GLN:HE22  | 12       | 0.28          |
| (2,684)  | 1:30:A:ARG:HG2   | 1:34:A:GLU:HG3   | 1        | 0.27          |
| (2,661)  | 1:30:A:ARG:HA    | 1:32:A:LEU:HD11  | 15       | 0.27          |
| (2,661)  | 1:30:A:ARG:HA    | 1:32:A:LEU:HD12  | 15       | 0.27          |
| (2,661)  | 1:30:A:ARG:HA    | 1:32:A:LEU:HD13  | 15       | 0.27          |
| (2,661)  | 1:30:A:ARG:HA    | 1:32:A:LEU:HD11  | 18       | 0.27          |
| (2,661)  | 1:30:A:ARG:HA    | 1:32:A:LEU:HD12  | 18       | 0.27          |
| (2,661)  | 1:30:A:ARG:HA    | 1:32:A:LEU:HD13  | 18       | 0.27          |
| (2,22)   | 1:32:A:LEU:H     | 1:49:A:PHE:HE1   | 2        | 0.27          |
| (2,22)   | 1:32:A:LEU:H     | 1:49:A:PHE:HE2   | 2        | 0.27          |
| (1,4021) | 1:19:A:PRO:HG2   | 1:22:A:LYS:HG3   | 2        | 0.27          |
| (1,4021) | 1:19:A:PRO:HG2   | 1:22:A:LYS:HG3   | 5        | 0.27          |
| (1,4021) | 1:19:A:PRO:HG2   | 1:22:A:LYS:HG3   | 19       | 0.27          |
| (1,3296) | 1:9:A:LYS:HA     | 1:122:A:SER:HB3  | 4        | 0.27          |
| (1,3277) | 1:12:A:PHE:HB2   | 1:120:A:SER:HB3  | 10       | 0.27          |
| (1,3277) | 1:12:A:PHE:HB2   | 1:120:A:SER:HB3  | 12       | 0.27          |
| (1,3155) | 1:83:A:ILE:HG21  | 1:106:A:THR:HG21 | 1        | 0.27          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3155) | 1:83:A:ILE:HG21  | 1:106:A:THR:HG22 | 1        | 0.27          |
| (1,3155) | 1:83:A:ILE:HG21  | 1:106:A:THR:HG23 | 1        | 0.27          |
| (1,3155) | 1:83:A:ILE:HG22  | 1:106:A:THR:HG21 | 1        | 0.27          |
| (1,3155) | 1:83:A:ILE:HG22  | 1:106:A:THR:HG22 | 1        | 0.27          |
| (1,3155) | 1:83:A:ILE:HG22  | 1:106:A:THR:HG23 | 1        | 0.27          |
| (1,3155) | 1:83:A:ILE:HG23  | 1:106:A:THR:HG21 | 1        | 0.27          |
| (1,3155) | 1:83:A:ILE:HG23  | 1:106:A:THR:HG22 | 1        | 0.27          |
| (1,3155) | 1:83:A:ILE:HG23  | 1:106:A:THR:HG23 | 1        | 0.27          |
| (1,2535) | 1:125:A:PRO:HD2  | 1:130:A:ALA:HB1  | 1        | 0.27          |
| (1,2535) | 1:125:A:PRO:HD2  | 1:130:A:ALA:HB2  | 1        | 0.27          |
| (1,2535) | 1:125:A:PRO:HD2  | 1:130:A:ALA:HB3  | 1        | 0.27          |
| (1,2535) | 1:125:A:PRO:HD2  | 1:130:A:ALA:HB1  | 3        | 0.27          |
| (1,2535) | 1:125:A:PRO:HD2  | 1:130:A:ALA:HB2  | 3        | 0.27          |
| (1,2535) | 1:125:A:PRO:HD2  | 1:130:A:ALA:HB3  | 3        | 0.27          |
| (1,2535) | 1:125:A:PRO:HD2  | 1:130:A:ALA:HB1  | 6        | 0.27          |
| (1,2535) | 1:125:A:PRO:HD2  | 1:130:A:ALA:HB2  | 6        | 0.27          |
| (1,2535) | 1:125:A:PRO:HD2  | 1:130:A:ALA:HB3  | 6        | 0.27          |
| (1,2535) | 1:125:A:PRO:HD2  | 1:130:A:ALA:HB1  | 15       | 0.27          |
| (1,2535) | 1:125:A:PRO:HD2  | 1:130:A:ALA:HB2  | 15       | 0.27          |
| (1,2535) | 1:125:A:PRO:HD2  | 1:130:A:ALA:HB3  | 15       | 0.27          |
| (1,2535) | 1:125:A:PRO:HD2  | 1:130:A:ALA:HB1  | 17       | 0.27          |
| (1,2535) | 1:125:A:PRO:HD2  | 1:130:A:ALA:HB2  | 17       | 0.27          |
| (1,2535) | 1:125:A:PRO:HD2  | 1:130:A:ALA:HB3  | 17       | 0.27          |
| (1,2410) | 1:12:A:PHE:HE1   | 1:146:A:LEU:HD21 | 15       | 0.27          |
| (1,2410) | 1:12:A:PHE:HE1   | 1:146:A:LEU:HD22 | 15       | 0.27          |
| (1,2410) | 1:12:A:PHE:HE1   | 1:146:A:LEU:HD23 | 15       | 0.27          |
| (1,2410) | 1:12:A:PHE:HE2   | 1:146:A:LEU:HD21 | 15       | 0.27          |
| (1,2410) | 1:12:A:PHE:HE2   | 1:146:A:LEU:HD22 | 15       | 0.27          |
| (1,2410) | 1:12:A:PHE:HE2   | 1:146:A:LEU:HD23 | 15       | 0.27          |
| (1,1988) | 1:27:A:TYR:HB3   | 1:28:A:THR:HG21  | 3        | 0.27          |
| (1,1988) | 1:27:A:TYR:HB3   | 1:28:A:THR:HG22  | 3        | 0.27          |
| (1,1988) | 1:27:A:TYR:HB3   | 1:28:A:THR:HG23  | 3        | 0.27          |
| (1,1496) | 1:28:A:THR:HB    | 1:29:A:LYS:HG2   | 20       | 0.27          |
| (1,1496) | 1:28:A:THR:HB    | 1:29:A:LYS:HG3   | 20       | 0.27          |
| (1,999)  | 1:126:A:THR:HA   | 1:130:A:ALA:H    | 5        | 0.27          |
| (1,572)  | 1:62:A:GLN:HA    | 1:62:A:GLN:HE22  | 16       | 0.27          |
| (2,801)  | 1:96:A:LYS:HD3   | 1:97:A:ASP:HA    | 5        | 0.26          |
| (2,661)  | 1:30:A:ARG:HA    | 1:32:A:LEU:HD11  | 6        | 0.26          |
| (2,661)  | 1:30:A:ARG:HA    | 1:32:A:LEU:HD12  | 6        | 0.26          |
| (2,661)  | 1:30:A:ARG:HA    | 1:32:A:LEU:HD13  | 6        | 0.26          |
| (1,4229) | 1:152:A:LEU:HD11 | 1:153:A:LEU:HD11 | 4        | 0.26          |
| (1,4229) | 1:152:A:LEU:HD11 | 1:153:A:LEU:HD12 | 4        | 0.26          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,4229) | 1:152:A:LEU:HD11 | 1:153:A:LEU:HD13 | 4        | 0.26          |
| (1,4229) | 1:152:A:LEU:HD12 | 1:153:A:LEU:HD11 | 4        | 0.26          |
| (1,4229) | 1:152:A:LEU:HD12 | 1:153:A:LEU:HD12 | 4        | 0.26          |
| (1,4229) | 1:152:A:LEU:HD12 | 1:153:A:LEU:HD13 | 4        | 0.26          |
| (1,4229) | 1:152:A:LEU:HD13 | 1:153:A:LEU:HD11 | 4        | 0.26          |
| (1,4229) | 1:152:A:LEU:HD13 | 1:153:A:LEU:HD12 | 4        | 0.26          |
| (1,4229) | 1:152:A:LEU:HD13 | 1:153:A:LEU:HD13 | 4        | 0.26          |
| (1,3972) | 1:5:A:LYS:HB3    | 1:6:A:LYS:HA     | 12       | 0.26          |
| (1,3391) | 1:131:A:GLN:HG2  | 1:132:A:GLN:HA   | 4        | 0.26          |
| (1,3391) | 1:131:A:GLN:HG2  | 1:132:A:GLN:HA   | 14       | 0.26          |
| (1,3296) | 1:9:A:LYS:HA     | 1:122:A:SER:HB3  | 12       | 0.26          |
| (1,3293) | 1:9:A:LYS:HD3    | 1:121:A:THR:HG21 | 13       | 0.26          |
| (1,3293) | 1:9:A:LYS:HD3    | 1:121:A:THR:HG22 | 13       | 0.26          |
| (1,3293) | 1:9:A:LYS:HD3    | 1:121:A:THR:HG23 | 13       | 0.26          |
| (1,3277) | 1:12:A:PHE:HB2   | 1:120:A:SER:HB3  | 9        | 0.26          |
| (1,3249) | 1:118:A:VAL:HG11 | 1:119:A:THR:HB   | 12       | 0.26          |
| (1,3249) | 1:118:A:VAL:HG12 | 1:119:A:THR:HB   | 12       | 0.26          |
| (1,3249) | 1:118:A:VAL:HG13 | 1:119:A:THR:HB   | 12       | 0.26          |
| (1,2835) | 1:93:A:LYS:HB3   | 1:95:A:GLU:HG2   | 8        | 0.26          |
| (1,2410) | 1:12:A:PHE:HE1   | 1:146:A:LEU:HD21 | 20       | 0.26          |
| (1,2410) | 1:12:A:PHE:HE1   | 1:146:A:LEU:HD22 | 20       | 0.26          |
| (1,2410) | 1:12:A:PHE:HE1   | 1:146:A:LEU:HD23 | 20       | 0.26          |
| (1,2410) | 1:12:A:PHE:HE2   | 1:146:A:LEU:HD21 | 20       | 0.26          |
| (1,2410) | 1:12:A:PHE:HE2   | 1:146:A:LEU:HD22 | 20       | 0.26          |
| (1,2410) | 1:12:A:PHE:HE2   | 1:146:A:LEU:HD23 | 20       | 0.26          |
| (1,1988) | 1:27:A:TYR:HB3   | 1:28:A:THR:HG21  | 6        | 0.26          |
| (1,1988) | 1:27:A:TYR:HB3   | 1:28:A:THR:HG22  | 6        | 0.26          |
| (1,1988) | 1:27:A:TYR:HB3   | 1:28:A:THR:HG23  | 6        | 0.26          |
| (1,999)  | 1:126:A:THR:HA   | 1:130:A:ALA:H    | 11       | 0.26          |
| (1,937)  | 1:117:A:THR:H    | 1:118:A:VAL:HB   | 16       | 0.26          |
| (2,684)  | 1:30:A:ARG:HG2   | 1:34:A:GLU:HG3   | 17       | 0.25          |
| (2,661)  | 1:30:A:ARG:HA    | 1:32:A:LEU:HD11  | 12       | 0.25          |
| (2,661)  | 1:30:A:ARG:HA    | 1:32:A:LEU:HD12  | 12       | 0.25          |
| (2,661)  | 1:30:A:ARG:HA    | 1:32:A:LEU:HD13  | 12       | 0.25          |
| (1,4021) | 1:19:A:PRO:HG2   | 1:22:A:LYS:HG3   | 18       | 0.25          |
| (1,3391) | 1:131:A:GLN:HG2  | 1:132:A:GLN:HA   | 16       | 0.25          |
| (1,3391) | 1:131:A:GLN:HG2  | 1:132:A:GLN:HA   | 17       | 0.25          |
| (1,3277) | 1:12:A:PHE:HB2   | 1:120:A:SER:HB3  | 1        | 0.25          |
| (1,3277) | 1:12:A:PHE:HB2   | 1:120:A:SER:HB3  | 13       | 0.25          |
| (1,3141) | 1:105:A:ILE:HG13 | 1:107:A:LEU:HG   | 4        | 0.25          |
| (1,3141) | 1:105:A:ILE:HG13 | 1:107:A:LEU:HG   | 10       | 0.25          |
| (1,1988) | 1:27:A:TYR:HB3   | 1:28:A:THR:HG21  | 1        | 0.25          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1988) | 1:27:A:TYR:HB3   | 1:28:A:THR:HG22  | 1        | 0.25          |
| (1,1988) | 1:27:A:TYR:HB3   | 1:28:A:THR:HG23  | 1        | 0.25          |
| (1,1988) | 1:27:A:TYR:HB3   | 1:28:A:THR:HG21  | 19       | 0.25          |
| (1,1988) | 1:27:A:TYR:HB3   | 1:28:A:THR:HG22  | 19       | 0.25          |
| (1,1988) | 1:27:A:TYR:HB3   | 1:28:A:THR:HG23  | 19       | 0.25          |
| (1,572)  | 1:62:A:GLN:HA    | 1:62:A:GLN:HE22  | 8        | 0.25          |
| (1,486)  | 1:53:A:LYS:HD2   | 1:54:A:GLY:H     | 1        | 0.25          |
| (1,486)  | 1:53:A:LYS:HD3   | 1:54:A:GLY:H     | 1        | 0.25          |
| (1,320)  | 1:154:A:ASN:HA   | 1:154:A:ASN:HD22 | 10       | 0.25          |
| (1,150)  | 1:21:A:ASN:H     | 1:23:A:VAL:HB    | 17       | 0.25          |
| (2,661)  | 1:30:A:ARG:HA    | 1:32:A:LEU:HD11  | 19       | 0.24          |
| (2,661)  | 1:30:A:ARG:HA    | 1:32:A:LEU:HD12  | 19       | 0.24          |
| (2,661)  | 1:30:A:ARG:HA    | 1:32:A:LEU:HD13  | 19       | 0.24          |
| (1,4257) | 1:24:A:PHE:HD1   | 1:27:A:TYR:H     | 14       | 0.24          |
| (1,4257) | 1:24:A:PHE:HD2   | 1:27:A:TYR:H     | 14       | 0.24          |
| (1,4229) | 1:152:A:LEU:HD11 | 1:153:A:LEU:HD11 | 9        | 0.24          |
| (1,4229) | 1:152:A:LEU:HD11 | 1:153:A:LEU:HD12 | 9        | 0.24          |
| (1,4229) | 1:152:A:LEU:HD11 | 1:153:A:LEU:HD13 | 9        | 0.24          |
| (1,4229) | 1:152:A:LEU:HD12 | 1:153:A:LEU:HD11 | 9        | 0.24          |
| (1,4229) | 1:152:A:LEU:HD12 | 1:153:A:LEU:HD12 | 9        | 0.24          |
| (1,4229) | 1:152:A:LEU:HD12 | 1:153:A:LEU:HD13 | 9        | 0.24          |
| (1,4229) | 1:152:A:LEU:HD13 | 1:153:A:LEU:HD11 | 9        | 0.24          |
| (1,4229) | 1:152:A:LEU:HD13 | 1:153:A:LEU:HD12 | 9        | 0.24          |
| (1,4229) | 1:152:A:LEU:HD13 | 1:153:A:LEU:HD13 | 9        | 0.24          |
| (1,4229) | 1:152:A:LEU:HD11 | 1:153:A:LEU:HD11 | 18       | 0.24          |
| (1,4229) | 1:152:A:LEU:HD11 | 1:153:A:LEU:HD12 | 18       | 0.24          |
| (1,4229) | 1:152:A:LEU:HD11 | 1:153:A:LEU:HD13 | 18       | 0.24          |
| (1,4229) | 1:152:A:LEU:HD12 | 1:153:A:LEU:HD11 | 18       | 0.24          |
| (1,4229) | 1:152:A:LEU:HD12 | 1:153:A:LEU:HD12 | 18       | 0.24          |
| (1,4229) | 1:152:A:LEU:HD12 | 1:153:A:LEU:HD13 | 18       | 0.24          |
| (1,4229) | 1:152:A:LEU:HD13 | 1:153:A:LEU:HD11 | 18       | 0.24          |
| (1,4229) | 1:152:A:LEU:HD13 | 1:153:A:LEU:HD12 | 18       | 0.24          |
| (1,4229) | 1:152:A:LEU:HD13 | 1:153:A:LEU:HD13 | 18       | 0.24          |
| (1,3462) | 1:136:A:MET:HB3  | 1:138:A:VAL:HG11 | 10       | 0.24          |
| (1,3462) | 1:136:A:MET:HB3  | 1:138:A:VAL:HG12 | 10       | 0.24          |
| (1,3462) | 1:136:A:MET:HB3  | 1:138:A:VAL:HG13 | 10       | 0.24          |
| (1,3391) | 1:131:A:GLN:HG2  | 1:132:A:GLN:HA   | 8        | 0.24          |
| (1,3391) | 1:131:A:GLN:HG2  | 1:132:A:GLN:HA   | 15       | 0.24          |
| (1,3391) | 1:131:A:GLN:HG2  | 1:132:A:GLN:HA   | 20       | 0.24          |
| (1,3277) | 1:12:A:PHE:HB2   | 1:120:A:SER:HB3  | 11       | 0.24          |
| (1,3026) | 1:91:A:THR:HG21  | 1:97:A:ASP:HB3   | 1        | 0.24          |
| (1,3026) | 1:91:A:THR:HG22  | 1:97:A:ASP:HB3   | 1        | 0.24          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3026) | 1:91:A:THR:HG23  | 1:97:A:ASP:HB3   | 1        | 0.24          |
| (1,3008) | 1:95:A:GLU:HB2   | 1:96:A:LYS:HB2   | 13       | 0.24          |
| (1,3008) | 1:95:A:GLU:HB2   | 1:96:A:LYS:HB3   | 13       | 0.24          |
| (1,2929) | 1:91:A:THR:HG21  | 1:96:A:LYS:HD2   | 8        | 0.24          |
| (1,2929) | 1:91:A:THR:HG22  | 1:96:A:LYS:HD2   | 8        | 0.24          |
| (1,2929) | 1:91:A:THR:HG23  | 1:96:A:LYS:HD2   | 8        | 0.24          |
| (1,2535) | 1:125:A:PRO:HD2  | 1:130:A:ALA:HB1  | 14       | 0.24          |
| (1,2535) | 1:125:A:PRO:HD2  | 1:130:A:ALA:HB2  | 14       | 0.24          |
| (1,2535) | 1:125:A:PRO:HD2  | 1:130:A:ALA:HB3  | 14       | 0.24          |
| (1,1988) | 1:27:A:TYR:HB3   | 1:28:A:THR:HG21  | 17       | 0.24          |
| (1,1988) | 1:27:A:TYR:HB3   | 1:28:A:THR:HG22  | 17       | 0.24          |
| (1,1988) | 1:27:A:TYR:HB3   | 1:28:A:THR:HG23  | 17       | 0.24          |
| (1,320)  | 1:154:A:ASN:HA   | 1:154:A:ASN:HD22 | 5        | 0.24          |
| (2,676)  | 1:32:A:LEU:HD11  | 1:149:A:LEU:HD21 | 10       | 0.23          |
| (2,676)  | 1:32:A:LEU:HD11  | 1:149:A:LEU:HD22 | 10       | 0.23          |
| (2,676)  | 1:32:A:LEU:HD11  | 1:149:A:LEU:HD23 | 10       | 0.23          |
| (2,676)  | 1:32:A:LEU:HD12  | 1:149:A:LEU:HD21 | 10       | 0.23          |
| (2,676)  | 1:32:A:LEU:HD12  | 1:149:A:LEU:HD22 | 10       | 0.23          |
| (2,676)  | 1:32:A:LEU:HD12  | 1:149:A:LEU:HD23 | 10       | 0.23          |
| (2,676)  | 1:32:A:LEU:HD13  | 1:149:A:LEU:HD21 | 10       | 0.23          |
| (2,676)  | 1:32:A:LEU:HD13  | 1:149:A:LEU:HD22 | 10       | 0.23          |
| (2,676)  | 1:32:A:LEU:HD13  | 1:149:A:LEU:HD23 | 10       | 0.23          |
| (2,661)  | 1:30:A:ARG:HA    | 1:32:A:LEU:HD11  | 1        | 0.23          |
| (2,661)  | 1:30:A:ARG:HA    | 1:32:A:LEU:HD12  | 1        | 0.23          |
| (2,661)  | 1:30:A:ARG:HA    | 1:32:A:LEU:HD13  | 1        | 0.23          |
| (2,641)  | 1:20:A:ILE:HG21  | 1:21:A:ASN:HD22  | 16       | 0.23          |
| (2,641)  | 1:20:A:ILE:HG22  | 1:21:A:ASN:HD22  | 16       | 0.23          |
| (2,641)  | 1:20:A:ILE:HG23  | 1:21:A:ASN:HD22  | 16       | 0.23          |
| (2,22)   | 1:32:A:LEU:H     | 1:49:A:PHE:HE1   | 20       | 0.23          |
| (2,22)   | 1:32:A:LEU:H     | 1:49:A:PHE:HE2   | 20       | 0.23          |
| (1,4229) | 1:152:A:LEU:HD11 | 1:153:A:LEU:HD11 | 3        | 0.23          |
| (1,4229) | 1:152:A:LEU:HD11 | 1:153:A:LEU:HD12 | 3        | 0.23          |
| (1,4229) | 1:152:A:LEU:HD11 | 1:153:A:LEU:HD13 | 3        | 0.23          |
| (1,4229) | 1:152:A:LEU:HD12 | 1:153:A:LEU:HD11 | 3        | 0.23          |
| (1,4229) | 1:152:A:LEU:HD12 | 1:153:A:LEU:HD12 | 3        | 0.23          |
| (1,4229) | 1:152:A:LEU:HD12 | 1:153:A:LEU:HD13 | 3        | 0.23          |
| (1,4229) | 1:152:A:LEU:HD13 | 1:153:A:LEU:HD11 | 3        | 0.23          |
| (1,4229) | 1:152:A:LEU:HD13 | 1:153:A:LEU:HD12 | 3        | 0.23          |
| (1,4229) | 1:152:A:LEU:HD13 | 1:153:A:LEU:HD13 | 3        | 0.23          |
| (1,4206) | 1:126:A:THR:HG21 | 1:129:A:ALA:HB1  | 17       | 0.23          |
| (1,4206) | 1:126:A:THR:HG21 | 1:129:A:ALA:HB2  | 17       | 0.23          |
| (1,4206) | 1:126:A:THR:HG21 | 1:129:A:ALA:HB3  | 17       | 0.23          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,4206) | 1:126:A:THR:HG22 | 1:129:A:ALA:HB1  | 17       | 0.23          |
| (1,4206) | 1:126:A:THR:HG22 | 1:129:A:ALA:HB2  | 17       | 0.23          |
| (1,4206) | 1:126:A:THR:HG22 | 1:129:A:ALA:HB3  | 17       | 0.23          |
| (1,4206) | 1:126:A:THR:HG23 | 1:129:A:ALA:HB1  | 17       | 0.23          |
| (1,4206) | 1:126:A:THR:HG23 | 1:129:A:ALA:HB2  | 17       | 0.23          |
| (1,4206) | 1:126:A:THR:HG23 | 1:129:A:ALA:HB3  | 17       | 0.23          |
| (1,4021) | 1:19:A:PRO:HG2   | 1:22:A:LYS:HG3   | 8        | 0.23          |
| (1,4021) | 1:19:A:PRO:HG2   | 1:22:A:LYS:HG3   | 14       | 0.23          |
| (1,3897) | 1:89:A:PHE:HD1   | 1:100:A:MET:HB2  | 3        | 0.23          |
| (1,3897) | 1:89:A:PHE:HD2   | 1:100:A:MET:HB2  | 3        | 0.23          |
| (1,3740) | 1:154:A:ASN:HA   | 1:157:A:LEU:HB3  | 13       | 0.23          |
| (1,3391) | 1:131:A:GLN:HG2  | 1:132:A:GLN:HA   | 7        | 0.23          |
| (1,3277) | 1:12:A:PHE:HB2   | 1:120:A:SER:HB3  | 2        | 0.23          |
| (1,3249) | 1:118:A:VAL:HG11 | 1:119:A:THR:HB   | 18       | 0.23          |
| (1,3249) | 1:118:A:VAL:HG12 | 1:119:A:THR:HB   | 18       | 0.23          |
| (1,3249) | 1:118:A:VAL:HG13 | 1:119:A:THR:HB   | 18       | 0.23          |
| (1,3155) | 1:83:A:ILE:HG21  | 1:106:A:THR:HG21 | 4        | 0.23          |
| (1,3155) | 1:83:A:ILE:HG21  | 1:106:A:THR:HG22 | 4        | 0.23          |
| (1,3155) | 1:83:A:ILE:HG21  | 1:106:A:THR:HG23 | 4        | 0.23          |
| (1,3155) | 1:83:A:ILE:HG22  | 1:106:A:THR:HG21 | 4        | 0.23          |
| (1,3155) | 1:83:A:ILE:HG22  | 1:106:A:THR:HG22 | 4        | 0.23          |
| (1,3155) | 1:83:A:ILE:HG22  | 1:106:A:THR:HG23 | 4        | 0.23          |
| (1,3155) | 1:83:A:ILE:HG23  | 1:106:A:THR:HG21 | 4        | 0.23          |
| (1,3155) | 1:83:A:ILE:HG23  | 1:106:A:THR:HG22 | 4        | 0.23          |
| (1,3155) | 1:83:A:ILE:HG23  | 1:106:A:THR:HG23 | 4        | 0.23          |
| (1,2889) | 1:87:A:ASP:HB2   | 1:103:A:MET:HB2  | 15       | 0.23          |
| (1,2889) | 1:87:A:ASP:HB2   | 1:103:A:MET:HB2  | 16       | 0.23          |
| (1,2410) | 1:12:A:PHE:HE1   | 1:146:A:LEU:HD21 | 5        | 0.23          |
| (1,2410) | 1:12:A:PHE:HE1   | 1:146:A:LEU:HD22 | 5        | 0.23          |
| (1,2410) | 1:12:A:PHE:HE1   | 1:146:A:LEU:HD23 | 5        | 0.23          |
| (1,2410) | 1:12:A:PHE:HE2   | 1:146:A:LEU:HD21 | 5        | 0.23          |
| (1,2410) | 1:12:A:PHE:HE2   | 1:146:A:LEU:HD22 | 5        | 0.23          |
| (1,2410) | 1:12:A:PHE:HE2   | 1:146:A:LEU:HD23 | 5        | 0.23          |
| (1,2410) | 1:12:A:PHE:HE1   | 1:146:A:LEU:HD21 | 9        | 0.23          |
| (1,2410) | 1:12:A:PHE:HE1   | 1:146:A:LEU:HD22 | 9        | 0.23          |
| (1,2410) | 1:12:A:PHE:HE1   | 1:146:A:LEU:HD23 | 9        | 0.23          |
| (1,2410) | 1:12:A:PHE:HE2   | 1:146:A:LEU:HD21 | 9        | 0.23          |
| (1,2410) | 1:12:A:PHE:HE2   | 1:146:A:LEU:HD22 | 9        | 0.23          |
| (1,2410) | 1:12:A:PHE:HE2   | 1:146:A:LEU:HD23 | 9        | 0.23          |
| (1,1988) | 1:27:A:TYR:HB3   | 1:28:A:THR:HG21  | 2        | 0.23          |
| (1,1988) | 1:27:A:TYR:HB3   | 1:28:A:THR:HG22  | 2        | 0.23          |
| (1,1988) | 1:27:A:TYR:HB3   | 1:28:A:THR:HG23  | 2        | 0.23          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1988) | 1:27:A:TYR:HB3  | 1:28:A:THR:HG21  | 15       | 0.23          |
| (1,1988) | 1:27:A:TYR:HB3  | 1:28:A:THR:HG22  | 15       | 0.23          |
| (1,1988) | 1:27:A:TYR:HB3  | 1:28:A:THR:HG23  | 15       | 0.23          |
| (1,1546) | 1:22:A:LYS:HG3  | 1:23:A:VAL:HB    | 6        | 0.23          |
| (1,1019) | 1:124:A:PHE:HB2 | 1:131:A:GLN:H    | 7        | 0.23          |
| (1,937)  | 1:117:A:THR:H   | 1:118:A:VAL:HB   | 2        | 0.23          |
| (1,320)  | 1:154:A:ASN:HA  | 1:154:A:ASN:HD22 | 7        | 0.23          |
| (1,9)    | 1:4:A:GLU:H     | 1:13:A:THR:HG21  | 17       | 0.23          |
| (1,9)    | 1:4:A:GLU:H     | 1:13:A:THR:HG22  | 17       | 0.23          |
| (1,9)    | 1:4:A:GLU:H     | 1:13:A:THR:HG23  | 17       | 0.23          |
| (2,676)  | 1:32:A:LEU:HD11 | 1:149:A:LEU:HD21 | 8        | 0.22          |
| (2,676)  | 1:32:A:LEU:HD11 | 1:149:A:LEU:HD22 | 8        | 0.22          |
| (2,676)  | 1:32:A:LEU:HD11 | 1:149:A:LEU:HD23 | 8        | 0.22          |
| (2,676)  | 1:32:A:LEU:HD12 | 1:149:A:LEU:HD21 | 8        | 0.22          |
| (2,676)  | 1:32:A:LEU:HD12 | 1:149:A:LEU:HD22 | 8        | 0.22          |
| (2,676)  | 1:32:A:LEU:HD12 | 1:149:A:LEU:HD23 | 8        | 0.22          |
| (2,676)  | 1:32:A:LEU:HD13 | 1:149:A:LEU:HD21 | 8        | 0.22          |
| (2,676)  | 1:32:A:LEU:HD13 | 1:149:A:LEU:HD22 | 8        | 0.22          |
| (2,676)  | 1:32:A:LEU:HD13 | 1:149:A:LEU:HD23 | 8        | 0.22          |
| (2,661)  | 1:30:A:ARG:HA   | 1:32:A:LEU:HD11  | 3        | 0.22          |
| (2,661)  | 1:30:A:ARG:HA   | 1:32:A:LEU:HD12  | 3        | 0.22          |
| (2,661)  | 1:30:A:ARG:HA   | 1:32:A:LEU:HD13  | 3        | 0.22          |
| (2,661)  | 1:30:A:ARG:HA   | 1:32:A:LEU:HD11  | 14       | 0.22          |
| (2,661)  | 1:30:A:ARG:HA   | 1:32:A:LEU:HD12  | 14       | 0.22          |
| (2,661)  | 1:30:A:ARG:HA   | 1:32:A:LEU:HD13  | 14       | 0.22          |
| (2,661)  | 1:30:A:ARG:HA   | 1:32:A:LEU:HD11  | 16       | 0.22          |
| (2,661)  | 1:30:A:ARG:HA   | 1:32:A:LEU:HD12  | 16       | 0.22          |
| (2,661)  | 1:30:A:ARG:HA   | 1:32:A:LEU:HD13  | 16       | 0.22          |
| (2,641)  | 1:20:A:ILE:HG21 | 1:21:A:ASN:HD22  | 3        | 0.22          |
| (2,641)  | 1:20:A:ILE:HG22 | 1:21:A:ASN:HD22  | 3        | 0.22          |
| (2,641)  | 1:20:A:ILE:HG23 | 1:21:A:ASN:HD22  | 3        | 0.22          |
| (2,22)   | 1:32:A:LEU:H    | 1:49:A:PHE:HE1   | 18       | 0.22          |
| (2,22)   | 1:32:A:LEU:H    | 1:49:A:PHE:HE2   | 18       | 0.22          |
| (1,4021) | 1:19:A:PRO:HG2  | 1:22:A:LYS:HG3   | 1        | 0.22          |
| (1,3897) | 1:89:A:PHE:HD1  | 1:100:A:MET:HB2  | 6        | 0.22          |
| (1,3897) | 1:89:A:PHE:HD2  | 1:100:A:MET:HB2  | 6        | 0.22          |
| (1,3749) | 1:3:A:ILE:HB    | 1:4:A:GLU:HA     | 7        | 0.22          |
| (1,3391) | 1:131:A:GLN:HG2 | 1:132:A:GLN:HA   | 6        | 0.22          |
| (1,3277) | 1:12:A:PHE:HB2  | 1:120:A:SER:HB3  | 19       | 0.22          |
| (1,3277) | 1:12:A:PHE:HB2  | 1:120:A:SER:HB3  | 20       | 0.22          |
| (1,3155) | 1:83:A:ILE:HG21 | 1:106:A:THR:HG21 | 2        | 0.22          |
| (1,3155) | 1:83:A:ILE:HG21 | 1:106:A:THR:HG22 | 2        | 0.22          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3155) | 1:83:A:ILE:HG21  | 1:106:A:THR:HG23 | 2        | 0.22          |
| (1,3155) | 1:83:A:ILE:HG22  | 1:106:A:THR:HG21 | 2        | 0.22          |
| (1,3155) | 1:83:A:ILE:HG22  | 1:106:A:THR:HG22 | 2        | 0.22          |
| (1,3155) | 1:83:A:ILE:HG22  | 1:106:A:THR:HG23 | 2        | 0.22          |
| (1,3155) | 1:83:A:ILE:HG23  | 1:106:A:THR:HG21 | 2        | 0.22          |
| (1,3155) | 1:83:A:ILE:HG23  | 1:106:A:THR:HG22 | 2        | 0.22          |
| (1,3155) | 1:83:A:ILE:HG23  | 1:106:A:THR:HG23 | 2        | 0.22          |
| (1,3155) | 1:83:A:ILE:HG21  | 1:106:A:THR:HG21 | 16       | 0.22          |
| (1,3155) | 1:83:A:ILE:HG21  | 1:106:A:THR:HG22 | 16       | 0.22          |
| (1,3155) | 1:83:A:ILE:HG21  | 1:106:A:THR:HG23 | 16       | 0.22          |
| (1,3155) | 1:83:A:ILE:HG22  | 1:106:A:THR:HG21 | 16       | 0.22          |
| (1,3155) | 1:83:A:ILE:HG22  | 1:106:A:THR:HG22 | 16       | 0.22          |
| (1,3155) | 1:83:A:ILE:HG22  | 1:106:A:THR:HG23 | 16       | 0.22          |
| (1,3155) | 1:83:A:ILE:HG23  | 1:106:A:THR:HG21 | 16       | 0.22          |
| (1,3155) | 1:83:A:ILE:HG23  | 1:106:A:THR:HG22 | 16       | 0.22          |
| (1,3155) | 1:83:A:ILE:HG23  | 1:106:A:THR:HG23 | 16       | 0.22          |
| (1,3155) | 1:83:A:ILE:HG21  | 1:106:A:THR:HG21 | 18       | 0.22          |
| (1,3155) | 1:83:A:ILE:HG21  | 1:106:A:THR:HG22 | 18       | 0.22          |
| (1,3155) | 1:83:A:ILE:HG21  | 1:106:A:THR:HG23 | 18       | 0.22          |
| (1,3155) | 1:83:A:ILE:HG22  | 1:106:A:THR:HG21 | 18       | 0.22          |
| (1,3155) | 1:83:A:ILE:HG22  | 1:106:A:THR:HG22 | 18       | 0.22          |
| (1,3155) | 1:83:A:ILE:HG22  | 1:106:A:THR:HG23 | 18       | 0.22          |
| (1,3155) | 1:83:A:ILE:HG23  | 1:106:A:THR:HG21 | 18       | 0.22          |
| (1,3155) | 1:83:A:ILE:HG23  | 1:106:A:THR:HG22 | 18       | 0.22          |
| (1,3155) | 1:83:A:ILE:HG23  | 1:106:A:THR:HG23 | 18       | 0.22          |
| (1,3141) | 1:105:A:ILE:HG13 | 1:107:A:LEU:HG   | 12       | 0.22          |
| (1,3026) | 1:91:A:THR:HG21  | 1:97:A:ASP:HB3   | 5        | 0.22          |
| (1,3026) | 1:91:A:THR:HG22  | 1:97:A:ASP:HB3   | 5        | 0.22          |
| (1,3026) | 1:91:A:THR:HG23  | 1:97:A:ASP:HB3   | 5        | 0.22          |
| (1,2930) | 1:71:A:ILE:HD11  | 1:91:A:THR:HG21  | 5        | 0.22          |
| (1,2930) | 1:71:A:ILE:HD11  | 1:91:A:THR:HG22  | 5        | 0.22          |
| (1,2930) | 1:71:A:ILE:HD11  | 1:91:A:THR:HG23  | 5        | 0.22          |
| (1,2930) | 1:71:A:ILE:HD12  | 1:91:A:THR:HG21  | 5        | 0.22          |
| (1,2930) | 1:71:A:ILE:HD12  | 1:91:A:THR:HG22  | 5        | 0.22          |
| (1,2930) | 1:71:A:ILE:HD12  | 1:91:A:THR:HG23  | 5        | 0.22          |
| (1,2930) | 1:71:A:ILE:HD13  | 1:91:A:THR:HG21  | 5        | 0.22          |
| (1,2930) | 1:71:A:ILE:HD13  | 1:91:A:THR:HG22  | 5        | 0.22          |
| (1,2930) | 1:71:A:ILE:HD13  | 1:91:A:THR:HG23  | 5        | 0.22          |
| (1,2930) | 1:71:A:ILE:HD11  | 1:91:A:THR:HG21  | 20       | 0.22          |
| (1,2930) | 1:71:A:ILE:HD11  | 1:91:A:THR:HG22  | 20       | 0.22          |
| (1,2930) | 1:71:A:ILE:HD11  | 1:91:A:THR:HG23  | 20       | 0.22          |
| (1,2930) | 1:71:A:ILE:HD12  | 1:91:A:THR:HG21  | 20       | 0.22          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2930) | 1:71:A:ILE:HD12  | 1:91:A:THR:HG22  | 20       | 0.22          |
| (1,2930) | 1:71:A:ILE:HD12  | 1:91:A:THR:HG23  | 20       | 0.22          |
| (1,2930) | 1:71:A:ILE:HD13  | 1:91:A:THR:HG21  | 20       | 0.22          |
| (1,2930) | 1:71:A:ILE:HD13  | 1:91:A:THR:HG22  | 20       | 0.22          |
| (1,2930) | 1:71:A:ILE:HD13  | 1:91:A:THR:HG23  | 20       | 0.22          |
| (1,2535) | 1:125:A:PRO:HD2  | 1:130:A:ALA:HB1  | 5        | 0.22          |
| (1,2535) | 1:125:A:PRO:HD2  | 1:130:A:ALA:HB2  | 5        | 0.22          |
| (1,2535) | 1:125:A:PRO:HD2  | 1:130:A:ALA:HB3  | 5        | 0.22          |
| (1,1675) | 1:53:A:LYS:HD2   | 1:77:A:VAL:HG11  | 9        | 0.22          |
| (1,1675) | 1:53:A:LYS:HD2   | 1:77:A:VAL:HG12  | 9        | 0.22          |
| (1,1675) | 1:53:A:LYS:HD2   | 1:77:A:VAL:HG13  | 9        | 0.22          |
| (1,1675) | 1:53:A:LYS:HD3   | 1:77:A:VAL:HG11  | 9        | 0.22          |
| (1,1675) | 1:53:A:LYS:HD3   | 1:77:A:VAL:HG12  | 9        | 0.22          |
| (1,1675) | 1:53:A:LYS:HD3   | 1:77:A:VAL:HG13  | 9        | 0.22          |
| (1,1546) | 1:22:A:LYS:HG3   | 1:23:A:VAL:HB    | 11       | 0.22          |
| (1,1546) | 1:22:A:LYS:HG3   | 1:23:A:VAL:HB    | 15       | 0.22          |
| (1,1247) | 1:128:A:SER:HA   | 1:132:A:GLN:H    | 20       | 0.22          |
| (1,1163) | 1:149:A:LEU:H    | 1:153:A:LEU:HD11 | 17       | 0.22          |
| (1,1163) | 1:149:A:LEU:H    | 1:153:A:LEU:HD12 | 17       | 0.22          |
| (1,1163) | 1:149:A:LEU:H    | 1:153:A:LEU:HD13 | 17       | 0.22          |
| (1,999)  | 1:126:A:THR:HA   | 1:130:A:ALA:H    | 15       | 0.22          |
| (1,937)  | 1:117:A:THR:H    | 1:118:A:VAL:HB   | 20       | 0.22          |
| (2,684)  | 1:30:A:ARG:HG2   | 1:34:A:GLU:HG3   | 15       | 0.21          |
| (2,661)  | 1:30:A:ARG:HA    | 1:32:A:LEU:HD11  | 8        | 0.21          |
| (2,661)  | 1:30:A:ARG:HA    | 1:32:A:LEU:HD12  | 8        | 0.21          |
| (2,661)  | 1:30:A:ARG:HA    | 1:32:A:LEU:HD13  | 8        | 0.21          |
| (2,661)  | 1:30:A:ARG:HA    | 1:32:A:LEU:HD11  | 10       | 0.21          |
| (2,661)  | 1:30:A:ARG:HA    | 1:32:A:LEU:HD12  | 10       | 0.21          |
| (2,661)  | 1:30:A:ARG:HA    | 1:32:A:LEU:HD13  | 10       | 0.21          |
| (2,661)  | 1:30:A:ARG:HA    | 1:32:A:LEU:HD11  | 11       | 0.21          |
| (2,661)  | 1:30:A:ARG:HA    | 1:32:A:LEU:HD12  | 11       | 0.21          |
| (2,661)  | 1:30:A:ARG:HA    | 1:32:A:LEU:HD13  | 11       | 0.21          |
| (2,252)  | 1:134:A:ILE:H    | 1:138:A:VAL:HG21 | 10       | 0.21          |
| (2,252)  | 1:134:A:ILE:H    | 1:138:A:VAL:HG22 | 10       | 0.21          |
| (2,252)  | 1:134:A:ILE:H    | 1:138:A:VAL:HG23 | 10       | 0.21          |
| (2,22)   | 1:32:A:LEU:H     | 1:49:A:PHE:HE1   | 1        | 0.21          |
| (2,22)   | 1:32:A:LEU:H     | 1:49:A:PHE:HE2   | 1        | 0.21          |
| (1,4362) | 1:68:A:SER:HA    | 1:69:A:TYR:HE1   | 7        | 0.21          |
| (1,4362) | 1:68:A:SER:HA    | 1:69:A:TYR:HE2   | 7        | 0.21          |
| (1,4362) | 1:68:A:SER:HA    | 1:69:A:TYR:HE1   | 12       | 0.21          |
| (1,4362) | 1:68:A:SER:HA    | 1:69:A:TYR:HE2   | 12       | 0.21          |
| (1,4229) | 1:152:A:LEU:HD11 | 1:153:A:LEU:HD11 | 13       | 0.21          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,4229) | 1:152:A:LEU:HD11 | 1:153:A:LEU:HD12 | 13       | 0.21          |
| (1,4229) | 1:152:A:LEU:HD11 | 1:153:A:LEU:HD13 | 13       | 0.21          |
| (1,4229) | 1:152:A:LEU:HD12 | 1:153:A:LEU:HD11 | 13       | 0.21          |
| (1,4229) | 1:152:A:LEU:HD12 | 1:153:A:LEU:HD12 | 13       | 0.21          |
| (1,4229) | 1:152:A:LEU:HD12 | 1:153:A:LEU:HD13 | 13       | 0.21          |
| (1,4229) | 1:152:A:LEU:HD13 | 1:153:A:LEU:HD11 | 13       | 0.21          |
| (1,4229) | 1:152:A:LEU:HD13 | 1:153:A:LEU:HD12 | 13       | 0.21          |
| (1,4229) | 1:152:A:LEU:HD13 | 1:153:A:LEU:HD13 | 13       | 0.21          |
| (1,4229) | 1:152:A:LEU:HD11 | 1:153:A:LEU:HD11 | 16       | 0.21          |
| (1,4229) | 1:152:A:LEU:HD11 | 1:153:A:LEU:HD12 | 16       | 0.21          |
| (1,4229) | 1:152:A:LEU:HD11 | 1:153:A:LEU:HD13 | 16       | 0.21          |
| (1,4229) | 1:152:A:LEU:HD12 | 1:153:A:LEU:HD11 | 16       | 0.21          |
| (1,4229) | 1:152:A:LEU:HD12 | 1:153:A:LEU:HD12 | 16       | 0.21          |
| (1,4229) | 1:152:A:LEU:HD12 | 1:153:A:LEU:HD13 | 16       | 0.21          |
| (1,4229) | 1:152:A:LEU:HD13 | 1:153:A:LEU:HD11 | 16       | 0.21          |
| (1,4229) | 1:152:A:LEU:HD13 | 1:153:A:LEU:HD12 | 16       | 0.21          |
| (1,4229) | 1:152:A:LEU:HD13 | 1:153:A:LEU:HD13 | 16       | 0.21          |
| (1,4016) | 1:20:A:ILE:HD11  | 1:23:A:VAL:HB    | 2        | 0.21          |
| (1,4016) | 1:20:A:ILE:HD12  | 1:23:A:VAL:HB    | 2        | 0.21          |
| (1,4016) | 1:20:A:ILE:HD13  | 1:23:A:VAL:HB    | 2        | 0.21          |
| (1,4016) | 1:20:A:ILE:HD11  | 1:23:A:VAL:HB    | 3        | 0.21          |
| (1,4016) | 1:20:A:ILE:HD12  | 1:23:A:VAL:HB    | 3        | 0.21          |
| (1,4016) | 1:20:A:ILE:HD13  | 1:23:A:VAL:HB    | 3        | 0.21          |
| (1,3391) | 1:131:A:GLN:HG2  | 1:132:A:GLN:HA   | 10       | 0.21          |
| (1,3277) | 1:12:A:PHE:HB2   | 1:120:A:SER:HB3  | 7        | 0.21          |
| (1,3277) | 1:12:A:PHE:HB2   | 1:120:A:SER:HB3  | 8        | 0.21          |
| (1,3277) | 1:12:A:PHE:HB2   | 1:120:A:SER:HB3  | 16       | 0.21          |
| (1,3155) | 1:83:A:ILE:HG21  | 1:106:A:THR:HG21 | 7        | 0.21          |
| (1,3155) | 1:83:A:ILE:HG21  | 1:106:A:THR:HG22 | 7        | 0.21          |
| (1,3155) | 1:83:A:ILE:HG21  | 1:106:A:THR:HG23 | 7        | 0.21          |
| (1,3155) | 1:83:A:ILE:HG22  | 1:106:A:THR:HG21 | 7        | 0.21          |
| (1,3155) | 1:83:A:ILE:HG22  | 1:106:A:THR:HG22 | 7        | 0.21          |
| (1,3155) | 1:83:A:ILE:HG22  | 1:106:A:THR:HG23 | 7        | 0.21          |
| (1,3155) | 1:83:A:ILE:HG23  | 1:106:A:THR:HG21 | 7        | 0.21          |
| (1,3155) | 1:83:A:ILE:HG23  | 1:106:A:THR:HG22 | 7        | 0.21          |
| (1,3155) | 1:83:A:ILE:HG23  | 1:106:A:THR:HG23 | 7        | 0.21          |
| (1,3155) | 1:83:A:ILE:HG21  | 1:106:A:THR:HG21 | 12       | 0.21          |
| (1,3155) | 1:83:A:ILE:HG21  | 1:106:A:THR:HG22 | 12       | 0.21          |
| (1,3155) | 1:83:A:ILE:HG21  | 1:106:A:THR:HG23 | 12       | 0.21          |
| (1,3155) | 1:83:A:ILE:HG22  | 1:106:A:THR:HG21 | 12       | 0.21          |
| (1,3155) | 1:83:A:ILE:HG22  | 1:106:A:THR:HG22 | 12       | 0.21          |
| (1,3155) | 1:83:A:ILE:HG22  | 1:106:A:THR:HG23 | 12       | 0.21          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3155) | 1:83:A:ILE:HG23 | 1:106:A:THR:HG21 | 12       | 0.21          |
| (1,3155) | 1:83:A:ILE:HG23 | 1:106:A:THR:HG22 | 12       | 0.21          |
| (1,3155) | 1:83:A:ILE:HG23 | 1:106:A:THR:HG23 | 12       | 0.21          |
| (1,3026) | 1:91:A:THR:HG21 | 1:97:A:ASP:HB3   | 15       | 0.21          |
| (1,3026) | 1:91:A:THR:HG22 | 1:97:A:ASP:HB3   | 15       | 0.21          |
| (1,3026) | 1:91:A:THR:HG23 | 1:97:A:ASP:HB3   | 15       | 0.21          |
| (1,2535) | 1:125:A:PRO:HD2 | 1:130:A:ALA:HB1  | 7        | 0.21          |
| (1,2535) | 1:125:A:PRO:HD2 | 1:130:A:ALA:HB2  | 7        | 0.21          |
| (1,2535) | 1:125:A:PRO:HD2 | 1:130:A:ALA:HB3  | 7        | 0.21          |
| (1,2535) | 1:125:A:PRO:HD2 | 1:130:A:ALA:HB1  | 11       | 0.21          |
| (1,2535) | 1:125:A:PRO:HD2 | 1:130:A:ALA:HB2  | 11       | 0.21          |
| (1,2535) | 1:125:A:PRO:HD2 | 1:130:A:ALA:HB3  | 11       | 0.21          |
| (1,2410) | 1:12:A:PHE:HE1  | 1:146:A:LEU:HD21 | 13       | 0.21          |
| (1,2410) | 1:12:A:PHE:HE1  | 1:146:A:LEU:HD22 | 13       | 0.21          |
| (1,2410) | 1:12:A:PHE:HE1  | 1:146:A:LEU:HD23 | 13       | 0.21          |
| (1,2410) | 1:12:A:PHE:HE2  | 1:146:A:LEU:HD21 | 13       | 0.21          |
| (1,2410) | 1:12:A:PHE:HE2  | 1:146:A:LEU:HD22 | 13       | 0.21          |
| (1,2410) | 1:12:A:PHE:HE2  | 1:146:A:LEU:HD23 | 13       | 0.21          |
| (1,2134) | 1:36:A:TRP:HH2  | 1:37:A:PHE:HA    | 13       | 0.21          |
| (1,1988) | 1:27:A:TYR:HB3  | 1:28:A:THR:HG21  | 7        | 0.21          |
| (1,1988) | 1:27:A:TYR:HB3  | 1:28:A:THR:HG22  | 7        | 0.21          |
| (1,1988) | 1:27:A:TYR:HB3  | 1:28:A:THR:HG23  | 7        | 0.21          |
| (1,1988) | 1:27:A:TYR:HB3  | 1:28:A:THR:HG21  | 12       | 0.21          |
| (1,1988) | 1:27:A:TYR:HB3  | 1:28:A:THR:HG22  | 12       | 0.21          |
| (1,1988) | 1:27:A:TYR:HB3  | 1:28:A:THR:HG23  | 12       | 0.21          |
| (1,1247) | 1:128:A:SER:HA  | 1:132:A:GLN:H    | 4        | 0.21          |
| (1,1136) | 1:144:A:SER:HA  | 1:147:A:ASN:HD22 | 17       | 0.21          |
| (1,1019) | 1:124:A:PHE:HB2 | 1:131:A:GLN:H    | 14       | 0.21          |
| (1,195)  | 1:108:A:ASN:H   | 1:118:A:VAL:HG21 | 1        | 0.21          |
| (1,195)  | 1:108:A:ASN:H   | 1:118:A:VAL:HG22 | 1        | 0.21          |
| (1,195)  | 1:108:A:ASN:H   | 1:118:A:VAL:HG23 | 1        | 0.21          |
| (1,150)  | 1:21:A:ASN:H    | 1:23:A:VAL:HB    | 9        | 0.21          |
| (2,661)  | 1:30:A:ARG:HA   | 1:32:A:LEU:HD11  | 4        | 0.2           |
| (2,661)  | 1:30:A:ARG:HA   | 1:32:A:LEU:HD12  | 4        | 0.2           |
| (2,661)  | 1:30:A:ARG:HA   | 1:32:A:LEU:HD13  | 4        | 0.2           |
| (2,22)   | 1:32:A:LEU:H    | 1:49:A:PHE:HE1   | 5        | 0.2           |
| (2,22)   | 1:32:A:LEU:H    | 1:49:A:PHE:HE2   | 5        | 0.2           |
| (2,22)   | 1:32:A:LEU:H    | 1:49:A:PHE:HE1   | 6        | 0.2           |
| (2,22)   | 1:32:A:LEU:H    | 1:49:A:PHE:HE2   | 6        | 0.2           |
| (2,22)   | 1:32:A:LEU:H    | 1:49:A:PHE:HE1   | 12       | 0.2           |
| (2,22)   | 1:32:A:LEU:H    | 1:49:A:PHE:HE2   | 12       | 0.2           |
| (2,22)   | 1:32:A:LEU:H    | 1:49:A:PHE:HE1   | 15       | 0.2           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,22)   | 1:32:A:LEU:H     | 1:49:A:PHE:HE2   | 15       | 0.2           |
| (2,22)   | 1:32:A:LEU:H     | 1:49:A:PHE:HE1   | 17       | 0.2           |
| (2,22)   | 1:32:A:LEU:H     | 1:49:A:PHE:HE2   | 17       | 0.2           |
| (2,22)   | 1:32:A:LEU:H     | 1:49:A:PHE:HE1   | 19       | 0.2           |
| (2,22)   | 1:32:A:LEU:H     | 1:49:A:PHE:HE2   | 19       | 0.2           |
| (1,4362) | 1:68:A:SER:HA    | 1:69:A:TYR:HE1   | 2        | 0.2           |
| (1,4362) | 1:68:A:SER:HA    | 1:69:A:TYR:HE2   | 2        | 0.2           |
| (1,4229) | 1:152:A:LEU:HD11 | 1:153:A:LEU:HD11 | 1        | 0.2           |
| (1,4229) | 1:152:A:LEU:HD11 | 1:153:A:LEU:HD12 | 1        | 0.2           |
| (1,4229) | 1:152:A:LEU:HD11 | 1:153:A:LEU:HD13 | 1        | 0.2           |
| (1,4229) | 1:152:A:LEU:HD12 | 1:153:A:LEU:HD11 | 1        | 0.2           |
| (1,4229) | 1:152:A:LEU:HD12 | 1:153:A:LEU:HD12 | 1        | 0.2           |
| (1,4229) | 1:152:A:LEU:HD12 | 1:153:A:LEU:HD13 | 1        | 0.2           |
| (1,4229) | 1:152:A:LEU:HD13 | 1:153:A:LEU:HD11 | 1        | 0.2           |
| (1,4229) | 1:152:A:LEU:HD13 | 1:153:A:LEU:HD12 | 1        | 0.2           |
| (1,4229) | 1:152:A:LEU:HD13 | 1:153:A:LEU:HD13 | 1        | 0.2           |
| (1,4229) | 1:152:A:LEU:HD11 | 1:153:A:LEU:HD11 | 8        | 0.2           |
| (1,4229) | 1:152:A:LEU:HD11 | 1:153:A:LEU:HD12 | 8        | 0.2           |
| (1,4229) | 1:152:A:LEU:HD11 | 1:153:A:LEU:HD13 | 8        | 0.2           |
| (1,4229) | 1:152:A:LEU:HD12 | 1:153:A:LEU:HD11 | 8        | 0.2           |
| (1,4229) | 1:152:A:LEU:HD12 | 1:153:A:LEU:HD12 | 8        | 0.2           |
| (1,4229) | 1:152:A:LEU:HD12 | 1:153:A:LEU:HD13 | 8        | 0.2           |
| (1,4229) | 1:152:A:LEU:HD13 | 1:153:A:LEU:HD11 | 8        | 0.2           |
| (1,4229) | 1:152:A:LEU:HD13 | 1:153:A:LEU:HD12 | 8        | 0.2           |
| (1,4229) | 1:152:A:LEU:HD13 | 1:153:A:LEU:HD13 | 8        | 0.2           |
| (1,4229) | 1:152:A:LEU:HD11 | 1:153:A:LEU:HD11 | 20       | 0.2           |
| (1,4229) | 1:152:A:LEU:HD11 | 1:153:A:LEU:HD12 | 20       | 0.2           |
| (1,4229) | 1:152:A:LEU:HD11 | 1:153:A:LEU:HD13 | 20       | 0.2           |
| (1,4229) | 1:152:A:LEU:HD12 | 1:153:A:LEU:HD11 | 20       | 0.2           |
| (1,4229) | 1:152:A:LEU:HD12 | 1:153:A:LEU:HD12 | 20       | 0.2           |
| (1,4229) | 1:152:A:LEU:HD12 | 1:153:A:LEU:HD13 | 20       | 0.2           |
| (1,4229) | 1:152:A:LEU:HD13 | 1:153:A:LEU:HD11 | 20       | 0.2           |
| (1,4229) | 1:152:A:LEU:HD13 | 1:153:A:LEU:HD12 | 20       | 0.2           |
| (1,4229) | 1:152:A:LEU:HD13 | 1:153:A:LEU:HD13 | 20       | 0.2           |
| (1,4021) | 1:19:A:PRO:HG2   | 1:22:A:LYS:HG3   | 7        | 0.2           |
| (1,3277) | 1:12:A:PHE:HB2   | 1:120:A:SER:HB3  | 18       | 0.2           |
| (1,3176) | 1:108:A:ASN:HA   | 1:109:A:PHE:HD1  | 5        | 0.2           |
| (1,3176) | 1:108:A:ASN:HA   | 1:109:A:PHE:HD2  | 5        | 0.2           |
| (1,3155) | 1:83:A:ILE:HG21  | 1:106:A:THR:HG21 | 11       | 0.2           |
| (1,3155) | 1:83:A:ILE:HG21  | 1:106:A:THR:HG22 | 11       | 0.2           |
| (1,3155) | 1:83:A:ILE:HG21  | 1:106:A:THR:HG23 | 11       | 0.2           |
| (1,3155) | 1:83:A:ILE:HG22  | 1:106:A:THR:HG21 | 11       | 0.2           |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3155) | 1:83:A:ILE:HG22 | 1:106:A:THR:HG22 | 11       | 0.2           |
| (1,3155) | 1:83:A:ILE:HG22 | 1:106:A:THR:HG23 | 11       | 0.2           |
| (1,3155) | 1:83:A:ILE:HG23 | 1:106:A:THR:HG21 | 11       | 0.2           |
| (1,3155) | 1:83:A:ILE:HG23 | 1:106:A:THR:HG22 | 11       | 0.2           |
| (1,3155) | 1:83:A:ILE:HG23 | 1:106:A:THR:HG23 | 11       | 0.2           |
| (1,3143) | 1:103:A:MET:HG3 | 1:105:A:ILE:HG12 | 4        | 0.2           |
| (1,3143) | 1:103:A:MET:HG3 | 1:105:A:ILE:HG12 | 11       | 0.2           |
| (1,3026) | 1:91:A:THR:HG21 | 1:97:A:ASP:HB3   | 2        | 0.2           |
| (1,3026) | 1:91:A:THR:HG22 | 1:97:A:ASP:HB3   | 2        | 0.2           |
| (1,3026) | 1:91:A:THR:HG23 | 1:97:A:ASP:HB3   | 2        | 0.2           |
| (1,2911) | 1:89:A:PHE:HB2  | 1:97:A:ASP:HB2   | 15       | 0.2           |
| (1,2552) | 1:100:A:MET:HB2 | 1:101:A:PRO:HD2  | 14       | 0.2           |
| (1,2535) | 1:125:A:PRO:HD2 | 1:130:A:ALA:HB1  | 9        | 0.2           |
| (1,2535) | 1:125:A:PRO:HD2 | 1:130:A:ALA:HB2  | 9        | 0.2           |
| (1,2535) | 1:125:A:PRO:HD2 | 1:130:A:ALA:HB3  | 9        | 0.2           |
| (1,2410) | 1:12:A:PHE:HE1  | 1:146:A:LEU:HD21 | 19       | 0.2           |
| (1,2410) | 1:12:A:PHE:HE1  | 1:146:A:LEU:HD22 | 19       | 0.2           |
| (1,2410) | 1:12:A:PHE:HE1  | 1:146:A:LEU:HD23 | 19       | 0.2           |
| (1,2410) | 1:12:A:PHE:HE2  | 1:146:A:LEU:HD21 | 19       | 0.2           |
| (1,2410) | 1:12:A:PHE:HE2  | 1:146:A:LEU:HD22 | 19       | 0.2           |
| (1,2410) | 1:12:A:PHE:HE2  | 1:146:A:LEU:HD23 | 19       | 0.2           |
| (1,2134) | 1:36:A:TRP:HH2  | 1:37:A:PHE:HA    | 19       | 0.2           |
| (1,1739) | 1:15:A:THR:HB   | 1:115:A:LYS:HE2  | 10       | 0.2           |
| (1,1739) | 1:15:A:THR:HB   | 1:115:A:LYS:HE3  | 10       | 0.2           |
| (1,1676) | 1:13:A:THR:HG21 | 1:14:A:ARG:HB2   | 16       | 0.2           |
| (1,1676) | 1:13:A:THR:HG22 | 1:14:A:ARG:HB2   | 16       | 0.2           |
| (1,1676) | 1:13:A:THR:HG23 | 1:14:A:ARG:HB2   | 16       | 0.2           |
| (1,937)  | 1:117:A:THR:H   | 1:118:A:VAL:HB   | 17       | 0.2           |
| (1,320)  | 1:154:A:ASN:HA  | 1:154:A:ASN:HD22 | 11       | 0.2           |
| (1,195)  | 1:108:A:ASN:H   | 1:118:A:VAL:HG21 | 5        | 0.2           |
| (1,195)  | 1:108:A:ASN:H   | 1:118:A:VAL:HG22 | 5        | 0.2           |
| (1,195)  | 1:108:A:ASN:H   | 1:118:A:VAL:HG23 | 5        | 0.2           |
| (2,684)  | 1:30:A:ARG:HG2  | 1:34:A:GLU:HG3   | 2        | 0.19          |
| (2,684)  | 1:30:A:ARG:HG2  | 1:34:A:GLU:HG3   | 12       | 0.19          |
| (2,661)  | 1:30:A:ARG:HA   | 1:32:A:LEU:HD11  | 13       | 0.19          |
| (2,661)  | 1:30:A:ARG:HA   | 1:32:A:LEU:HD12  | 13       | 0.19          |
| (2,661)  | 1:30:A:ARG:HA   | 1:32:A:LEU:HD13  | 13       | 0.19          |
| (2,661)  | 1:30:A:ARG:HA   | 1:32:A:LEU:HD11  | 17       | 0.19          |
| (2,661)  | 1:30:A:ARG:HA   | 1:32:A:LEU:HD12  | 17       | 0.19          |
| (2,661)  | 1:30:A:ARG:HA   | 1:32:A:LEU:HD13  | 17       | 0.19          |
| (2,22)   | 1:32:A:LEU:H    | 1:49:A:PHE:HE1   | 7        | 0.19          |
| (2,22)   | 1:32:A:LEU:H    | 1:49:A:PHE:HE2   | 7        | 0.19          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,22)   | 1:32:A:LEU:H    | 1:49:A:PHE:HE1   | 14       | 0.19          |
| (2,22)   | 1:32:A:LEU:H    | 1:49:A:PHE:HE2   | 14       | 0.19          |
| (1,4362) | 1:68:A:SER:HA   | 1:69:A:TYR:HE1   | 10       | 0.19          |
| (1,4362) | 1:68:A:SER:HA   | 1:69:A:TYR:HE2   | 10       | 0.19          |
| (1,3391) | 1:131:A:GLN:HG2 | 1:132:A:GLN:HA   | 5        | 0.19          |
| (1,3391) | 1:131:A:GLN:HG2 | 1:132:A:GLN:HA   | 13       | 0.19          |
| (1,3296) | 1:9:A:LYS:HA    | 1:122:A:SER:HB3  | 16       | 0.19          |
| (1,3277) | 1:12:A:PHE:HB2  | 1:120:A:SER:HB3  | 15       | 0.19          |
| (1,3191) | 1:108:A:ASN:HB3 | 1:119:A:THR:HB   | 6        | 0.19          |
| (1,3155) | 1:83:A:ILE:HG21 | 1:106:A:THR:HG21 | 5        | 0.19          |
| (1,3155) | 1:83:A:ILE:HG21 | 1:106:A:THR:HG22 | 5        | 0.19          |
| (1,3155) | 1:83:A:ILE:HG21 | 1:106:A:THR:HG23 | 5        | 0.19          |
| (1,3155) | 1:83:A:ILE:HG22 | 1:106:A:THR:HG21 | 5        | 0.19          |
| (1,3155) | 1:83:A:ILE:HG22 | 1:106:A:THR:HG22 | 5        | 0.19          |
| (1,3155) | 1:83:A:ILE:HG22 | 1:106:A:THR:HG23 | 5        | 0.19          |
| (1,3155) | 1:83:A:ILE:HG23 | 1:106:A:THR:HG21 | 5        | 0.19          |
| (1,3155) | 1:83:A:ILE:HG23 | 1:106:A:THR:HG22 | 5        | 0.19          |
| (1,3155) | 1:83:A:ILE:HG23 | 1:106:A:THR:HG23 | 5        | 0.19          |
| (1,3155) | 1:83:A:ILE:HG21 | 1:106:A:THR:HG21 | 17       | 0.19          |
| (1,3155) | 1:83:A:ILE:HG21 | 1:106:A:THR:HG22 | 17       | 0.19          |
| (1,3155) | 1:83:A:ILE:HG21 | 1:106:A:THR:HG23 | 17       | 0.19          |
| (1,3155) | 1:83:A:ILE:HG22 | 1:106:A:THR:HG21 | 17       | 0.19          |
| (1,3155) | 1:83:A:ILE:HG22 | 1:106:A:THR:HG22 | 17       | 0.19          |
| (1,3155) | 1:83:A:ILE:HG22 | 1:106:A:THR:HG23 | 17       | 0.19          |
| (1,3155) | 1:83:A:ILE:HG23 | 1:106:A:THR:HG21 | 17       | 0.19          |
| (1,3155) | 1:83:A:ILE:HG23 | 1:106:A:THR:HG22 | 17       | 0.19          |
| (1,3155) | 1:83:A:ILE:HG23 | 1:106:A:THR:HG23 | 17       | 0.19          |
| (1,2410) | 1:12:A:PHE:HE1  | 1:146:A:LEU:HD21 | 8        | 0.19          |
| (1,2410) | 1:12:A:PHE:HE1  | 1:146:A:LEU:HD22 | 8        | 0.19          |
| (1,2410) | 1:12:A:PHE:HE1  | 1:146:A:LEU:HD23 | 8        | 0.19          |
| (1,2410) | 1:12:A:PHE:HE2  | 1:146:A:LEU:HD21 | 8        | 0.19          |
| (1,2410) | 1:12:A:PHE:HE2  | 1:146:A:LEU:HD22 | 8        | 0.19          |
| (1,2410) | 1:12:A:PHE:HE2  | 1:146:A:LEU:HD23 | 8        | 0.19          |
| (1,2134) | 1:36:A:TRP:HH2  | 1:37:A:PHE:HA    | 14       | 0.19          |
| (1,1772) | 1:18:A:ALA:HB1  | 1:22:A:LYS:HB3   | 18       | 0.19          |
| (1,1772) | 1:18:A:ALA:HB2  | 1:22:A:LYS:HB3   | 18       | 0.19          |
| (1,1772) | 1:18:A:ALA:HB3  | 1:22:A:LYS:HB3   | 18       | 0.19          |
| (1,1675) | 1:53:A:LYS:HD2  | 1:77:A:VAL:HG11  | 15       | 0.19          |
| (1,1675) | 1:53:A:LYS:HD2  | 1:77:A:VAL:HG12  | 15       | 0.19          |
| (1,1675) | 1:53:A:LYS:HD2  | 1:77:A:VAL:HG13  | 15       | 0.19          |
| (1,1675) | 1:53:A:LYS:HD3  | 1:77:A:VAL:HG11  | 15       | 0.19          |
| (1,1675) | 1:53:A:LYS:HD3  | 1:77:A:VAL:HG12  | 15       | 0.19          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1675) | 1:53:A:LYS:HD3   | 1:77:A:VAL:HG13  | 15       | 0.19          |
| (1,1546) | 1:22:A:LYS:HG3   | 1:23:A:VAL:HB    | 4        | 0.19          |
| (1,1399) | 1:20:A:ILE:HD11  | 1:81:A:TYR:HD1   | 2        | 0.19          |
| (1,1399) | 1:20:A:ILE:HD11  | 1:81:A:TYR:HD2   | 2        | 0.19          |
| (1,1399) | 1:20:A:ILE:HD12  | 1:81:A:TYR:HD1   | 2        | 0.19          |
| (1,1399) | 1:20:A:ILE:HD12  | 1:81:A:TYR:HD2   | 2        | 0.19          |
| (1,1399) | 1:20:A:ILE:HD13  | 1:81:A:TYR:HD1   | 2        | 0.19          |
| (1,1399) | 1:20:A:ILE:HD13  | 1:81:A:TYR:HD2   | 2        | 0.19          |
| (1,1019) | 1:124:A:PHE:HB2  | 1:131:A:GLN:H    | 3        | 0.19          |
| (1,999)  | 1:126:A:THR:HA   | 1:130:A:ALA:H    | 12       | 0.19          |
| (1,486)  | 1:53:A:LYS:HD2   | 1:54:A:GLY:H     | 12       | 0.19          |
| (1,486)  | 1:53:A:LYS:HD3   | 1:54:A:GLY:H     | 12       | 0.19          |
| (1,226)  | 1:27:A:TYR:H     | 1:28:A:THR:HG21  | 15       | 0.19          |
| (1,226)  | 1:27:A:TYR:H     | 1:28:A:THR:HG22  | 15       | 0.19          |
| (1,226)  | 1:27:A:TYR:H     | 1:28:A:THR:HG23  | 15       | 0.19          |
| (1,226)  | 1:27:A:TYR:H     | 1:28:A:THR:HG21  | 17       | 0.19          |
| (1,226)  | 1:27:A:TYR:H     | 1:28:A:THR:HG22  | 17       | 0.19          |
| (1,226)  | 1:27:A:TYR:H     | 1:28:A:THR:HG23  | 17       | 0.19          |
| (2,22)   | 1:32:A:LEU:H     | 1:49:A:PHE:HE1   | 13       | 0.18          |
| (2,22)   | 1:32:A:LEU:H     | 1:49:A:PHE:HE2   | 13       | 0.18          |
| (1,4362) | 1:68:A:SER:HA    | 1:69:A:TYR:HE1   | 17       | 0.18          |
| (1,4362) | 1:68:A:SER:HA    | 1:69:A:TYR:HE2   | 17       | 0.18          |
| (1,4229) | 1:152:A:LEU:HD11 | 1:153:A:LEU:HD11 | 19       | 0.18          |
| (1,4229) | 1:152:A:LEU:HD11 | 1:153:A:LEU:HD12 | 19       | 0.18          |
| (1,4229) | 1:152:A:LEU:HD11 | 1:153:A:LEU:HD13 | 19       | 0.18          |
| (1,4229) | 1:152:A:LEU:HD12 | 1:153:A:LEU:HD11 | 19       | 0.18          |
| (1,4229) | 1:152:A:LEU:HD12 | 1:153:A:LEU:HD12 | 19       | 0.18          |
| (1,4229) | 1:152:A:LEU:HD12 | 1:153:A:LEU:HD13 | 19       | 0.18          |
| (1,4229) | 1:152:A:LEU:HD13 | 1:153:A:LEU:HD11 | 19       | 0.18          |
| (1,4229) | 1:152:A:LEU:HD13 | 1:153:A:LEU:HD12 | 19       | 0.18          |
| (1,4229) | 1:152:A:LEU:HD13 | 1:153:A:LEU:HD13 | 19       | 0.18          |
| (1,4052) | 1:34:A:GLU:HG2   | 1:35:A:GLN:HG3   | 10       | 0.18          |
| (1,4020) | 1:19:A:PRO:HG2   | 1:22:A:LYS:HG2   | 6        | 0.18          |
| (1,3897) | 1:89:A:PHE:HD1   | 1:100:A:MET:HB2  | 7        | 0.18          |
| (1,3897) | 1:89:A:PHE:HD2   | 1:100:A:MET:HB2  | 7        | 0.18          |
| (1,3391) | 1:131:A:GLN:HG2  | 1:132:A:GLN:HA   | 3        | 0.18          |
| (1,3249) | 1:118:A:VAL:HG11 | 1:119:A:THR:HB   | 9        | 0.18          |
| (1,3249) | 1:118:A:VAL:HG12 | 1:119:A:THR:HB   | 9        | 0.18          |
| (1,3249) | 1:118:A:VAL:HG13 | 1:119:A:THR:HB   | 9        | 0.18          |
| (1,3155) | 1:83:A:ILE:HG21  | 1:106:A:THR:HG21 | 13       | 0.18          |
| (1,3155) | 1:83:A:ILE:HG21  | 1:106:A:THR:HG22 | 13       | 0.18          |
| (1,3155) | 1:83:A:ILE:HG21  | 1:106:A:THR:HG23 | 13       | 0.18          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3155) | 1:83:A:ILE:HG22  | 1:106:A:THR:HG21 | 13       | 0.18          |
| (1,3155) | 1:83:A:ILE:HG22  | 1:106:A:THR:HG22 | 13       | 0.18          |
| (1,3155) | 1:83:A:ILE:HG22  | 1:106:A:THR:HG23 | 13       | 0.18          |
| (1,3155) | 1:83:A:ILE:HG23  | 1:106:A:THR:HG21 | 13       | 0.18          |
| (1,3155) | 1:83:A:ILE:HG23  | 1:106:A:THR:HG22 | 13       | 0.18          |
| (1,3155) | 1:83:A:ILE:HG23  | 1:106:A:THR:HG23 | 13       | 0.18          |
| (1,3155) | 1:83:A:ILE:HG21  | 1:106:A:THR:HG21 | 20       | 0.18          |
| (1,3155) | 1:83:A:ILE:HG21  | 1:106:A:THR:HG22 | 20       | 0.18          |
| (1,3155) | 1:83:A:ILE:HG21  | 1:106:A:THR:HG23 | 20       | 0.18          |
| (1,3155) | 1:83:A:ILE:HG22  | 1:106:A:THR:HG21 | 20       | 0.18          |
| (1,3155) | 1:83:A:ILE:HG22  | 1:106:A:THR:HG22 | 20       | 0.18          |
| (1,3155) | 1:83:A:ILE:HG22  | 1:106:A:THR:HG23 | 20       | 0.18          |
| (1,3155) | 1:83:A:ILE:HG23  | 1:106:A:THR:HG21 | 20       | 0.18          |
| (1,3155) | 1:83:A:ILE:HG23  | 1:106:A:THR:HG22 | 20       | 0.18          |
| (1,3155) | 1:83:A:ILE:HG23  | 1:106:A:THR:HG23 | 20       | 0.18          |
| (1,2889) | 1:87:A:ASP:HB2   | 1:103:A:MET:HB2  | 10       | 0.18          |
| (1,2410) | 1:12:A:PHE:HE1   | 1:146:A:LEU:HD21 | 1        | 0.18          |
| (1,2410) | 1:12:A:PHE:HE1   | 1:146:A:LEU:HD22 | 1        | 0.18          |
| (1,2410) | 1:12:A:PHE:HE1   | 1:146:A:LEU:HD23 | 1        | 0.18          |
| (1,2410) | 1:12:A:PHE:HE2   | 1:146:A:LEU:HD21 | 1        | 0.18          |
| (1,2410) | 1:12:A:PHE:HE2   | 1:146:A:LEU:HD22 | 1        | 0.18          |
| (1,2410) | 1:12:A:PHE:HE2   | 1:146:A:LEU:HD23 | 1        | 0.18          |
| (1,2410) | 1:12:A:PHE:HE1   | 1:146:A:LEU:HD21 | 10       | 0.18          |
| (1,2410) | 1:12:A:PHE:HE1   | 1:146:A:LEU:HD22 | 10       | 0.18          |
| (1,2410) | 1:12:A:PHE:HE1   | 1:146:A:LEU:HD23 | 10       | 0.18          |
| (1,2410) | 1:12:A:PHE:HE2   | 1:146:A:LEU:HD21 | 10       | 0.18          |
| (1,2410) | 1:12:A:PHE:HE2   | 1:146:A:LEU:HD22 | 10       | 0.18          |
| (1,2410) | 1:12:A:PHE:HE2   | 1:146:A:LEU:HD23 | 10       | 0.18          |
| (1,2134) | 1:36:A:TRP:HH2   | 1:37:A:PHE:HA    | 4        | 0.18          |
| (1,1832) | 1:35:A:GLN:HB3   | 1:152:A:LEU:HA   | 2        | 0.18          |
| (1,1832) | 1:35:A:GLN:HB3   | 1:152:A:LEU:HA   | 14       | 0.18          |
| (1,1382) | 1:117:A:THR:HG21 | 1:119:A:THR:H    | 4        | 0.18          |
| (1,1382) | 1:117:A:THR:HG22 | 1:119:A:THR:H    | 4        | 0.18          |
| (1,1382) | 1:117:A:THR:HG23 | 1:119:A:THR:H    | 4        | 0.18          |
| (1,1247) | 1:128:A:SER:HA   | 1:132:A:GLN:H    | 12       | 0.18          |
| (1,395)  | 1:53:A:LYS:HB2   | 1:77:A:VAL:H     | 7        | 0.18          |
| (1,320)  | 1:154:A:ASN:HA   | 1:154:A:ASN:HD22 | 18       | 0.18          |
| (1,226)  | 1:27:A:TYR:H     | 1:28:A:THR:HG21  | 4        | 0.18          |
| (1,226)  | 1:27:A:TYR:H     | 1:28:A:THR:HG22  | 4        | 0.18          |
| (1,226)  | 1:27:A:TYR:H     | 1:28:A:THR:HG23  | 4        | 0.18          |
| (2,676)  | 1:32:A:LEU:HD11  | 1:149:A:LEU:HD21 | 11       | 0.17          |
| (2,676)  | 1:32:A:LEU:HD11  | 1:149:A:LEU:HD22 | 11       | 0.17          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,676)  | 1:32:A:LEU:HD11 | 1:149:A:LEU:HD23 | 11       | 0.17          |
| (2,676)  | 1:32:A:LEU:HD12 | 1:149:A:LEU:HD21 | 11       | 0.17          |
| (2,676)  | 1:32:A:LEU:HD12 | 1:149:A:LEU:HD22 | 11       | 0.17          |
| (2,676)  | 1:32:A:LEU:HD12 | 1:149:A:LEU:HD23 | 11       | 0.17          |
| (2,676)  | 1:32:A:LEU:HD13 | 1:149:A:LEU:HD21 | 11       | 0.17          |
| (2,676)  | 1:32:A:LEU:HD13 | 1:149:A:LEU:HD22 | 11       | 0.17          |
| (2,676)  | 1:32:A:LEU:HD13 | 1:149:A:LEU:HD23 | 11       | 0.17          |
| (2,22)   | 1:32:A:LEU:H    | 1:49:A:PHE:HE1   | 9        | 0.17          |
| (2,22)   | 1:32:A:LEU:H    | 1:49:A:PHE:HE2   | 9        | 0.17          |
| (2,22)   | 1:32:A:LEU:H    | 1:49:A:PHE:HE1   | 10       | 0.17          |
| (2,22)   | 1:32:A:LEU:H    | 1:49:A:PHE:HE2   | 10       | 0.17          |
| (2,22)   | 1:32:A:LEU:H    | 1:49:A:PHE:HE1   | 16       | 0.17          |
| (2,22)   | 1:32:A:LEU:H    | 1:49:A:PHE:HE2   | 16       | 0.17          |
| (1,4410) | 1:79:A:ALA:HA   | 1:81:A:TYR:HD1   | 11       | 0.17          |
| (1,4410) | 1:79:A:ALA:HA   | 1:81:A:TYR:HD2   | 11       | 0.17          |
| (1,4401) | 1:82:A:TYR:HE1  | 1:108:A:ASN:HB2  | 6        | 0.17          |
| (1,4401) | 1:82:A:TYR:HE2  | 1:108:A:ASN:HB2  | 6        | 0.17          |
| (1,4362) | 1:68:A:SER:HA   | 1:69:A:TYR:HE1   | 5        | 0.17          |
| (1,4362) | 1:68:A:SER:HA   | 1:69:A:TYR:HE2   | 5        | 0.17          |
| (1,4362) | 1:68:A:SER:HA   | 1:69:A:TYR:HE1   | 6        | 0.17          |
| (1,4362) | 1:68:A:SER:HA   | 1:69:A:TYR:HE2   | 6        | 0.17          |
| (1,4203) | 1:128:A:SER:HB3 | 1:131:A:GLN:HG2  | 9        | 0.17          |
| (1,4104) | 1:66:A:MET:HA   | 1:66:A:MET:HE1   | 15       | 0.17          |
| (1,4104) | 1:66:A:MET:HA   | 1:66:A:MET:HE2   | 15       | 0.17          |
| (1,4104) | 1:66:A:MET:HA   | 1:66:A:MET:HE3   | 15       | 0.17          |
| (1,4020) | 1:19:A:PRO:HG2  | 1:22:A:LYS:HG2   | 3        | 0.17          |
| (1,4020) | 1:19:A:PRO:HG2  | 1:22:A:LYS:HG2   | 20       | 0.17          |
| (1,4016) | 1:20:A:ILE:HD11 | 1:23:A:VAL:HB    | 10       | 0.17          |
| (1,4016) | 1:20:A:ILE:HD12 | 1:23:A:VAL:HB    | 10       | 0.17          |
| (1,4016) | 1:20:A:ILE:HD13 | 1:23:A:VAL:HB    | 10       | 0.17          |
| (1,3797) | 1:34:A:GLU:HG2  | 1:35:A:GLN:HA    | 11       | 0.17          |
| (1,3277) | 1:12:A:PHE:HB2  | 1:120:A:SER:HB3  | 3        | 0.17          |
| (1,3246) | 1:24:A:PHE:HD1  | 1:118:A:VAL:HG11 | 18       | 0.17          |
| (1,3246) | 1:24:A:PHE:HD1  | 1:118:A:VAL:HG12 | 18       | 0.17          |
| (1,3246) | 1:24:A:PHE:HD1  | 1:118:A:VAL:HG13 | 18       | 0.17          |
| (1,3246) | 1:24:A:PHE:HD2  | 1:118:A:VAL:HG11 | 18       | 0.17          |
| (1,3246) | 1:24:A:PHE:HD2  | 1:118:A:VAL:HG12 | 18       | 0.17          |
| (1,3246) | 1:24:A:PHE:HD2  | 1:118:A:VAL:HG13 | 18       | 0.17          |
| (1,3155) | 1:83:A:ILE:HG21 | 1:106:A:THR:HG21 | 19       | 0.17          |
| (1,3155) | 1:83:A:ILE:HG21 | 1:106:A:THR:HG22 | 19       | 0.17          |
| (1,3155) | 1:83:A:ILE:HG21 | 1:106:A:THR:HG23 | 19       | 0.17          |
| (1,3155) | 1:83:A:ILE:HG22 | 1:106:A:THR:HG21 | 19       | 0.17          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3155) | 1:83:A:ILE:HG22  | 1:106:A:THR:HG22 | 19       | 0.17          |
| (1,3155) | 1:83:A:ILE:HG22  | 1:106:A:THR:HG23 | 19       | 0.17          |
| (1,3155) | 1:83:A:ILE:HG23  | 1:106:A:THR:HG21 | 19       | 0.17          |
| (1,3155) | 1:83:A:ILE:HG23  | 1:106:A:THR:HG22 | 19       | 0.17          |
| (1,3155) | 1:83:A:ILE:HG23  | 1:106:A:THR:HG23 | 19       | 0.17          |
| (1,3143) | 1:103:A:MET:HG3  | 1:105:A:ILE:HG12 | 3        | 0.17          |
| (1,3143) | 1:103:A:MET:HG3  | 1:105:A:ILE:HG12 | 7        | 0.17          |
| (1,3141) | 1:105:A:ILE:HG13 | 1:107:A:LEU:HG   | 7        | 0.17          |
| (1,3008) | 1:95:A:GLU:HB2   | 1:96:A:LYS:HB2   | 5        | 0.17          |
| (1,3008) | 1:95:A:GLU:HB2   | 1:96:A:LYS:HB3   | 5        | 0.17          |
| (1,2835) | 1:93:A:LYS:HB3   | 1:95:A:GLU:HG2   | 15       | 0.17          |
| (1,2739) | 1:53:A:LYS:HD2   | 1:76:A:GLN:HG3   | 19       | 0.17          |
| (1,2739) | 1:53:A:LYS:HD3   | 1:76:A:GLN:HG3   | 19       | 0.17          |
| (1,2667) | 1:70:A:THR:H     | 1:71:A:ILE:HD11  | 15       | 0.17          |
| (1,2667) | 1:70:A:THR:H     | 1:71:A:ILE:HD12  | 15       | 0.17          |
| (1,2667) | 1:70:A:THR:H     | 1:71:A:ILE:HD13  | 15       | 0.17          |
| (1,2591) | 1:61:A:ILE:HG21  | 1:66:A:MET:HE1   | 3        | 0.17          |
| (1,2591) | 1:61:A:ILE:HG21  | 1:66:A:MET:HE2   | 3        | 0.17          |
| (1,2591) | 1:61:A:ILE:HG21  | 1:66:A:MET:HE3   | 3        | 0.17          |
| (1,2591) | 1:61:A:ILE:HG22  | 1:66:A:MET:HE1   | 3        | 0.17          |
| (1,2591) | 1:61:A:ILE:HG22  | 1:66:A:MET:HE2   | 3        | 0.17          |
| (1,2591) | 1:61:A:ILE:HG22  | 1:66:A:MET:HE3   | 3        | 0.17          |
| (1,2591) | 1:61:A:ILE:HG23  | 1:66:A:MET:HE1   | 3        | 0.17          |
| (1,2591) | 1:61:A:ILE:HG23  | 1:66:A:MET:HE2   | 3        | 0.17          |
| (1,2591) | 1:61:A:ILE:HG23  | 1:66:A:MET:HE3   | 3        | 0.17          |
| (1,2134) | 1:36:A:TRP:HH2   | 1:37:A:PHE:HA    | 2        | 0.17          |
| (1,1772) | 1:18:A:ALA:HB1   | 1:22:A:LYS:HB3   | 8        | 0.17          |
| (1,1772) | 1:18:A:ALA:HB2   | 1:22:A:LYS:HB3   | 8        | 0.17          |
| (1,1772) | 1:18:A:ALA:HB3   | 1:22:A:LYS:HB3   | 8        | 0.17          |
| (1,1675) | 1:53:A:LYS:HD2   | 1:77:A:VAL:HG11  | 1        | 0.17          |
| (1,1675) | 1:53:A:LYS:HD2   | 1:77:A:VAL:HG12  | 1        | 0.17          |
| (1,1675) | 1:53:A:LYS:HD2   | 1:77:A:VAL:HG13  | 1        | 0.17          |
| (1,1675) | 1:53:A:LYS:HD3   | 1:77:A:VAL:HG11  | 1        | 0.17          |
| (1,1675) | 1:53:A:LYS:HD3   | 1:77:A:VAL:HG12  | 1        | 0.17          |
| (1,1675) | 1:53:A:LYS:HD3   | 1:77:A:VAL:HG13  | 1        | 0.17          |
| (1,1546) | 1:22:A:LYS:HG3   | 1:23:A:VAL:HB    | 13       | 0.17          |
| (1,1402) | 1:3:A:ILE:HG12   | 1:139:A:GLU:HA   | 10       | 0.17          |
| (1,1163) | 1:149:A:LEU:H    | 1:153:A:LEU:HD11 | 3        | 0.17          |
| (1,1163) | 1:149:A:LEU:H    | 1:153:A:LEU:HD12 | 3        | 0.17          |
| (1,1163) | 1:149:A:LEU:H    | 1:153:A:LEU:HD13 | 3        | 0.17          |
| (1,1163) | 1:149:A:LEU:H    | 1:153:A:LEU:HD11 | 15       | 0.17          |
| (1,1163) | 1:149:A:LEU:H    | 1:153:A:LEU:HD12 | 15       | 0.17          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1163) | 1:149:A:LEU:H    | 1:153:A:LEU:HD13 | 15       | 0.17          |
| (1,1136) | 1:144:A:SER:HA   | 1:147:A:ASN:HD22 | 12       | 0.17          |
| (1,999)  | 1:126:A:THR:HA   | 1:130:A:ALA:H    | 4        | 0.17          |
| (1,937)  | 1:117:A:THR:H    | 1:118:A:VAL:HB   | 7        | 0.17          |
| (1,811)  | 1:91:A:THR:H     | 1:95:A:GLU:H     | 11       | 0.17          |
| (1,811)  | 1:91:A:THR:H     | 1:95:A:GLU:H     | 17       | 0.17          |
| (1,320)  | 1:154:A:ASN:HA   | 1:154:A:ASN:HD22 | 4        | 0.17          |
| (1,270)  | 1:31:A:GLU:HG3   | 1:32:A:LEU:H     | 12       | 0.17          |
| (1,226)  | 1:27:A:TYR:H     | 1:28:A:THR:HG21  | 3        | 0.17          |
| (1,226)  | 1:27:A:TYR:H     | 1:28:A:THR:HG22  | 3        | 0.17          |
| (1,226)  | 1:27:A:TYR:H     | 1:28:A:THR:HG23  | 3        | 0.17          |
| (1,226)  | 1:27:A:TYR:H     | 1:28:A:THR:HG21  | 7        | 0.17          |
| (1,226)  | 1:27:A:TYR:H     | 1:28:A:THR:HG22  | 7        | 0.17          |
| (1,226)  | 1:27:A:TYR:H     | 1:28:A:THR:HG23  | 7        | 0.17          |
| (1,195)  | 1:108:A:ASN:H    | 1:118:A:VAL:HG21 | 8        | 0.17          |
| (1,195)  | 1:108:A:ASN:H    | 1:118:A:VAL:HG22 | 8        | 0.17          |
| (1,195)  | 1:108:A:ASN:H    | 1:118:A:VAL:HG23 | 8        | 0.17          |
| (2,816)  | 1:105:A:ILE:HG12 | 1:123:A:THR:H    | 13       | 0.16          |
| (2,676)  | 1:32:A:LEU:HD11  | 1:149:A:LEU:HD21 | 14       | 0.16          |
| (2,676)  | 1:32:A:LEU:HD11  | 1:149:A:LEU:HD22 | 14       | 0.16          |
| (2,676)  | 1:32:A:LEU:HD11  | 1:149:A:LEU:HD23 | 14       | 0.16          |
| (2,676)  | 1:32:A:LEU:HD12  | 1:149:A:LEU:HD21 | 14       | 0.16          |
| (2,676)  | 1:32:A:LEU:HD12  | 1:149:A:LEU:HD22 | 14       | 0.16          |
| (2,676)  | 1:32:A:LEU:HD12  | 1:149:A:LEU:HD23 | 14       | 0.16          |
| (2,676)  | 1:32:A:LEU:HD13  | 1:149:A:LEU:HD21 | 14       | 0.16          |
| (2,676)  | 1:32:A:LEU:HD13  | 1:149:A:LEU:HD22 | 14       | 0.16          |
| (2,676)  | 1:32:A:LEU:HD13  | 1:149:A:LEU:HD23 | 14       | 0.16          |
| (2,449)  | 1:154:A:ASN:HA   | 1:157:A:LEU:HG   | 10       | 0.16          |
| (2,449)  | 1:154:A:ASN:HA   | 1:157:A:LEU:HG   | 18       | 0.16          |
| (2,243)  | 1:91:A:THR:HB    | 1:97:A:ASP:H     | 9        | 0.16          |
| (2,86)   | 1:9:A:LYS:HD3    | 1:122:A:SER:H    | 13       | 0.16          |
| (2,43)   | 1:49:A:PHE:HB3   | 1:58:A:PHE:H     | 12       | 0.16          |
| (2,22)   | 1:32:A:LEU:H     | 1:49:A:PHE:HE1   | 3        | 0.16          |
| (2,22)   | 1:32:A:LEU:H     | 1:49:A:PHE:HE2   | 3        | 0.16          |
| (2,22)   | 1:32:A:LEU:H     | 1:49:A:PHE:HE1   | 8        | 0.16          |
| (2,22)   | 1:32:A:LEU:H     | 1:49:A:PHE:HE2   | 8        | 0.16          |
| (1,4362) | 1:68:A:SER:HA    | 1:69:A:TYR:HE1   | 1        | 0.16          |
| (1,4362) | 1:68:A:SER:HA    | 1:69:A:TYR:HE2   | 1        | 0.16          |
| (1,4362) | 1:68:A:SER:HA    | 1:69:A:TYR:HE1   | 3        | 0.16          |
| (1,4362) | 1:68:A:SER:HA    | 1:69:A:TYR:HE2   | 3        | 0.16          |
| (1,4362) | 1:68:A:SER:HA    | 1:69:A:TYR:HE1   | 15       | 0.16          |
| (1,4362) | 1:68:A:SER:HA    | 1:69:A:TYR:HE2   | 15       | 0.16          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,4196) | 1:8:A:ASN:HB2   | 1:125:A:PRO:HD2  | 16       | 0.16          |
| (1,4136) | 1:73:A:GLU:HA   | 1:86:A:LEU:HD11  | 15       | 0.16          |
| (1,4136) | 1:73:A:GLU:HA   | 1:86:A:LEU:HD12  | 15       | 0.16          |
| (1,4136) | 1:73:A:GLU:HA   | 1:86:A:LEU:HD13  | 15       | 0.16          |
| (1,4104) | 1:66:A:MET:HA   | 1:66:A:MET:HE1   | 17       | 0.16          |
| (1,4104) | 1:66:A:MET:HA   | 1:66:A:MET:HE2   | 17       | 0.16          |
| (1,4104) | 1:66:A:MET:HA   | 1:66:A:MET:HE3   | 17       | 0.16          |
| (1,4020) | 1:19:A:PRO:HG2  | 1:22:A:LYS:HG2   | 10       | 0.16          |
| (1,4020) | 1:19:A:PRO:HG2  | 1:22:A:LYS:HG2   | 15       | 0.16          |
| (1,4016) | 1:20:A:ILE:HD11 | 1:23:A:VAL:HB    | 16       | 0.16          |
| (1,4016) | 1:20:A:ILE:HD12 | 1:23:A:VAL:HB    | 16       | 0.16          |
| (1,4016) | 1:20:A:ILE:HD13 | 1:23:A:VAL:HB    | 16       | 0.16          |
| (1,3897) | 1:89:A:PHE:HD1  | 1:100:A:MET:HB2  | 9        | 0.16          |
| (1,3897) | 1:89:A:PHE:HD2  | 1:100:A:MET:HB2  | 9        | 0.16          |
| (1,3897) | 1:89:A:PHE:HD1  | 1:100:A:MET:HB2  | 13       | 0.16          |
| (1,3897) | 1:89:A:PHE:HD2  | 1:100:A:MET:HB2  | 13       | 0.16          |
| (1,3659) | 1:151:A:LYS:HB2 | 1:157:A:LEU:HB3  | 10       | 0.16          |
| (1,3659) | 1:151:A:LYS:HB3 | 1:157:A:LEU:HB3  | 10       | 0.16          |
| (1,3524) | 1:133:A:ALA:HB1 | 1:142:A:MET:HE1  | 6        | 0.16          |
| (1,3524) | 1:133:A:ALA:HB1 | 1:142:A:MET:HE2  | 6        | 0.16          |
| (1,3524) | 1:133:A:ALA:HB1 | 1:142:A:MET:HE3  | 6        | 0.16          |
| (1,3524) | 1:133:A:ALA:HB2 | 1:142:A:MET:HE1  | 6        | 0.16          |
| (1,3524) | 1:133:A:ALA:HB2 | 1:142:A:MET:HE2  | 6        | 0.16          |
| (1,3524) | 1:133:A:ALA:HB2 | 1:142:A:MET:HE3  | 6        | 0.16          |
| (1,3524) | 1:133:A:ALA:HB3 | 1:142:A:MET:HE1  | 6        | 0.16          |
| (1,3524) | 1:133:A:ALA:HB3 | 1:142:A:MET:HE2  | 6        | 0.16          |
| (1,3524) | 1:133:A:ALA:HB3 | 1:142:A:MET:HE3  | 6        | 0.16          |
| (1,3291) | 1:6:A:LYS:HE2   | 1:121:A:THR:HG21 | 9        | 0.16          |
| (1,3291) | 1:6:A:LYS:HE2   | 1:121:A:THR:HG22 | 9        | 0.16          |
| (1,3291) | 1:6:A:LYS:HE2   | 1:121:A:THR:HG23 | 9        | 0.16          |
| (1,3291) | 1:6:A:LYS:HE3   | 1:121:A:THR:HG21 | 9        | 0.16          |
| (1,3291) | 1:6:A:LYS:HE3   | 1:121:A:THR:HG22 | 9        | 0.16          |
| (1,3291) | 1:6:A:LYS:HE3   | 1:121:A:THR:HG23 | 9        | 0.16          |
| (1,3277) | 1:12:A:PHE:HB2  | 1:120:A:SER:HB3  | 6        | 0.16          |
| (1,3155) | 1:83:A:ILE:HG21 | 1:106:A:THR:HG21 | 6        | 0.16          |
| (1,3155) | 1:83:A:ILE:HG21 | 1:106:A:THR:HG22 | 6        | 0.16          |
| (1,3155) | 1:83:A:ILE:HG21 | 1:106:A:THR:HG23 | 6        | 0.16          |
| (1,3155) | 1:83:A:ILE:HG22 | 1:106:A:THR:HG21 | 6        | 0.16          |
| (1,3155) | 1:83:A:ILE:HG22 | 1:106:A:THR:HG22 | 6        | 0.16          |
| (1,3155) | 1:83:A:ILE:HG22 | 1:106:A:THR:HG23 | 6        | 0.16          |
| (1,3155) | 1:83:A:ILE:HG23 | 1:106:A:THR:HG21 | 6        | 0.16          |
| (1,3155) | 1:83:A:ILE:HG23 | 1:106:A:THR:HG22 | 6        | 0.16          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3155) | 1:83:A:ILE:HG23 | 1:106:A:THR:HG23 | 6        | 0.16          |
| (1,2991) | 1:88:A:TYR:HD1  | 1:96:A:LYS:HE3   | 9        | 0.16          |
| (1,2991) | 1:88:A:TYR:HD2  | 1:96:A:LYS:HE3   | 9        | 0.16          |
| (1,2929) | 1:91:A:THR:HG21 | 1:96:A:LYS:HD2   | 20       | 0.16          |
| (1,2929) | 1:91:A:THR:HG22 | 1:96:A:LYS:HD2   | 20       | 0.16          |
| (1,2929) | 1:91:A:THR:HG23 | 1:96:A:LYS:HD2   | 20       | 0.16          |
| (1,2911) | 1:89:A:PHE:HB2  | 1:97:A:ASP:HB2   | 2        | 0.16          |
| (1,2889) | 1:87:A:ASP:HB2  | 1:103:A:MET:HB2  | 8        | 0.16          |
| (1,2417) | 1:45:A:THR:HB   | 1:60:A:ALA:HB1   | 20       | 0.16          |
| (1,2417) | 1:45:A:THR:HB   | 1:60:A:ALA:HB2   | 20       | 0.16          |
| (1,2417) | 1:45:A:THR:HB   | 1:60:A:ALA:HB3   | 20       | 0.16          |
| (1,1988) | 1:27:A:TYR:HB3  | 1:28:A:THR:HG21  | 4        | 0.16          |
| (1,1988) | 1:27:A:TYR:HB3  | 1:28:A:THR:HG22  | 4        | 0.16          |
| (1,1988) | 1:27:A:TYR:HB3  | 1:28:A:THR:HG23  | 4        | 0.16          |
| (1,1858) | 1:28:A:THR:HB   | 1:29:A:LYS:HD2   | 4        | 0.16          |
| (1,1858) | 1:28:A:THR:HB   | 1:29:A:LYS:HD3   | 4        | 0.16          |
| (1,1832) | 1:35:A:GLN:HB3  | 1:152:A:LEU:HA   | 6        | 0.16          |
| (1,1739) | 1:15:A:THR:HB   | 1:115:A:LYS:HE2  | 7        | 0.16          |
| (1,1739) | 1:15:A:THR:HB   | 1:115:A:LYS:HE3  | 7        | 0.16          |
| (1,1546) | 1:22:A:LYS:HG3  | 1:23:A:VAL:HB    | 20       | 0.16          |
| (1,1542) | 1:6:A:LYS:HG2   | 1:9:A:LYS:HE2    | 10       | 0.16          |
| (1,1542) | 1:6:A:LYS:HG2   | 1:9:A:LYS:HE3    | 10       | 0.16          |
| (1,1542) | 1:6:A:LYS:HG3   | 1:9:A:LYS:HE2    | 10       | 0.16          |
| (1,1542) | 1:6:A:LYS:HG3   | 1:9:A:LYS:HE3    | 10       | 0.16          |
| (1,1542) | 1:6:A:LYS:HG2   | 1:9:A:LYS:HE2    | 19       | 0.16          |
| (1,1542) | 1:6:A:LYS:HG2   | 1:9:A:LYS:HE3    | 19       | 0.16          |
| (1,1542) | 1:6:A:LYS:HG3   | 1:9:A:LYS:HE2    | 19       | 0.16          |
| (1,1542) | 1:6:A:LYS:HG3   | 1:9:A:LYS:HE3    | 19       | 0.16          |
| (1,1394) | 1:3:A:ILE:HG21  | 1:4:A:GLU:HA     | 15       | 0.16          |
| (1,1394) | 1:3:A:ILE:HG22  | 1:4:A:GLU:HA     | 15       | 0.16          |
| (1,1394) | 1:3:A:ILE:HG23  | 1:4:A:GLU:HA     | 15       | 0.16          |
| (1,1247) | 1:128:A:SER:HA  | 1:132:A:GLN:H    | 13       | 0.16          |
| (1,1163) | 1:149:A:LEU:H   | 1:153:A:LEU:HD11 | 20       | 0.16          |
| (1,1163) | 1:149:A:LEU:H   | 1:153:A:LEU:HD12 | 20       | 0.16          |
| (1,1163) | 1:149:A:LEU:H   | 1:153:A:LEU:HD13 | 20       | 0.16          |
| (1,1019) | 1:124:A:PHE:HB2 | 1:131:A:GLN:H    | 8        | 0.16          |
| (1,1019) | 1:124:A:PHE:HB2 | 1:131:A:GLN:H    | 9        | 0.16          |
| (1,937)  | 1:117:A:THR:H   | 1:118:A:VAL:HB   | 15       | 0.16          |
| (1,840)  | 1:88:A:TYR:HA   | 1:102:A:GLY:H    | 2        | 0.16          |
| (1,786)  | 1:91:A:THR:H    | 1:95:A:GLU:H     | 11       | 0.16          |
| (1,786)  | 1:91:A:THR:H    | 1:95:A:GLU:H     | 17       | 0.16          |
| (1,436)  | 1:50:A:ASN:HD21 | 1:55:A:GLY:HA3   | 1        | 0.16          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,320)  | 1:154:A:ASN:HA   | 1:154:A:ASN:HD22 | 6        | 0.16          |
| (1,195)  | 1:108:A:ASN:H    | 1:118:A:VAL:HG21 | 7        | 0.16          |
| (1,195)  | 1:108:A:ASN:H    | 1:118:A:VAL:HG22 | 7        | 0.16          |
| (1,195)  | 1:108:A:ASN:H    | 1:118:A:VAL:HG23 | 7        | 0.16          |
| (1,195)  | 1:108:A:ASN:H    | 1:118:A:VAL:HG21 | 14       | 0.16          |
| (1,195)  | 1:108:A:ASN:H    | 1:118:A:VAL:HG22 | 14       | 0.16          |
| (1,195)  | 1:108:A:ASN:H    | 1:118:A:VAL:HG23 | 14       | 0.16          |
| (2,684)  | 1:30:A:ARG:HG2   | 1:34:A:GLU:HG3   | 19       | 0.15          |
| (2,661)  | 1:30:A:ARG:HA    | 1:32:A:LEU:HD11  | 5        | 0.15          |
| (2,661)  | 1:30:A:ARG:HA    | 1:32:A:LEU:HD12  | 5        | 0.15          |
| (2,661)  | 1:30:A:ARG:HA    | 1:32:A:LEU:HD13  | 5        | 0.15          |
| (2,641)  | 1:20:A:ILE:HG21  | 1:21:A:ASN:HD22  | 1        | 0.15          |
| (2,641)  | 1:20:A:ILE:HG22  | 1:21:A:ASN:HD22  | 1        | 0.15          |
| (2,641)  | 1:20:A:ILE:HG23  | 1:21:A:ASN:HD22  | 1        | 0.15          |
| (2,641)  | 1:20:A:ILE:HG21  | 1:21:A:ASN:HD22  | 12       | 0.15          |
| (2,641)  | 1:20:A:ILE:HG22  | 1:21:A:ASN:HD22  | 12       | 0.15          |
| (2,641)  | 1:20:A:ILE:HG23  | 1:21:A:ASN:HD22  | 12       | 0.15          |
| (1,4401) | 1:82:A:TYR:HE1   | 1:108:A:ASN:HB2  | 9        | 0.15          |
| (1,4401) | 1:82:A:TYR:HE2   | 1:108:A:ASN:HB2  | 9        | 0.15          |
| (1,4362) | 1:68:A:SER:HA    | 1:69:A:TYR:HE1   | 14       | 0.15          |
| (1,4362) | 1:68:A:SER:HA    | 1:69:A:TYR:HE2   | 14       | 0.15          |
| (1,4229) | 1:152:A:LEU:HD11 | 1:153:A:LEU:HD11 | 2        | 0.15          |
| (1,4229) | 1:152:A:LEU:HD11 | 1:153:A:LEU:HD12 | 2        | 0.15          |
| (1,4229) | 1:152:A:LEU:HD11 | 1:153:A:LEU:HD13 | 2        | 0.15          |
| (1,4229) | 1:152:A:LEU:HD12 | 1:153:A:LEU:HD11 | 2        | 0.15          |
| (1,4229) | 1:152:A:LEU:HD12 | 1:153:A:LEU:HD12 | 2        | 0.15          |
| (1,4229) | 1:152:A:LEU:HD12 | 1:153:A:LEU:HD13 | 2        | 0.15          |
| (1,4229) | 1:152:A:LEU:HD13 | 1:153:A:LEU:HD11 | 2        | 0.15          |
| (1,4229) | 1:152:A:LEU:HD13 | 1:153:A:LEU:HD12 | 2        | 0.15          |
| (1,4229) | 1:152:A:LEU:HD13 | 1:153:A:LEU:HD13 | 2        | 0.15          |
| (1,4020) | 1:19:A:PRO:HG2   | 1:22:A:LYS:HG2   | 13       | 0.15          |
| (1,4014) | 1:20:A:ILE:HD11  | 1:80:A:PRO:HB2   | 13       | 0.15          |
| (1,4014) | 1:20:A:ILE:HD12  | 1:80:A:PRO:HB2   | 13       | 0.15          |
| (1,4014) | 1:20:A:ILE:HD13  | 1:80:A:PRO:HB2   | 13       | 0.15          |
| (1,3797) | 1:34:A:GLU:HG2   | 1:35:A:GLN:HA    | 14       | 0.15          |
| (1,3659) | 1:151:A:LYS:HB2  | 1:157:A:LEU:HB3  | 17       | 0.15          |
| (1,3659) | 1:151:A:LYS:HB3  | 1:157:A:LEU:HB3  | 17       | 0.15          |
| (1,3524) | 1:133:A:ALA:HB1  | 1:142:A:MET:HE1  | 14       | 0.15          |
| (1,3524) | 1:133:A:ALA:HB1  | 1:142:A:MET:HE2  | 14       | 0.15          |
| (1,3524) | 1:133:A:ALA:HB1  | 1:142:A:MET:HE3  | 14       | 0.15          |
| (1,3524) | 1:133:A:ALA:HB2  | 1:142:A:MET:HE1  | 14       | 0.15          |
| (1,3524) | 1:133:A:ALA:HB2  | 1:142:A:MET:HE2  | 14       | 0.15          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3524) | 1:133:A:ALA:HB2 | 1:142:A:MET:HE3  | 14       | 0.15          |
| (1,3524) | 1:133:A:ALA:HB3 | 1:142:A:MET:HE1  | 14       | 0.15          |
| (1,3524) | 1:133:A:ALA:HB3 | 1:142:A:MET:HE2  | 14       | 0.15          |
| (1,3524) | 1:133:A:ALA:HB3 | 1:142:A:MET:HE3  | 14       | 0.15          |
| (1,3272) | 1:107:A:LEU:HB3 | 1:120:A:SER:HB2  | 16       | 0.15          |
| (1,3246) | 1:24:A:PHE:HD1  | 1:118:A:VAL:HG11 | 6        | 0.15          |
| (1,3246) | 1:24:A:PHE:HD1  | 1:118:A:VAL:HG12 | 6        | 0.15          |
| (1,3246) | 1:24:A:PHE:HD1  | 1:118:A:VAL:HG13 | 6        | 0.15          |
| (1,3246) | 1:24:A:PHE:HD2  | 1:118:A:VAL:HG11 | 6        | 0.15          |
| (1,3246) | 1:24:A:PHE:HD2  | 1:118:A:VAL:HG12 | 6        | 0.15          |
| (1,3246) | 1:24:A:PHE:HD2  | 1:118:A:VAL:HG13 | 6        | 0.15          |
| (1,3246) | 1:24:A:PHE:HD1  | 1:118:A:VAL:HG11 | 13       | 0.15          |
| (1,3246) | 1:24:A:PHE:HD1  | 1:118:A:VAL:HG12 | 13       | 0.15          |
| (1,3246) | 1:24:A:PHE:HD1  | 1:118:A:VAL:HG13 | 13       | 0.15          |
| (1,3246) | 1:24:A:PHE:HD2  | 1:118:A:VAL:HG11 | 13       | 0.15          |
| (1,3246) | 1:24:A:PHE:HD2  | 1:118:A:VAL:HG12 | 13       | 0.15          |
| (1,3246) | 1:24:A:PHE:HD2  | 1:118:A:VAL:HG13 | 13       | 0.15          |
| (1,3176) | 1:108:A:ASN:HA  | 1:109:A:PHE:HD1  | 9        | 0.15          |
| (1,3176) | 1:108:A:ASN:HA  | 1:109:A:PHE:HD2  | 9        | 0.15          |
| (1,3026) | 1:91:A:THR:HG21 | 1:97:A:ASP:HB3   | 11       | 0.15          |
| (1,3026) | 1:91:A:THR:HG22 | 1:97:A:ASP:HB3   | 11       | 0.15          |
| (1,3026) | 1:91:A:THR:HG23 | 1:97:A:ASP:HB3   | 11       | 0.15          |
| (1,2930) | 1:71:A:ILE:HD11 | 1:91:A:THR:HG21  | 16       | 0.15          |
| (1,2930) | 1:71:A:ILE:HD11 | 1:91:A:THR:HG22  | 16       | 0.15          |
| (1,2930) | 1:71:A:ILE:HD11 | 1:91:A:THR:HG23  | 16       | 0.15          |
| (1,2930) | 1:71:A:ILE:HD12 | 1:91:A:THR:HG21  | 16       | 0.15          |
| (1,2930) | 1:71:A:ILE:HD12 | 1:91:A:THR:HG22  | 16       | 0.15          |
| (1,2930) | 1:71:A:ILE:HD12 | 1:91:A:THR:HG23  | 16       | 0.15          |
| (1,2930) | 1:71:A:ILE:HD13 | 1:91:A:THR:HG21  | 16       | 0.15          |
| (1,2930) | 1:71:A:ILE:HD13 | 1:91:A:THR:HG22  | 16       | 0.15          |
| (1,2930) | 1:71:A:ILE:HD13 | 1:91:A:THR:HG23  | 16       | 0.15          |
| (1,2929) | 1:91:A:THR:HG21 | 1:96:A:LYS:HD2   | 12       | 0.15          |
| (1,2929) | 1:91:A:THR:HG22 | 1:96:A:LYS:HD2   | 12       | 0.15          |
| (1,2929) | 1:91:A:THR:HG23 | 1:96:A:LYS:HD2   | 12       | 0.15          |
| (1,2911) | 1:89:A:PHE:HB2  | 1:97:A:ASP:HB2   | 7        | 0.15          |
| (1,2889) | 1:87:A:ASP:HB2  | 1:103:A:MET:HB2  | 2        | 0.15          |
| (1,2889) | 1:87:A:ASP:HB2  | 1:103:A:MET:HB2  | 18       | 0.15          |
| (1,2566) | 1:129:A:ALA:HA  | 1:132:A:GLN:HG2  | 7        | 0.15          |
| (1,2566) | 1:129:A:ALA:HA  | 1:132:A:GLN:HG2  | 14       | 0.15          |
| (1,2552) | 1:100:A:MET:HB2 | 1:101:A:PRO:HD2  | 8        | 0.15          |
| (1,2410) | 1:12:A:PHE:HE1  | 1:146:A:LEU:HD21 | 6        | 0.15          |
| (1,2410) | 1:12:A:PHE:HE1  | 1:146:A:LEU:HD22 | 6        | 0.15          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2410) | 1:12:A:PHE:HE1  | 1:146:A:LEU:HD23 | 6        | 0.15          |
| (1,2410) | 1:12:A:PHE:HE2  | 1:146:A:LEU:HD21 | 6        | 0.15          |
| (1,2410) | 1:12:A:PHE:HE2  | 1:146:A:LEU:HD22 | 6        | 0.15          |
| (1,2410) | 1:12:A:PHE:HE2  | 1:146:A:LEU:HD23 | 6        | 0.15          |
| (1,2134) | 1:36:A:TRP:HH2  | 1:37:A:PHE:HA    | 17       | 0.15          |
| (1,2134) | 1:36:A:TRP:HH2  | 1:37:A:PHE:HA    | 20       | 0.15          |
| (1,2042) | 1:31:A:GLU:HG3  | 1:32:A:LEU:HA    | 8        | 0.15          |
| (1,1832) | 1:35:A:GLN:HB3  | 1:152:A:LEU:HA   | 11       | 0.15          |
| (1,1772) | 1:18:A:ALA:HB1  | 1:22:A:LYS:HB3   | 16       | 0.15          |
| (1,1772) | 1:18:A:ALA:HB2  | 1:22:A:LYS:HB3   | 16       | 0.15          |
| (1,1772) | 1:18:A:ALA:HB3  | 1:22:A:LYS:HB3   | 16       | 0.15          |
| (1,1712) | 1:14:A:ARG:HD2  | 1:15:A:THR:H     | 16       | 0.15          |
| (1,1542) | 1:6:A:LYS:HG2   | 1:9:A:LYS:HE2    | 3        | 0.15          |
| (1,1542) | 1:6:A:LYS:HG2   | 1:9:A:LYS:HE3    | 3        | 0.15          |
| (1,1542) | 1:6:A:LYS:HG3   | 1:9:A:LYS:HE2    | 3        | 0.15          |
| (1,1542) | 1:6:A:LYS:HG3   | 1:9:A:LYS:HE3    | 3        | 0.15          |
| (1,1291) | 1:91:A:THR:HB   | 1:92:A:SER:H     | 12       | 0.15          |
| (1,1163) | 1:149:A:LEU:H   | 1:153:A:LEU:HD11 | 6        | 0.15          |
| (1,1163) | 1:149:A:LEU:H   | 1:153:A:LEU:HD12 | 6        | 0.15          |
| (1,1163) | 1:149:A:LEU:H   | 1:153:A:LEU:HD13 | 6        | 0.15          |
| (1,1163) | 1:149:A:LEU:H   | 1:153:A:LEU:HD11 | 8        | 0.15          |
| (1,1163) | 1:149:A:LEU:H   | 1:153:A:LEU:HD12 | 8        | 0.15          |
| (1,1163) | 1:149:A:LEU:H   | 1:153:A:LEU:HD13 | 8        | 0.15          |
| (1,1163) | 1:149:A:LEU:H   | 1:153:A:LEU:HD11 | 11       | 0.15          |
| (1,1163) | 1:149:A:LEU:H   | 1:153:A:LEU:HD12 | 11       | 0.15          |
| (1,1163) | 1:149:A:LEU:H   | 1:153:A:LEU:HD13 | 11       | 0.15          |
| (1,1019) | 1:124:A:PHE:HB2 | 1:131:A:GLN:H    | 5        | 0.15          |
| (1,1019) | 1:124:A:PHE:HB2 | 1:131:A:GLN:H    | 6        | 0.15          |
| (1,999)  | 1:126:A:THR:HA  | 1:130:A:ALA:H    | 17       | 0.15          |
| (1,289)  | 1:34:A:GLU:H    | 1:49:A:PHE:HE1   | 3        | 0.15          |
| (1,289)  | 1:34:A:GLU:H    | 1:49:A:PHE:HE2   | 3        | 0.15          |
| (1,289)  | 1:34:A:GLU:H    | 1:49:A:PHE:HE1   | 18       | 0.15          |
| (1,289)  | 1:34:A:GLU:H    | 1:49:A:PHE:HE2   | 18       | 0.15          |
| (1,270)  | 1:31:A:GLU:HG3  | 1:32:A:LEU:H     | 9        | 0.15          |
| (1,226)  | 1:27:A:TYR:H    | 1:28:A:THR:HG21  | 2        | 0.15          |
| (1,226)  | 1:27:A:TYR:H    | 1:28:A:THR:HG22  | 2        | 0.15          |
| (1,226)  | 1:27:A:TYR:H    | 1:28:A:THR:HG23  | 2        | 0.15          |
| (1,195)  | 1:108:A:ASN:H   | 1:118:A:VAL:HG21 | 15       | 0.15          |
| (1,195)  | 1:108:A:ASN:H   | 1:118:A:VAL:HG22 | 15       | 0.15          |
| (1,195)  | 1:108:A:ASN:H   | 1:118:A:VAL:HG23 | 15       | 0.15          |
| (1,150)  | 1:21:A:ASN:H    | 1:23:A:VAL:HB    | 4        | 0.15          |
| (1,124)  | 1:14:A:ARG:HG3  | 1:15:A:THR:H     | 12       | 0.15          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,676)  | 1:32:A:LEU:HD11  | 1:149:A:LEU:HD21 | 16       | 0.14          |
| (2,676)  | 1:32:A:LEU:HD11  | 1:149:A:LEU:HD22 | 16       | 0.14          |
| (2,676)  | 1:32:A:LEU:HD11  | 1:149:A:LEU:HD23 | 16       | 0.14          |
| (2,676)  | 1:32:A:LEU:HD12  | 1:149:A:LEU:HD21 | 16       | 0.14          |
| (2,676)  | 1:32:A:LEU:HD12  | 1:149:A:LEU:HD22 | 16       | 0.14          |
| (2,676)  | 1:32:A:LEU:HD12  | 1:149:A:LEU:HD23 | 16       | 0.14          |
| (2,676)  | 1:32:A:LEU:HD13  | 1:149:A:LEU:HD21 | 16       | 0.14          |
| (2,676)  | 1:32:A:LEU:HD13  | 1:149:A:LEU:HD22 | 16       | 0.14          |
| (2,676)  | 1:32:A:LEU:HD13  | 1:149:A:LEU:HD23 | 16       | 0.14          |
| (1,4412) | 1:20:A:ILE:HG21  | 1:81:A:TYR:HD1   | 18       | 0.14          |
| (1,4412) | 1:20:A:ILE:HG21  | 1:81:A:TYR:HD2   | 18       | 0.14          |
| (1,4412) | 1:20:A:ILE:HG22  | 1:81:A:TYR:HD1   | 18       | 0.14          |
| (1,4412) | 1:20:A:ILE:HG22  | 1:81:A:TYR:HD2   | 18       | 0.14          |
| (1,4412) | 1:20:A:ILE:HG23  | 1:81:A:TYR:HD1   | 18       | 0.14          |
| (1,4412) | 1:20:A:ILE:HG23  | 1:81:A:TYR:HD2   | 18       | 0.14          |
| (1,4229) | 1:152:A:LEU:HD11 | 1:153:A:LEU:HD11 | 5        | 0.14          |
| (1,4229) | 1:152:A:LEU:HD11 | 1:153:A:LEU:HD12 | 5        | 0.14          |
| (1,4229) | 1:152:A:LEU:HD11 | 1:153:A:LEU:HD13 | 5        | 0.14          |
| (1,4229) | 1:152:A:LEU:HD12 | 1:153:A:LEU:HD11 | 5        | 0.14          |
| (1,4229) | 1:152:A:LEU:HD12 | 1:153:A:LEU:HD12 | 5        | 0.14          |
| (1,4229) | 1:152:A:LEU:HD12 | 1:153:A:LEU:HD13 | 5        | 0.14          |
| (1,4229) | 1:152:A:LEU:HD13 | 1:153:A:LEU:HD11 | 5        | 0.14          |
| (1,4229) | 1:152:A:LEU:HD13 | 1:153:A:LEU:HD12 | 5        | 0.14          |
| (1,4229) | 1:152:A:LEU:HD13 | 1:153:A:LEU:HD13 | 5        | 0.14          |
| (1,4229) | 1:152:A:LEU:HD11 | 1:153:A:LEU:HD11 | 14       | 0.14          |
| (1,4229) | 1:152:A:LEU:HD11 | 1:153:A:LEU:HD12 | 14       | 0.14          |
| (1,4229) | 1:152:A:LEU:HD11 | 1:153:A:LEU:HD13 | 14       | 0.14          |
| (1,4229) | 1:152:A:LEU:HD12 | 1:153:A:LEU:HD11 | 14       | 0.14          |
| (1,4229) | 1:152:A:LEU:HD12 | 1:153:A:LEU:HD12 | 14       | 0.14          |
| (1,4229) | 1:152:A:LEU:HD12 | 1:153:A:LEU:HD13 | 14       | 0.14          |
| (1,4229) | 1:152:A:LEU:HD13 | 1:153:A:LEU:HD11 | 14       | 0.14          |
| (1,4229) | 1:152:A:LEU:HD13 | 1:153:A:LEU:HD12 | 14       | 0.14          |
| (1,4229) | 1:152:A:LEU:HD13 | 1:153:A:LEU:HD13 | 14       | 0.14          |
| (1,4229) | 1:152:A:LEU:HD11 | 1:153:A:LEU:HD11 | 17       | 0.14          |
| (1,4229) | 1:152:A:LEU:HD11 | 1:153:A:LEU:HD12 | 17       | 0.14          |
| (1,4229) | 1:152:A:LEU:HD11 | 1:153:A:LEU:HD13 | 17       | 0.14          |
| (1,4229) | 1:152:A:LEU:HD12 | 1:153:A:LEU:HD11 | 17       | 0.14          |
| (1,4229) | 1:152:A:LEU:HD12 | 1:153:A:LEU:HD12 | 17       | 0.14          |
| (1,4229) | 1:152:A:LEU:HD12 | 1:153:A:LEU:HD13 | 17       | 0.14          |
| (1,4229) | 1:152:A:LEU:HD13 | 1:153:A:LEU:HD11 | 17       | 0.14          |
| (1,4229) | 1:152:A:LEU:HD13 | 1:153:A:LEU:HD12 | 17       | 0.14          |
| (1,4229) | 1:152:A:LEU:HD13 | 1:153:A:LEU:HD13 | 17       | 0.14          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,4203) | 1:128:A:SER:HB3 | 1:131:A:GLN:HG2  | 3        | 0.14          |
| (1,4202) | 1:125:A:PRO:HB3 | 1:126:A:THR:HG21 | 6        | 0.14          |
| (1,4202) | 1:125:A:PRO:HB3 | 1:126:A:THR:HG22 | 6        | 0.14          |
| (1,4202) | 1:125:A:PRO:HB3 | 1:126:A:THR:HG23 | 6        | 0.14          |
| (1,4196) | 1:8:A:ASN:HB2   | 1:125:A:PRO:HD2  | 18       | 0.14          |
| (1,4049) | 1:30:A:ARG:HB3  | 1:31:A:GLU:HA    | 9        | 0.14          |
| (1,3797) | 1:34:A:GLU:HG2  | 1:35:A:GLN:HA    | 5        | 0.14          |
| (1,3668) | 1:154:A:ASN:HA  | 1:157:A:LEU:HD11 | 15       | 0.14          |
| (1,3668) | 1:154:A:ASN:HA  | 1:157:A:LEU:HD12 | 15       | 0.14          |
| (1,3668) | 1:154:A:ASN:HA  | 1:157:A:LEU:HD13 | 15       | 0.14          |
| (1,3433) | 1:5:A:LYS:HB2   | 1:134:A:ILE:HD11 | 16       | 0.14          |
| (1,3433) | 1:5:A:LYS:HB2   | 1:134:A:ILE:HD12 | 16       | 0.14          |
| (1,3433) | 1:5:A:LYS:HB2   | 1:134:A:ILE:HD13 | 16       | 0.14          |
| (1,3405) | 1:132:A:GLN:HG3 | 1:135:A:ASP:HB2  | 19       | 0.14          |
| (1,3391) | 1:131:A:GLN:HG2 | 1:132:A:GLN:HA   | 19       | 0.14          |
| (1,3236) | 1:108:A:ASN:HB2 | 1:119:A:THR:HB   | 2        | 0.14          |
| (1,3155) | 1:83:A:ILE:HG21 | 1:106:A:THR:HG21 | 15       | 0.14          |
| (1,3155) | 1:83:A:ILE:HG21 | 1:106:A:THR:HG22 | 15       | 0.14          |
| (1,3155) | 1:83:A:ILE:HG21 | 1:106:A:THR:HG23 | 15       | 0.14          |
| (1,3155) | 1:83:A:ILE:HG22 | 1:106:A:THR:HG21 | 15       | 0.14          |
| (1,3155) | 1:83:A:ILE:HG22 | 1:106:A:THR:HG22 | 15       | 0.14          |
| (1,3155) | 1:83:A:ILE:HG22 | 1:106:A:THR:HG23 | 15       | 0.14          |
| (1,3155) | 1:83:A:ILE:HG23 | 1:106:A:THR:HG21 | 15       | 0.14          |
| (1,3155) | 1:83:A:ILE:HG23 | 1:106:A:THR:HG22 | 15       | 0.14          |
| (1,3155) | 1:83:A:ILE:HG23 | 1:106:A:THR:HG23 | 15       | 0.14          |
| (1,2930) | 1:71:A:ILE:HD11 | 1:91:A:THR:HG21  | 2        | 0.14          |
| (1,2930) | 1:71:A:ILE:HD11 | 1:91:A:THR:HG22  | 2        | 0.14          |
| (1,2930) | 1:71:A:ILE:HD11 | 1:91:A:THR:HG23  | 2        | 0.14          |
| (1,2930) | 1:71:A:ILE:HD12 | 1:91:A:THR:HG21  | 2        | 0.14          |
| (1,2930) | 1:71:A:ILE:HD12 | 1:91:A:THR:HG22  | 2        | 0.14          |
| (1,2930) | 1:71:A:ILE:HD12 | 1:91:A:THR:HG23  | 2        | 0.14          |
| (1,2930) | 1:71:A:ILE:HD13 | 1:91:A:THR:HG21  | 2        | 0.14          |
| (1,2930) | 1:71:A:ILE:HD13 | 1:91:A:THR:HG22  | 2        | 0.14          |
| (1,2930) | 1:71:A:ILE:HD13 | 1:91:A:THR:HG23  | 2        | 0.14          |
| (1,2911) | 1:89:A:PHE:HB2  | 1:97:A:ASP:HB2   | 8        | 0.14          |
| (1,2591) | 1:61:A:ILE:HG21 | 1:66:A:MET:HE1   | 9        | 0.14          |
| (1,2591) | 1:61:A:ILE:HG21 | 1:66:A:MET:HE2   | 9        | 0.14          |
| (1,2591) | 1:61:A:ILE:HG21 | 1:66:A:MET:HE3   | 9        | 0.14          |
| (1,2591) | 1:61:A:ILE:HG22 | 1:66:A:MET:HE1   | 9        | 0.14          |
| (1,2591) | 1:61:A:ILE:HG22 | 1:66:A:MET:HE2   | 9        | 0.14          |
| (1,2591) | 1:61:A:ILE:HG22 | 1:66:A:MET:HE3   | 9        | 0.14          |
| (1,2591) | 1:61:A:ILE:HG23 | 1:66:A:MET:HE1   | 9        | 0.14          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2591) | 1:61:A:ILE:HG23 | 1:66:A:MET:HE2   | 9        | 0.14          |
| (1,2591) | 1:61:A:ILE:HG23 | 1:66:A:MET:HE3   | 9        | 0.14          |
| (1,2410) | 1:12:A:PHE:HE1  | 1:146:A:LEU:HD21 | 12       | 0.14          |
| (1,2410) | 1:12:A:PHE:HE1  | 1:146:A:LEU:HD22 | 12       | 0.14          |
| (1,2410) | 1:12:A:PHE:HE1  | 1:146:A:LEU:HD23 | 12       | 0.14          |
| (1,2410) | 1:12:A:PHE:HE2  | 1:146:A:LEU:HD21 | 12       | 0.14          |
| (1,2410) | 1:12:A:PHE:HE2  | 1:146:A:LEU:HD22 | 12       | 0.14          |
| (1,2410) | 1:12:A:PHE:HE2  | 1:146:A:LEU:HD23 | 12       | 0.14          |
| (1,2134) | 1:36:A:TRP:HH2  | 1:37:A:PHE:HA    | 8        | 0.14          |
| (1,2075) | 1:31:A:GLU:HG3  | 1:32:A:LEU:HG    | 14       | 0.14          |
| (1,1832) | 1:35:A:GLN:HB3  | 1:152:A:LEU:HA   | 8        | 0.14          |
| (1,1832) | 1:35:A:GLN:HB3  | 1:152:A:LEU:HA   | 17       | 0.14          |
| (1,1542) | 1:6:A:LYS:HG2   | 1:9:A:LYS:HE2    | 2        | 0.14          |
| (1,1542) | 1:6:A:LYS:HG2   | 1:9:A:LYS:HE3    | 2        | 0.14          |
| (1,1542) | 1:6:A:LYS:HG3   | 1:9:A:LYS:HE2    | 2        | 0.14          |
| (1,1542) | 1:6:A:LYS:HG3   | 1:9:A:LYS:HE3    | 2        | 0.14          |
| (1,1479) | 1:30:A:ARG:HB3  | 1:49:A:PHE:HB2   | 4        | 0.14          |
| (1,1291) | 1:91:A:THR:HB   | 1:92:A:SER:H     | 20       | 0.14          |
| (1,1264) | 1:8:A:ASN:HD22  | 1:124:A:PHE:H    | 10       | 0.14          |
| (1,1247) | 1:128:A:SER:HA  | 1:132:A:GLN:H    | 5        | 0.14          |
| (1,1247) | 1:128:A:SER:HA  | 1:132:A:GLN:H    | 15       | 0.14          |
| (1,1163) | 1:149:A:LEU:H   | 1:153:A:LEU:HD11 | 1        | 0.14          |
| (1,1163) | 1:149:A:LEU:H   | 1:153:A:LEU:HD12 | 1        | 0.14          |
| (1,1163) | 1:149:A:LEU:H   | 1:153:A:LEU:HD13 | 1        | 0.14          |
| (1,1163) | 1:149:A:LEU:H   | 1:153:A:LEU:HD11 | 18       | 0.14          |
| (1,1163) | 1:149:A:LEU:H   | 1:153:A:LEU:HD12 | 18       | 0.14          |
| (1,1163) | 1:149:A:LEU:H   | 1:153:A:LEU:HD13 | 18       | 0.14          |
| (1,1163) | 1:149:A:LEU:H   | 1:153:A:LEU:HD11 | 19       | 0.14          |
| (1,1163) | 1:149:A:LEU:H   | 1:153:A:LEU:HD12 | 19       | 0.14          |
| (1,1163) | 1:149:A:LEU:H   | 1:153:A:LEU:HD13 | 19       | 0.14          |
| (1,1019) | 1:124:A:PHE:HB2 | 1:131:A:GLN:H    | 19       | 0.14          |
| (1,980)  | 1:9:A:LYS:HB2   | 1:122:A:SER:H    | 12       | 0.14          |
| (1,980)  | 1:9:A:LYS:HB2   | 1:122:A:SER:H    | 14       | 0.14          |
| (1,703)  | 1:79:A:ALA:HA   | 1:81:A:TYR:H     | 2        | 0.14          |
| (1,703)  | 1:79:A:ALA:HA   | 1:81:A:TYR:H     | 3        | 0.14          |
| (1,320)  | 1:154:A:ASN:HA  | 1:154:A:ASN:HD22 | 17       | 0.14          |
| (1,226)  | 1:27:A:TYR:H    | 1:28:A:THR:HG21  | 6        | 0.14          |
| (1,226)  | 1:27:A:TYR:H    | 1:28:A:THR:HG22  | 6        | 0.14          |
| (1,226)  | 1:27:A:TYR:H    | 1:28:A:THR:HG23  | 6        | 0.14          |
| (1,150)  | 1:21:A:ASN:H    | 1:23:A:VAL:HB    | 6        | 0.14          |
| (2,801)  | 1:96:A:LYS:HD3  | 1:97:A:ASP:HA    | 8        | 0.13          |
| (2,764)  | 1:73:A:GLU:HG2  | 1:88:A:TYR:HB3   | 6        | 0.13          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,676)  | 1:32:A:LEU:HD11  | 1:149:A:LEU:HD21 | 4        | 0.13          |
| (2,676)  | 1:32:A:LEU:HD11  | 1:149:A:LEU:HD22 | 4        | 0.13          |
| (2,676)  | 1:32:A:LEU:HD11  | 1:149:A:LEU:HD23 | 4        | 0.13          |
| (2,676)  | 1:32:A:LEU:HD12  | 1:149:A:LEU:HD21 | 4        | 0.13          |
| (2,676)  | 1:32:A:LEU:HD12  | 1:149:A:LEU:HD22 | 4        | 0.13          |
| (2,676)  | 1:32:A:LEU:HD12  | 1:149:A:LEU:HD23 | 4        | 0.13          |
| (2,676)  | 1:32:A:LEU:HD13  | 1:149:A:LEU:HD21 | 4        | 0.13          |
| (2,676)  | 1:32:A:LEU:HD13  | 1:149:A:LEU:HD22 | 4        | 0.13          |
| (2,676)  | 1:32:A:LEU:HD13  | 1:149:A:LEU:HD23 | 4        | 0.13          |
| (2,641)  | 1:20:A:ILE:HG21  | 1:21:A:ASN:HD22  | 18       | 0.13          |
| (2,641)  | 1:20:A:ILE:HG22  | 1:21:A:ASN:HD22  | 18       | 0.13          |
| (2,641)  | 1:20:A:ILE:HG23  | 1:21:A:ASN:HD22  | 18       | 0.13          |
| (1,4410) | 1:79:A:ALA:HA    | 1:81:A:TYR:HD1   | 3        | 0.13          |
| (1,4410) | 1:79:A:ALA:HA    | 1:81:A:TYR:HD2   | 3        | 0.13          |
| (1,4362) | 1:68:A:SER:HA    | 1:69:A:TYR:HE1   | 16       | 0.13          |
| (1,4362) | 1:68:A:SER:HA    | 1:69:A:TYR:HE2   | 16       | 0.13          |
| (1,4362) | 1:68:A:SER:HA    | 1:69:A:TYR:HE1   | 18       | 0.13          |
| (1,4362) | 1:68:A:SER:HA    | 1:69:A:TYR:HE2   | 18       | 0.13          |
| (1,4229) | 1:152:A:LEU:HD11 | 1:153:A:LEU:HD11 | 6        | 0.13          |
| (1,4229) | 1:152:A:LEU:HD11 | 1:153:A:LEU:HD12 | 6        | 0.13          |
| (1,4229) | 1:152:A:LEU:HD11 | 1:153:A:LEU:HD13 | 6        | 0.13          |
| (1,4229) | 1:152:A:LEU:HD12 | 1:153:A:LEU:HD11 | 6        | 0.13          |
| (1,4229) | 1:152:A:LEU:HD12 | 1:153:A:LEU:HD12 | 6        | 0.13          |
| (1,4229) | 1:152:A:LEU:HD12 | 1:153:A:LEU:HD13 | 6        | 0.13          |
| (1,4229) | 1:152:A:LEU:HD13 | 1:153:A:LEU:HD11 | 6        | 0.13          |
| (1,4229) | 1:152:A:LEU:HD13 | 1:153:A:LEU:HD12 | 6        | 0.13          |
| (1,4229) | 1:152:A:LEU:HD13 | 1:153:A:LEU:HD13 | 6        | 0.13          |
| (1,4202) | 1:125:A:PRO:HB3  | 1:126:A:THR:HG21 | 20       | 0.13          |
| (1,4202) | 1:125:A:PRO:HB3  | 1:126:A:THR:HG22 | 20       | 0.13          |
| (1,4202) | 1:125:A:PRO:HB3  | 1:126:A:THR:HG23 | 20       | 0.13          |
| (1,4098) | 1:62:A:GLN:HB2   | 1:67:A:ILE:HD11  | 20       | 0.13          |
| (1,4098) | 1:62:A:GLN:HB2   | 1:67:A:ILE:HD12  | 20       | 0.13          |
| (1,4098) | 1:62:A:GLN:HB2   | 1:67:A:ILE:HD13  | 20       | 0.13          |
| (1,4052) | 1:34:A:GLU:HG2   | 1:35:A:GLN:HG3   | 7        | 0.13          |
| (1,4020) | 1:19:A:PRO:HG2   | 1:22:A:LYS:HG2   | 4        | 0.13          |
| (1,4020) | 1:19:A:PRO:HG2   | 1:22:A:LYS:HG2   | 11       | 0.13          |
| (1,4020) | 1:19:A:PRO:HG2   | 1:22:A:LYS:HG2   | 17       | 0.13          |
| (1,4016) | 1:20:A:ILE:HD11  | 1:23:A:VAL:HB    | 13       | 0.13          |
| (1,4016) | 1:20:A:ILE:HD12  | 1:23:A:VAL:HB    | 13       | 0.13          |
| (1,4016) | 1:20:A:ILE:HD13  | 1:23:A:VAL:HB    | 13       | 0.13          |
| (1,4014) | 1:20:A:ILE:HD11  | 1:80:A:PRO:HB2   | 1        | 0.13          |
| (1,4014) | 1:20:A:ILE:HD12  | 1:80:A:PRO:HB2   | 1        | 0.13          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,4014) | 1:20:A:ILE:HD13  | 1:80:A:PRO:HB2   | 1        | 0.13          |
| (1,3897) | 1:89:A:PHE:HD1   | 1:100:A:MET:HB2  | 2        | 0.13          |
| (1,3897) | 1:89:A:PHE:HD2   | 1:100:A:MET:HB2  | 2        | 0.13          |
| (1,3797) | 1:34:A:GLU:HG2   | 1:35:A:GLN:HA    | 1        | 0.13          |
| (1,3740) | 1:154:A:ASN:HA   | 1:157:A:LEU:HB3  | 3        | 0.13          |
| (1,3740) | 1:154:A:ASN:HA   | 1:157:A:LEU:HB3  | 19       | 0.13          |
| (1,3296) | 1:9:A:LYS:HA     | 1:122:A:SER:HB3  | 8        | 0.13          |
| (1,3246) | 1:24:A:PHE:HD1   | 1:118:A:VAL:HG11 | 10       | 0.13          |
| (1,3246) | 1:24:A:PHE:HD1   | 1:118:A:VAL:HG12 | 10       | 0.13          |
| (1,3246) | 1:24:A:PHE:HD1   | 1:118:A:VAL:HG13 | 10       | 0.13          |
| (1,3246) | 1:24:A:PHE:HD2   | 1:118:A:VAL:HG11 | 10       | 0.13          |
| (1,3246) | 1:24:A:PHE:HD2   | 1:118:A:VAL:HG12 | 10       | 0.13          |
| (1,3246) | 1:24:A:PHE:HD2   | 1:118:A:VAL:HG13 | 10       | 0.13          |
| (1,3155) | 1:83:A:ILE:HG21  | 1:106:A:THR:HG21 | 9        | 0.13          |
| (1,3155) | 1:83:A:ILE:HG21  | 1:106:A:THR:HG22 | 9        | 0.13          |
| (1,3155) | 1:83:A:ILE:HG21  | 1:106:A:THR:HG23 | 9        | 0.13          |
| (1,3155) | 1:83:A:ILE:HG22  | 1:106:A:THR:HG21 | 9        | 0.13          |
| (1,3155) | 1:83:A:ILE:HG22  | 1:106:A:THR:HG22 | 9        | 0.13          |
| (1,3155) | 1:83:A:ILE:HG22  | 1:106:A:THR:HG23 | 9        | 0.13          |
| (1,3155) | 1:83:A:ILE:HG23  | 1:106:A:THR:HG21 | 9        | 0.13          |
| (1,3155) | 1:83:A:ILE:HG23  | 1:106:A:THR:HG22 | 9        | 0.13          |
| (1,3155) | 1:83:A:ILE:HG23  | 1:106:A:THR:HG23 | 9        | 0.13          |
| (1,3141) | 1:105:A:ILE:HG13 | 1:107:A:LEU:HG   | 3        | 0.13          |
| (1,3088) | 1:10:A:ILE:HD11  | 1:103:A:MET:HE1  | 14       | 0.13          |
| (1,3088) | 1:10:A:ILE:HD11  | 1:103:A:MET:HE2  | 14       | 0.13          |
| (1,3088) | 1:10:A:ILE:HD11  | 1:103:A:MET:HE3  | 14       | 0.13          |
| (1,3088) | 1:10:A:ILE:HD12  | 1:103:A:MET:HE1  | 14       | 0.13          |
| (1,3088) | 1:10:A:ILE:HD12  | 1:103:A:MET:HE2  | 14       | 0.13          |
| (1,3088) | 1:10:A:ILE:HD12  | 1:103:A:MET:HE3  | 14       | 0.13          |
| (1,3088) | 1:10:A:ILE:HD13  | 1:103:A:MET:HE1  | 14       | 0.13          |
| (1,3088) | 1:10:A:ILE:HD13  | 1:103:A:MET:HE2  | 14       | 0.13          |
| (1,3088) | 1:10:A:ILE:HD13  | 1:103:A:MET:HE3  | 14       | 0.13          |
| (1,3047) | 1:142:A:MET:HA   | 1:142:A:MET:HE1  | 1        | 0.13          |
| (1,3047) | 1:142:A:MET:HA   | 1:142:A:MET:HE2  | 1        | 0.13          |
| (1,3047) | 1:142:A:MET:HA   | 1:142:A:MET:HE3  | 1        | 0.13          |
| (1,3008) | 1:95:A:GLU:HB2   | 1:96:A:LYS:HB2   | 3        | 0.13          |
| (1,3008) | 1:95:A:GLU:HB2   | 1:96:A:LYS:HB3   | 3        | 0.13          |
| (1,2930) | 1:71:A:ILE:HD11  | 1:91:A:THR:HG21  | 4        | 0.13          |
| (1,2930) | 1:71:A:ILE:HD11  | 1:91:A:THR:HG22  | 4        | 0.13          |
| (1,2930) | 1:71:A:ILE:HD11  | 1:91:A:THR:HG23  | 4        | 0.13          |
| (1,2930) | 1:71:A:ILE:HD12  | 1:91:A:THR:HG21  | 4        | 0.13          |
| (1,2930) | 1:71:A:ILE:HD12  | 1:91:A:THR:HG22  | 4        | 0.13          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2930) | 1:71:A:ILE:HD12 | 1:91:A:THR:HG23 | 4        | 0.13          |
| (1,2930) | 1:71:A:ILE:HD13 | 1:91:A:THR:HG21 | 4        | 0.13          |
| (1,2930) | 1:71:A:ILE:HD13 | 1:91:A:THR:HG22 | 4        | 0.13          |
| (1,2930) | 1:71:A:ILE:HD13 | 1:91:A:THR:HG23 | 4        | 0.13          |
| (1,2930) | 1:71:A:ILE:HD11 | 1:91:A:THR:HG21 | 18       | 0.13          |
| (1,2930) | 1:71:A:ILE:HD11 | 1:91:A:THR:HG22 | 18       | 0.13          |
| (1,2930) | 1:71:A:ILE:HD11 | 1:91:A:THR:HG23 | 18       | 0.13          |
| (1,2930) | 1:71:A:ILE:HD12 | 1:91:A:THR:HG21 | 18       | 0.13          |
| (1,2930) | 1:71:A:ILE:HD12 | 1:91:A:THR:HG22 | 18       | 0.13          |
| (1,2930) | 1:71:A:ILE:HD12 | 1:91:A:THR:HG23 | 18       | 0.13          |
| (1,2930) | 1:71:A:ILE:HD13 | 1:91:A:THR:HG21 | 18       | 0.13          |
| (1,2930) | 1:71:A:ILE:HD13 | 1:91:A:THR:HG22 | 18       | 0.13          |
| (1,2930) | 1:71:A:ILE:HD13 | 1:91:A:THR:HG23 | 18       | 0.13          |
| (1,2930) | 1:71:A:ILE:HD11 | 1:91:A:THR:HG21 | 19       | 0.13          |
| (1,2930) | 1:71:A:ILE:HD11 | 1:91:A:THR:HG22 | 19       | 0.13          |
| (1,2930) | 1:71:A:ILE:HD11 | 1:91:A:THR:HG23 | 19       | 0.13          |
| (1,2930) | 1:71:A:ILE:HD12 | 1:91:A:THR:HG21 | 19       | 0.13          |
| (1,2930) | 1:71:A:ILE:HD12 | 1:91:A:THR:HG22 | 19       | 0.13          |
| (1,2930) | 1:71:A:ILE:HD12 | 1:91:A:THR:HG23 | 19       | 0.13          |
| (1,2930) | 1:71:A:ILE:HD13 | 1:91:A:THR:HG21 | 19       | 0.13          |
| (1,2930) | 1:71:A:ILE:HD13 | 1:91:A:THR:HG22 | 19       | 0.13          |
| (1,2930) | 1:71:A:ILE:HD13 | 1:91:A:THR:HG23 | 19       | 0.13          |
| (1,2889) | 1:87:A:ASP:HB2  | 1:103:A:MET:HB2 | 9        | 0.13          |
| (1,2667) | 1:70:A:THR:H    | 1:71:A:ILE:HD11 | 9        | 0.13          |
| (1,2667) | 1:70:A:THR:H    | 1:71:A:ILE:HD12 | 9        | 0.13          |
| (1,2667) | 1:70:A:THR:H    | 1:71:A:ILE:HD13 | 9        | 0.13          |
| (1,2529) | 1:100:A:MET:HG3 | 1:101:A:PRO:HD3 | 12       | 0.13          |
| (1,2134) | 1:36:A:TRP:HH2  | 1:37:A:PHE:HA   | 9        | 0.13          |
| (1,2036) | 1:4:A:GLU:HG2   | 1:6:A:LYS:HG2   | 12       | 0.13          |
| (1,2036) | 1:4:A:GLU:HG2   | 1:6:A:LYS:HG3   | 12       | 0.13          |
| (1,2036) | 1:4:A:GLU:HG2   | 1:6:A:LYS:HG2   | 15       | 0.13          |
| (1,2036) | 1:4:A:GLU:HG2   | 1:6:A:LYS:HG3   | 15       | 0.13          |
| (1,2036) | 1:4:A:GLU:HG2   | 1:6:A:LYS:HG2   | 20       | 0.13          |
| (1,2036) | 1:4:A:GLU:HG2   | 1:6:A:LYS:HG3   | 20       | 0.13          |
| (1,1832) | 1:35:A:GLN:HB3  | 1:152:A:LEU:HA  | 16       | 0.13          |
| (1,1676) | 1:13:A:THR:HG21 | 1:14:A:ARG:HB2  | 17       | 0.13          |
| (1,1676) | 1:13:A:THR:HG22 | 1:14:A:ARG:HB2  | 17       | 0.13          |
| (1,1676) | 1:13:A:THR:HG23 | 1:14:A:ARG:HB2  | 17       | 0.13          |
| (1,1675) | 1:53:A:LYS:HD2  | 1:77:A:VAL:HG11 | 20       | 0.13          |
| (1,1675) | 1:53:A:LYS:HD2  | 1:77:A:VAL:HG12 | 20       | 0.13          |
| (1,1675) | 1:53:A:LYS:HD2  | 1:77:A:VAL:HG13 | 20       | 0.13          |
| (1,1675) | 1:53:A:LYS:HD3  | 1:77:A:VAL:HG11 | 20       | 0.13          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1675) | 1:53:A:LYS:HD3  | 1:77:A:VAL:HG12  | 20       | 0.13          |
| (1,1675) | 1:53:A:LYS:HD3  | 1:77:A:VAL:HG13  | 20       | 0.13          |
| (1,1566) | 1:10:A:ILE:HD11 | 1:133:A:ALA:H    | 4        | 0.13          |
| (1,1566) | 1:10:A:ILE:HD12 | 1:133:A:ALA:H    | 4        | 0.13          |
| (1,1566) | 1:10:A:ILE:HD13 | 1:133:A:ALA:H    | 4        | 0.13          |
| (1,1542) | 1:6:A:LYS:HG2   | 1:9:A:LYS:HE2    | 6        | 0.13          |
| (1,1542) | 1:6:A:LYS:HG2   | 1:9:A:LYS:HE3    | 6        | 0.13          |
| (1,1542) | 1:6:A:LYS:HG3   | 1:9:A:LYS:HE2    | 6        | 0.13          |
| (1,1542) | 1:6:A:LYS:HG3   | 1:9:A:LYS:HE3    | 6        | 0.13          |
| (1,1394) | 1:3:A:ILE:HG21  | 1:4:A:GLU:HA     | 1        | 0.13          |
| (1,1394) | 1:3:A:ILE:HG22  | 1:4:A:GLU:HA     | 1        | 0.13          |
| (1,1394) | 1:3:A:ILE:HG23  | 1:4:A:GLU:HA     | 1        | 0.13          |
| (1,1394) | 1:3:A:ILE:HG21  | 1:4:A:GLU:HA     | 9        | 0.13          |
| (1,1394) | 1:3:A:ILE:HG22  | 1:4:A:GLU:HA     | 9        | 0.13          |
| (1,1394) | 1:3:A:ILE:HG23  | 1:4:A:GLU:HA     | 9        | 0.13          |
| (1,1163) | 1:149:A:LEU:H   | 1:153:A:LEU:HD11 | 4        | 0.13          |
| (1,1163) | 1:149:A:LEU:H   | 1:153:A:LEU:HD12 | 4        | 0.13          |
| (1,1163) | 1:149:A:LEU:H   | 1:153:A:LEU:HD13 | 4        | 0.13          |
| (1,1163) | 1:149:A:LEU:H   | 1:153:A:LEU:HD11 | 14       | 0.13          |
| (1,1163) | 1:149:A:LEU:H   | 1:153:A:LEU:HD12 | 14       | 0.13          |
| (1,1163) | 1:149:A:LEU:H   | 1:153:A:LEU:HD13 | 14       | 0.13          |
| (1,1136) | 1:144:A:SER:HA  | 1:147:A:ASN:HD22 | 16       | 0.13          |
| (1,1019) | 1:124:A:PHE:HB2 | 1:131:A:GLN:H    | 11       | 0.13          |
| (1,937)  | 1:117:A:THR:H   | 1:118:A:VAL:HB   | 8        | 0.13          |
| (1,937)  | 1:117:A:THR:H   | 1:118:A:VAL:HB   | 11       | 0.13          |
| (1,937)  | 1:117:A:THR:H   | 1:118:A:VAL:HB   | 14       | 0.13          |
| (1,937)  | 1:117:A:THR:H   | 1:118:A:VAL:HB   | 19       | 0.13          |
| (1,830)  | 1:99:A:SER:H    | 1:100:A:MET:HG2  | 17       | 0.13          |
| (1,817)  | 1:93:A:LYS:HB2  | 1:95:A:GLU:H     | 11       | 0.13          |
| (1,703)  | 1:79:A:ALA:HA   | 1:81:A:TYR:H     | 16       | 0.13          |
| (1,320)  | 1:154:A:ASN:HA  | 1:154:A:ASN:HD22 | 14       | 0.13          |
| (1,226)  | 1:27:A:TYR:H    | 1:28:A:THR:HG21  | 1        | 0.13          |
| (1,226)  | 1:27:A:TYR:H    | 1:28:A:THR:HG22  | 1        | 0.13          |
| (1,226)  | 1:27:A:TYR:H    | 1:28:A:THR:HG23  | 1        | 0.13          |
| (1,226)  | 1:27:A:TYR:H    | 1:28:A:THR:HG21  | 12       | 0.13          |
| (1,226)  | 1:27:A:TYR:H    | 1:28:A:THR:HG22  | 12       | 0.13          |
| (1,226)  | 1:27:A:TYR:H    | 1:28:A:THR:HG23  | 12       | 0.13          |
| (1,195)  | 1:108:A:ASN:H   | 1:118:A:VAL:HG21 | 3        | 0.13          |
| (1,195)  | 1:108:A:ASN:H   | 1:118:A:VAL:HG22 | 3        | 0.13          |
| (1,195)  | 1:108:A:ASN:H   | 1:118:A:VAL:HG23 | 3        | 0.13          |
| (1,150)  | 1:21:A:ASN:H    | 1:23:A:VAL:HB    | 5        | 0.13          |
| (1,150)  | 1:21:A:ASN:H    | 1:23:A:VAL:HB    | 14       | 0.13          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,9)    | 1:4:A:GLU:H     | 1:13:A:THR:HG21  | 9        | 0.13          |
| (1,9)    | 1:4:A:GLU:H     | 1:13:A:THR:HG22  | 9        | 0.13          |
| (1,9)    | 1:4:A:GLU:H     | 1:13:A:THR:HG23  | 9        | 0.13          |
| (2,764)  | 1:73:A:GLU:HG2  | 1:88:A:TYR:HB3   | 15       | 0.12          |
| (2,676)  | 1:32:A:LEU:HD11 | 1:149:A:LEU:HD21 | 7        | 0.12          |
| (2,676)  | 1:32:A:LEU:HD11 | 1:149:A:LEU:HD22 | 7        | 0.12          |
| (2,676)  | 1:32:A:LEU:HD11 | 1:149:A:LEU:HD23 | 7        | 0.12          |
| (2,676)  | 1:32:A:LEU:HD12 | 1:149:A:LEU:HD21 | 7        | 0.12          |
| (2,676)  | 1:32:A:LEU:HD12 | 1:149:A:LEU:HD22 | 7        | 0.12          |
| (2,676)  | 1:32:A:LEU:HD12 | 1:149:A:LEU:HD23 | 7        | 0.12          |
| (2,676)  | 1:32:A:LEU:HD13 | 1:149:A:LEU:HD21 | 7        | 0.12          |
| (2,676)  | 1:32:A:LEU:HD13 | 1:149:A:LEU:HD22 | 7        | 0.12          |
| (2,676)  | 1:32:A:LEU:HD13 | 1:149:A:LEU:HD23 | 7        | 0.12          |
| (2,676)  | 1:32:A:LEU:HD11 | 1:149:A:LEU:HD21 | 9        | 0.12          |
| (2,676)  | 1:32:A:LEU:HD11 | 1:149:A:LEU:HD22 | 9        | 0.12          |
| (2,676)  | 1:32:A:LEU:HD11 | 1:149:A:LEU:HD23 | 9        | 0.12          |
| (2,676)  | 1:32:A:LEU:HD12 | 1:149:A:LEU:HD21 | 9        | 0.12          |
| (2,676)  | 1:32:A:LEU:HD12 | 1:149:A:LEU:HD22 | 9        | 0.12          |
| (2,676)  | 1:32:A:LEU:HD12 | 1:149:A:LEU:HD23 | 9        | 0.12          |
| (2,676)  | 1:32:A:LEU:HD13 | 1:149:A:LEU:HD21 | 9        | 0.12          |
| (2,676)  | 1:32:A:LEU:HD13 | 1:149:A:LEU:HD22 | 9        | 0.12          |
| (2,676)  | 1:32:A:LEU:HD13 | 1:149:A:LEU:HD23 | 9        | 0.12          |
| (2,612)  | 1:7:A:LYS:HB2   | 1:8:A:ASN:HD21   | 10       | 0.12          |
| (2,449)  | 1:154:A:ASN:HA  | 1:157:A:LEU:HG   | 11       | 0.12          |
| (2,449)  | 1:154:A:ASN:HA  | 1:157:A:LEU:HG   | 16       | 0.12          |
| (2,251)  | 1:133:A:ALA:H   | 1:138:A:VAL:HG21 | 10       | 0.12          |
| (2,251)  | 1:133:A:ALA:H   | 1:138:A:VAL:HG22 | 10       | 0.12          |
| (2,251)  | 1:133:A:ALA:H   | 1:138:A:VAL:HG23 | 10       | 0.12          |
| (2,80)   | 1:82:A:TYR:HE1  | 1:108:A:ASN:HD21 | 12       | 0.12          |
| (2,80)   | 1:82:A:TYR:HE2  | 1:108:A:ASN:HD21 | 12       | 0.12          |
| (2,74)   | 1:97:A:ASP:HB2  | 1:100:A:MET:H    | 19       | 0.12          |
| (2,22)   | 1:32:A:LEU:H    | 1:49:A:PHE:HE1   | 4        | 0.12          |
| (2,22)   | 1:32:A:LEU:H    | 1:49:A:PHE:HE2   | 4        | 0.12          |
| (1,4412) | 1:20:A:ILE:HG21 | 1:81:A:TYR:HD1   | 2        | 0.12          |
| (1,4412) | 1:20:A:ILE:HG21 | 1:81:A:TYR:HD2   | 2        | 0.12          |
| (1,4412) | 1:20:A:ILE:HG22 | 1:81:A:TYR:HD1   | 2        | 0.12          |
| (1,4412) | 1:20:A:ILE:HG22 | 1:81:A:TYR:HD2   | 2        | 0.12          |
| (1,4412) | 1:20:A:ILE:HG23 | 1:81:A:TYR:HD1   | 2        | 0.12          |
| (1,4412) | 1:20:A:ILE:HG23 | 1:81:A:TYR:HD2   | 2        | 0.12          |
| (1,4410) | 1:79:A:ALA:HA   | 1:81:A:TYR:HD1   | 2        | 0.12          |
| (1,4410) | 1:79:A:ALA:HA   | 1:81:A:TYR:HD2   | 2        | 0.12          |
| (1,4362) | 1:68:A:SER:HA   | 1:69:A:TYR:HE1   | 11       | 0.12          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,4362) | 1:68:A:SER:HA    | 1:69:A:TYR:HE2   | 11       | 0.12          |
| (1,4362) | 1:68:A:SER:HA    | 1:69:A:TYR:HE1   | 20       | 0.12          |
| (1,4362) | 1:68:A:SER:HA    | 1:69:A:TYR:HE2   | 20       | 0.12          |
| (1,4206) | 1:126:A:THR:HG21 | 1:129:A:ALA:HB1  | 2        | 0.12          |
| (1,4206) | 1:126:A:THR:HG21 | 1:129:A:ALA:HB2  | 2        | 0.12          |
| (1,4206) | 1:126:A:THR:HG21 | 1:129:A:ALA:HB3  | 2        | 0.12          |
| (1,4206) | 1:126:A:THR:HG22 | 1:129:A:ALA:HB1  | 2        | 0.12          |
| (1,4206) | 1:126:A:THR:HG22 | 1:129:A:ALA:HB2  | 2        | 0.12          |
| (1,4206) | 1:126:A:THR:HG22 | 1:129:A:ALA:HB3  | 2        | 0.12          |
| (1,4206) | 1:126:A:THR:HG23 | 1:129:A:ALA:HB1  | 2        | 0.12          |
| (1,4206) | 1:126:A:THR:HG23 | 1:129:A:ALA:HB2  | 2        | 0.12          |
| (1,4206) | 1:126:A:THR:HG23 | 1:129:A:ALA:HB3  | 2        | 0.12          |
| (1,4136) | 1:73:A:GLU:HA    | 1:86:A:LEU:HD11  | 6        | 0.12          |
| (1,4136) | 1:73:A:GLU:HA    | 1:86:A:LEU:HD12  | 6        | 0.12          |
| (1,4136) | 1:73:A:GLU:HA    | 1:86:A:LEU:HD13  | 6        | 0.12          |
| (1,4136) | 1:73:A:GLU:HA    | 1:86:A:LEU:HD11  | 17       | 0.12          |
| (1,4136) | 1:73:A:GLU:HA    | 1:86:A:LEU:HD12  | 17       | 0.12          |
| (1,4136) | 1:73:A:GLU:HA    | 1:86:A:LEU:HD13  | 17       | 0.12          |
| (1,4057) | 1:34:A:GLU:HG3   | 1:35:A:GLN:HG2   | 3        | 0.12          |
| (1,3740) | 1:154:A:ASN:HA   | 1:157:A:LEU:HB3  | 7        | 0.12          |
| (1,3391) | 1:131:A:GLN:HG2  | 1:132:A:GLN:HA   | 9        | 0.12          |
| (1,3380) | 1:5:A:LYS:HE2    | 1:131:A:GLN:HA   | 11       | 0.12          |
| (1,3380) | 1:5:A:LYS:HE3    | 1:131:A:GLN:HA   | 11       | 0.12          |
| (1,3296) | 1:9:A:LYS:HA     | 1:122:A:SER:HB3  | 20       | 0.12          |
| (1,3272) | 1:107:A:LEU:HB3  | 1:120:A:SER:HB2  | 4        | 0.12          |
| (1,3272) | 1:107:A:LEU:HB3  | 1:120:A:SER:HB2  | 8        | 0.12          |
| (1,3272) | 1:107:A:LEU:HB3  | 1:120:A:SER:HB2  | 11       | 0.12          |
| (1,3272) | 1:107:A:LEU:HB3  | 1:120:A:SER:HB2  | 17       | 0.12          |
| (1,3246) | 1:24:A:PHE:HD1   | 1:118:A:VAL:HG11 | 7        | 0.12          |
| (1,3246) | 1:24:A:PHE:HD1   | 1:118:A:VAL:HG12 | 7        | 0.12          |
| (1,3246) | 1:24:A:PHE:HD1   | 1:118:A:VAL:HG13 | 7        | 0.12          |
| (1,3246) | 1:24:A:PHE:HD2   | 1:118:A:VAL:HG11 | 7        | 0.12          |
| (1,3246) | 1:24:A:PHE:HD2   | 1:118:A:VAL:HG12 | 7        | 0.12          |
| (1,3246) | 1:24:A:PHE:HD2   | 1:118:A:VAL:HG13 | 7        | 0.12          |
| (1,3246) | 1:24:A:PHE:HD1   | 1:118:A:VAL:HG11 | 20       | 0.12          |
| (1,3246) | 1:24:A:PHE:HD1   | 1:118:A:VAL:HG12 | 20       | 0.12          |
| (1,3246) | 1:24:A:PHE:HD1   | 1:118:A:VAL:HG13 | 20       | 0.12          |
| (1,3246) | 1:24:A:PHE:HD2   | 1:118:A:VAL:HG11 | 20       | 0.12          |
| (1,3246) | 1:24:A:PHE:HD2   | 1:118:A:VAL:HG12 | 20       | 0.12          |
| (1,3246) | 1:24:A:PHE:HD2   | 1:118:A:VAL:HG13 | 20       | 0.12          |
| (1,3236) | 1:108:A:ASN:HB2  | 1:119:A:THR:HB   | 19       | 0.12          |
| (1,3155) | 1:83:A:ILE:HG21  | 1:106:A:THR:HG21 | 3        | 0.12          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3155) | 1:83:A:ILE:HG21  | 1:106:A:THR:HG22 | 3        | 0.12          |
| (1,3155) | 1:83:A:ILE:HG21  | 1:106:A:THR:HG23 | 3        | 0.12          |
| (1,3155) | 1:83:A:ILE:HG22  | 1:106:A:THR:HG21 | 3        | 0.12          |
| (1,3155) | 1:83:A:ILE:HG22  | 1:106:A:THR:HG22 | 3        | 0.12          |
| (1,3155) | 1:83:A:ILE:HG22  | 1:106:A:THR:HG23 | 3        | 0.12          |
| (1,3155) | 1:83:A:ILE:HG23  | 1:106:A:THR:HG21 | 3        | 0.12          |
| (1,3155) | 1:83:A:ILE:HG23  | 1:106:A:THR:HG22 | 3        | 0.12          |
| (1,3155) | 1:83:A:ILE:HG23  | 1:106:A:THR:HG23 | 3        | 0.12          |
| (1,3141) | 1:105:A:ILE:HG13 | 1:107:A:LEU:HG   | 16       | 0.12          |
| (1,3087) | 1:103:A:MET:HE1  | 1:105:A:ILE:HG12 | 8        | 0.12          |
| (1,3087) | 1:103:A:MET:HE2  | 1:105:A:ILE:HG12 | 8        | 0.12          |
| (1,3087) | 1:103:A:MET:HE3  | 1:105:A:ILE:HG12 | 8        | 0.12          |
| (1,3078) | 1:87:A:ASP:H     | 1:103:A:MET:HE1  | 15       | 0.12          |
| (1,3078) | 1:87:A:ASP:H     | 1:103:A:MET:HE2  | 15       | 0.12          |
| (1,3078) | 1:87:A:ASP:H     | 1:103:A:MET:HE3  | 15       | 0.12          |
| (1,3026) | 1:91:A:THR:HG21  | 1:97:A:ASP:HB3   | 10       | 0.12          |
| (1,3026) | 1:91:A:THR:HG22  | 1:97:A:ASP:HB3   | 10       | 0.12          |
| (1,3026) | 1:91:A:THR:HG23  | 1:97:A:ASP:HB3   | 10       | 0.12          |
| (1,3026) | 1:91:A:THR:HG21  | 1:97:A:ASP:HB3   | 17       | 0.12          |
| (1,3026) | 1:91:A:THR:HG22  | 1:97:A:ASP:HB3   | 17       | 0.12          |
| (1,3026) | 1:91:A:THR:HG23  | 1:97:A:ASP:HB3   | 17       | 0.12          |
| (1,2930) | 1:71:A:ILE:HD11  | 1:91:A:THR:HG21  | 14       | 0.12          |
| (1,2930) | 1:71:A:ILE:HD11  | 1:91:A:THR:HG22  | 14       | 0.12          |
| (1,2930) | 1:71:A:ILE:HD11  | 1:91:A:THR:HG23  | 14       | 0.12          |
| (1,2930) | 1:71:A:ILE:HD12  | 1:91:A:THR:HG21  | 14       | 0.12          |
| (1,2930) | 1:71:A:ILE:HD12  | 1:91:A:THR:HG22  | 14       | 0.12          |
| (1,2930) | 1:71:A:ILE:HD12  | 1:91:A:THR:HG23  | 14       | 0.12          |
| (1,2930) | 1:71:A:ILE:HD13  | 1:91:A:THR:HG21  | 14       | 0.12          |
| (1,2930) | 1:71:A:ILE:HD13  | 1:91:A:THR:HG22  | 14       | 0.12          |
| (1,2930) | 1:71:A:ILE:HD13  | 1:91:A:THR:HG23  | 14       | 0.12          |
| (1,2911) | 1:89:A:PHE:HB2   | 1:97:A:ASP:HB2   | 6        | 0.12          |
| (1,2889) | 1:87:A:ASP:HB2   | 1:103:A:MET:HB2  | 5        | 0.12          |
| (1,2889) | 1:87:A:ASP:HB2   | 1:103:A:MET:HB2  | 20       | 0.12          |
| (1,2667) | 1:70:A:THR:H     | 1:71:A:ILE:HD11  | 12       | 0.12          |
| (1,2667) | 1:70:A:THR:H     | 1:71:A:ILE:HD12  | 12       | 0.12          |
| (1,2667) | 1:70:A:THR:H     | 1:71:A:ILE:HD13  | 12       | 0.12          |
| (1,2590) | 1:63:A:ALA:HB1   | 1:66:A:MET:HE1   | 6        | 0.12          |
| (1,2590) | 1:63:A:ALA:HB1   | 1:66:A:MET:HE2   | 6        | 0.12          |
| (1,2590) | 1:63:A:ALA:HB1   | 1:66:A:MET:HE3   | 6        | 0.12          |
| (1,2590) | 1:63:A:ALA:HB2   | 1:66:A:MET:HE1   | 6        | 0.12          |
| (1,2590) | 1:63:A:ALA:HB2   | 1:66:A:MET:HE2   | 6        | 0.12          |
| (1,2590) | 1:63:A:ALA:HB2   | 1:66:A:MET:HE3   | 6        | 0.12          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2590) | 1:63:A:ALA:HB3  | 1:66:A:MET:HE1   | 6        | 0.12          |
| (1,2590) | 1:63:A:ALA:HB3  | 1:66:A:MET:HE2   | 6        | 0.12          |
| (1,2590) | 1:63:A:ALA:HB3  | 1:66:A:MET:HE3   | 6        | 0.12          |
| (1,2529) | 1:100:A:MET:HG3 | 1:101:A:PRO:HD3  | 14       | 0.12          |
| (1,2466) | 1:61:A:ILE:HG12 | 1:69:A:TYR:HA    | 9        | 0.12          |
| (1,2410) | 1:12:A:PHE:HE1  | 1:146:A:LEU:HD21 | 3        | 0.12          |
| (1,2410) | 1:12:A:PHE:HE1  | 1:146:A:LEU:HD22 | 3        | 0.12          |
| (1,2410) | 1:12:A:PHE:HE1  | 1:146:A:LEU:HD23 | 3        | 0.12          |
| (1,2410) | 1:12:A:PHE:HE2  | 1:146:A:LEU:HD21 | 3        | 0.12          |
| (1,2410) | 1:12:A:PHE:HE2  | 1:146:A:LEU:HD22 | 3        | 0.12          |
| (1,2410) | 1:12:A:PHE:HE2  | 1:146:A:LEU:HD23 | 3        | 0.12          |
| (1,2134) | 1:36:A:TRP:HH2  | 1:37:A:PHE:HA    | 11       | 0.12          |
| (1,1832) | 1:35:A:GLN:HB3  | 1:152:A:LEU:HA   | 20       | 0.12          |
| (1,1804) | 1:20:A:ILE:HG21 | 1:23:A:VAL:H     | 19       | 0.12          |
| (1,1804) | 1:20:A:ILE:HG22 | 1:23:A:VAL:H     | 19       | 0.12          |
| (1,1804) | 1:20:A:ILE:HG23 | 1:23:A:VAL:H     | 19       | 0.12          |
| (1,1763) | 1:30:A:ARG:HG2  | 1:49:A:PHE:HB2   | 12       | 0.12          |
| (1,1731) | 1:14:A:ARG:HD3  | 1:146:A:LEU:HB3  | 16       | 0.12          |
| (1,1675) | 1:53:A:LYS:HD2  | 1:77:A:VAL:HG11  | 6        | 0.12          |
| (1,1675) | 1:53:A:LYS:HD2  | 1:77:A:VAL:HG12  | 6        | 0.12          |
| (1,1675) | 1:53:A:LYS:HD2  | 1:77:A:VAL:HG13  | 6        | 0.12          |
| (1,1675) | 1:53:A:LYS:HD3  | 1:77:A:VAL:HG11  | 6        | 0.12          |
| (1,1675) | 1:53:A:LYS:HD3  | 1:77:A:VAL:HG12  | 6        | 0.12          |
| (1,1675) | 1:53:A:LYS:HD3  | 1:77:A:VAL:HG13  | 6        | 0.12          |
| (1,1554) | 1:6:A:LYS:HE2   | 1:9:A:LYS:HD3    | 4        | 0.12          |
| (1,1554) | 1:6:A:LYS:HE3   | 1:9:A:LYS:HD3    | 4        | 0.12          |
| (1,1554) | 1:6:A:LYS:HE2   | 1:9:A:LYS:HD3    | 9        | 0.12          |
| (1,1554) | 1:6:A:LYS:HE3   | 1:9:A:LYS:HD3    | 9        | 0.12          |
| (1,1546) | 1:22:A:LYS:HG3  | 1:23:A:VAL:HB    | 10       | 0.12          |
| (1,1402) | 1:3:A:ILE:HG12  | 1:139:A:GLU:HA   | 15       | 0.12          |
| (1,1399) | 1:20:A:ILE:HD11 | 1:81:A:TYR:HD1   | 3        | 0.12          |
| (1,1399) | 1:20:A:ILE:HD11 | 1:81:A:TYR:HD2   | 3        | 0.12          |
| (1,1399) | 1:20:A:ILE:HD12 | 1:81:A:TYR:HD1   | 3        | 0.12          |
| (1,1399) | 1:20:A:ILE:HD12 | 1:81:A:TYR:HD2   | 3        | 0.12          |
| (1,1399) | 1:20:A:ILE:HD13 | 1:81:A:TYR:HD1   | 3        | 0.12          |
| (1,1399) | 1:20:A:ILE:HD13 | 1:81:A:TYR:HD2   | 3        | 0.12          |
| (1,1394) | 1:3:A:ILE:HG21  | 1:4:A:GLU:HA     | 3        | 0.12          |
| (1,1394) | 1:3:A:ILE:HG22  | 1:4:A:GLU:HA     | 3        | 0.12          |
| (1,1394) | 1:3:A:ILE:HG23  | 1:4:A:GLU:HA     | 3        | 0.12          |
| (1,1394) | 1:3:A:ILE:HG21  | 1:4:A:GLU:HA     | 10       | 0.12          |
| (1,1394) | 1:3:A:ILE:HG22  | 1:4:A:GLU:HA     | 10       | 0.12          |
| (1,1394) | 1:3:A:ILE:HG23  | 1:4:A:GLU:HA     | 10       | 0.12          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1394) | 1:3:A:ILE:HG21   | 1:4:A:GLU:HA     | 13       | 0.12          |
| (1,1394) | 1:3:A:ILE:HG22   | 1:4:A:GLU:HA     | 13       | 0.12          |
| (1,1394) | 1:3:A:ILE:HG23   | 1:4:A:GLU:HA     | 13       | 0.12          |
| (1,1394) | 1:3:A:ILE:HG21   | 1:4:A:GLU:HA     | 14       | 0.12          |
| (1,1394) | 1:3:A:ILE:HG22   | 1:4:A:GLU:HA     | 14       | 0.12          |
| (1,1394) | 1:3:A:ILE:HG23   | 1:4:A:GLU:HA     | 14       | 0.12          |
| (1,1382) | 1:117:A:THR:HG21 | 1:119:A:THR:H    | 9        | 0.12          |
| (1,1382) | 1:117:A:THR:HG22 | 1:119:A:THR:H    | 9        | 0.12          |
| (1,1382) | 1:117:A:THR:HG23 | 1:119:A:THR:H    | 9        | 0.12          |
| (1,1358) | 1:44:A:VAL:H     | 1:62:A:GLN:HB2   | 19       | 0.12          |
| (1,1163) | 1:149:A:LEU:H    | 1:153:A:LEU:HD11 | 12       | 0.12          |
| (1,1163) | 1:149:A:LEU:H    | 1:153:A:LEU:HD12 | 12       | 0.12          |
| (1,1163) | 1:149:A:LEU:H    | 1:153:A:LEU:HD13 | 12       | 0.12          |
| (1,1163) | 1:149:A:LEU:H    | 1:153:A:LEU:HD11 | 13       | 0.12          |
| (1,1163) | 1:149:A:LEU:H    | 1:153:A:LEU:HD12 | 13       | 0.12          |
| (1,1163) | 1:149:A:LEU:H    | 1:153:A:LEU:HD13 | 13       | 0.12          |
| (1,1140) | 1:147:A:ASN:HB2  | 1:148:A:GLN:HE21 | 13       | 0.12          |
| (1,1136) | 1:144:A:SER:HA   | 1:147:A:ASN:HD22 | 1        | 0.12          |
| (1,1019) | 1:124:A:PHE:HB2  | 1:131:A:GLN:H    | 13       | 0.12          |
| (1,999)  | 1:126:A:THR:HA   | 1:130:A:ALA:H    | 10       | 0.12          |
| (1,999)  | 1:126:A:THR:HA   | 1:130:A:ALA:H    | 13       | 0.12          |
| (1,980)  | 1:9:A:LYS:HB2    | 1:122:A:SER:H    | 10       | 0.12          |
| (1,937)  | 1:117:A:THR:H    | 1:118:A:VAL:HB   | 1        | 0.12          |
| (1,937)  | 1:117:A:THR:H    | 1:118:A:VAL:HB   | 3        | 0.12          |
| (1,937)  | 1:117:A:THR:H    | 1:118:A:VAL:HB   | 13       | 0.12          |
| (1,830)  | 1:99:A:SER:H     | 1:100:A:MET:HG2  | 12       | 0.12          |
| (1,703)  | 1:79:A:ALA:HA    | 1:81:A:TYR:H     | 11       | 0.12          |
| (1,378)  | 1:39:A:PRO:HG2   | 1:43:A:SER:H     | 12       | 0.12          |
| (1,378)  | 1:39:A:PRO:HG3   | 1:43:A:SER:H     | 12       | 0.12          |
| (2,801)  | 1:96:A:LYS:HD3   | 1:97:A:ASP:HA    | 10       | 0.11          |
| (2,801)  | 1:96:A:LYS:HD3   | 1:97:A:ASP:HA    | 12       | 0.11          |
| (2,684)  | 1:30:A:ARG:HG2   | 1:34:A:GLU:HG3   | 14       | 0.11          |
| (2,676)  | 1:32:A:LEU:HD11  | 1:149:A:LEU:HD21 | 12       | 0.11          |
| (2,676)  | 1:32:A:LEU:HD11  | 1:149:A:LEU:HD22 | 12       | 0.11          |
| (2,676)  | 1:32:A:LEU:HD11  | 1:149:A:LEU:HD23 | 12       | 0.11          |
| (2,676)  | 1:32:A:LEU:HD12  | 1:149:A:LEU:HD21 | 12       | 0.11          |
| (2,676)  | 1:32:A:LEU:HD12  | 1:149:A:LEU:HD22 | 12       | 0.11          |
| (2,676)  | 1:32:A:LEU:HD12  | 1:149:A:LEU:HD23 | 12       | 0.11          |
| (2,676)  | 1:32:A:LEU:HD13  | 1:149:A:LEU:HD21 | 12       | 0.11          |
| (2,676)  | 1:32:A:LEU:HD13  | 1:149:A:LEU:HD22 | 12       | 0.11          |
| (2,676)  | 1:32:A:LEU:HD13  | 1:149:A:LEU:HD23 | 12       | 0.11          |
| (2,676)  | 1:32:A:LEU:HD11  | 1:149:A:LEU:HD21 | 13       | 0.11          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,676)  | 1:32:A:LEU:HD11  | 1:149:A:LEU:HD22 | 13       | 0.11          |
| (2,676)  | 1:32:A:LEU:HD11  | 1:149:A:LEU:HD23 | 13       | 0.11          |
| (2,676)  | 1:32:A:LEU:HD12  | 1:149:A:LEU:HD21 | 13       | 0.11          |
| (2,676)  | 1:32:A:LEU:HD12  | 1:149:A:LEU:HD22 | 13       | 0.11          |
| (2,676)  | 1:32:A:LEU:HD12  | 1:149:A:LEU:HD23 | 13       | 0.11          |
| (2,676)  | 1:32:A:LEU:HD13  | 1:149:A:LEU:HD21 | 13       | 0.11          |
| (2,676)  | 1:32:A:LEU:HD13  | 1:149:A:LEU:HD22 | 13       | 0.11          |
| (2,676)  | 1:32:A:LEU:HD13  | 1:149:A:LEU:HD23 | 13       | 0.11          |
| (2,612)  | 1:7:A:LYS:HB2    | 1:8:A:ASN:HD21   | 16       | 0.11          |
| (2,449)  | 1:154:A:ASN:HA   | 1:157:A:LEU:HG   | 1        | 0.11          |
| (2,449)  | 1:154:A:ASN:HA   | 1:157:A:LEU:HG   | 19       | 0.11          |
| (1,4410) | 1:79:A:ALA:HA    | 1:81:A:TYR:HD1   | 18       | 0.11          |
| (1,4410) | 1:79:A:ALA:HA    | 1:81:A:TYR:HD2   | 18       | 0.11          |
| (1,4401) | 1:82:A:TYR:HE1   | 1:108:A:ASN:HB2  | 8        | 0.11          |
| (1,4401) | 1:82:A:TYR:HE2   | 1:108:A:ASN:HB2  | 8        | 0.11          |
| (1,4362) | 1:68:A:SER:HA    | 1:69:A:TYR:HE1   | 8        | 0.11          |
| (1,4362) | 1:68:A:SER:HA    | 1:69:A:TYR:HE2   | 8        | 0.11          |
| (1,4300) | 1:38:A:HIS:HD2   | 1:44:A:VAL:HG21  | 10       | 0.11          |
| (1,4300) | 1:38:A:HIS:HD2   | 1:44:A:VAL:HG22  | 10       | 0.11          |
| (1,4300) | 1:38:A:HIS:HD2   | 1:44:A:VAL:HG23  | 10       | 0.11          |
| (1,4300) | 1:38:A:HIS:HD2   | 1:44:A:VAL:HG21  | 17       | 0.11          |
| (1,4300) | 1:38:A:HIS:HD2   | 1:44:A:VAL:HG22  | 17       | 0.11          |
| (1,4300) | 1:38:A:HIS:HD2   | 1:44:A:VAL:HG23  | 17       | 0.11          |
| (1,4229) | 1:152:A:LEU:HD11 | 1:153:A:LEU:HD11 | 15       | 0.11          |
| (1,4229) | 1:152:A:LEU:HD11 | 1:153:A:LEU:HD12 | 15       | 0.11          |
| (1,4229) | 1:152:A:LEU:HD11 | 1:153:A:LEU:HD13 | 15       | 0.11          |
| (1,4229) | 1:152:A:LEU:HD12 | 1:153:A:LEU:HD11 | 15       | 0.11          |
| (1,4229) | 1:152:A:LEU:HD12 | 1:153:A:LEU:HD12 | 15       | 0.11          |
| (1,4229) | 1:152:A:LEU:HD12 | 1:153:A:LEU:HD13 | 15       | 0.11          |
| (1,4229) | 1:152:A:LEU:HD13 | 1:153:A:LEU:HD11 | 15       | 0.11          |
| (1,4229) | 1:152:A:LEU:HD13 | 1:153:A:LEU:HD12 | 15       | 0.11          |
| (1,4229) | 1:152:A:LEU:HD13 | 1:153:A:LEU:HD13 | 15       | 0.11          |
| (1,4202) | 1:125:A:PRO:HB3  | 1:126:A:THR:HG21 | 8        | 0.11          |
| (1,4202) | 1:125:A:PRO:HB3  | 1:126:A:THR:HG22 | 8        | 0.11          |
| (1,4202) | 1:125:A:PRO:HB3  | 1:126:A:THR:HG23 | 8        | 0.11          |
| (1,4196) | 1:8:A:ASN:HB2    | 1:125:A:PRO:HD2  | 17       | 0.11          |
| (1,4112) | 1:67:A:ILE:H     | 1:68:A:SER:HA    | 10       | 0.11          |
| (1,4098) | 1:62:A:GLN:HB2   | 1:67:A:ILE:HD11  | 4        | 0.11          |
| (1,4098) | 1:62:A:GLN:HB2   | 1:67:A:ILE:HD12  | 4        | 0.11          |
| (1,4098) | 1:62:A:GLN:HB2   | 1:67:A:ILE:HD13  | 4        | 0.11          |
| (1,4036) | 1:30:A:ARG:HA    | 1:49:A:PHE:HB3   | 20       | 0.11          |
| (1,3797) | 1:34:A:GLU:HG2   | 1:35:A:GLN:HA    | 7        | 0.11          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3797) | 1:34:A:GLU:HG2  | 1:35:A:GLN:HA    | 8        | 0.11          |
| (1,3797) | 1:34:A:GLU:HG2  | 1:35:A:GLN:HA    | 13       | 0.11          |
| (1,3659) | 1:151:A:LYS:HB2 | 1:157:A:LEU:HB3  | 15       | 0.11          |
| (1,3659) | 1:151:A:LYS:HB3 | 1:157:A:LEU:HB3  | 15       | 0.11          |
| (1,3433) | 1:5:A:LYS:HB2   | 1:134:A:ILE:HD11 | 1        | 0.11          |
| (1,3433) | 1:5:A:LYS:HB2   | 1:134:A:ILE:HD12 | 1        | 0.11          |
| (1,3433) | 1:5:A:LYS:HB2   | 1:134:A:ILE:HD13 | 1        | 0.11          |
| (1,3433) | 1:5:A:LYS:HB2   | 1:134:A:ILE:HD11 | 5        | 0.11          |
| (1,3433) | 1:5:A:LYS:HB2   | 1:134:A:ILE:HD12 | 5        | 0.11          |
| (1,3433) | 1:5:A:LYS:HB2   | 1:134:A:ILE:HD13 | 5        | 0.11          |
| (1,3272) | 1:107:A:LEU:HB3 | 1:120:A:SER:HB2  | 18       | 0.11          |
| (1,3155) | 1:83:A:ILE:HG21 | 1:106:A:THR:HG21 | 8        | 0.11          |
| (1,3155) | 1:83:A:ILE:HG21 | 1:106:A:THR:HG22 | 8        | 0.11          |
| (1,3155) | 1:83:A:ILE:HG21 | 1:106:A:THR:HG23 | 8        | 0.11          |
| (1,3155) | 1:83:A:ILE:HG22 | 1:106:A:THR:HG21 | 8        | 0.11          |
| (1,3155) | 1:83:A:ILE:HG22 | 1:106:A:THR:HG22 | 8        | 0.11          |
| (1,3155) | 1:83:A:ILE:HG22 | 1:106:A:THR:HG23 | 8        | 0.11          |
| (1,3155) | 1:83:A:ILE:HG23 | 1:106:A:THR:HG21 | 8        | 0.11          |
| (1,3155) | 1:83:A:ILE:HG23 | 1:106:A:THR:HG22 | 8        | 0.11          |
| (1,3155) | 1:83:A:ILE:HG23 | 1:106:A:THR:HG23 | 8        | 0.11          |
| (1,3155) | 1:83:A:ILE:HG21 | 1:106:A:THR:HG21 | 14       | 0.11          |
| (1,3155) | 1:83:A:ILE:HG21 | 1:106:A:THR:HG22 | 14       | 0.11          |
| (1,3155) | 1:83:A:ILE:HG21 | 1:106:A:THR:HG23 | 14       | 0.11          |
| (1,3155) | 1:83:A:ILE:HG22 | 1:106:A:THR:HG21 | 14       | 0.11          |
| (1,3155) | 1:83:A:ILE:HG22 | 1:106:A:THR:HG22 | 14       | 0.11          |
| (1,3155) | 1:83:A:ILE:HG22 | 1:106:A:THR:HG23 | 14       | 0.11          |
| (1,3155) | 1:83:A:ILE:HG23 | 1:106:A:THR:HG21 | 14       | 0.11          |
| (1,3155) | 1:83:A:ILE:HG23 | 1:106:A:THR:HG22 | 14       | 0.11          |
| (1,3155) | 1:83:A:ILE:HG23 | 1:106:A:THR:HG23 | 14       | 0.11          |
| (1,3047) | 1:142:A:MET:HA  | 1:142:A:MET:HE1  | 2        | 0.11          |
| (1,3047) | 1:142:A:MET:HA  | 1:142:A:MET:HE2  | 2        | 0.11          |
| (1,3047) | 1:142:A:MET:HA  | 1:142:A:MET:HE3  | 2        | 0.11          |
| (1,3008) | 1:95:A:GLU:HB2  | 1:96:A:LYS:HB2   | 6        | 0.11          |
| (1,3008) | 1:95:A:GLU:HB2  | 1:96:A:LYS:HB3   | 6        | 0.11          |
| (1,2930) | 1:71:A:ILE:HD11 | 1:91:A:THR:HG21  | 10       | 0.11          |
| (1,2930) | 1:71:A:ILE:HD11 | 1:91:A:THR:HG22  | 10       | 0.11          |
| (1,2930) | 1:71:A:ILE:HD11 | 1:91:A:THR:HG23  | 10       | 0.11          |
| (1,2930) | 1:71:A:ILE:HD12 | 1:91:A:THR:HG21  | 10       | 0.11          |
| (1,2930) | 1:71:A:ILE:HD12 | 1:91:A:THR:HG22  | 10       | 0.11          |
| (1,2930) | 1:71:A:ILE:HD12 | 1:91:A:THR:HG23  | 10       | 0.11          |
| (1,2930) | 1:71:A:ILE:HD13 | 1:91:A:THR:HG21  | 10       | 0.11          |
| (1,2930) | 1:71:A:ILE:HD13 | 1:91:A:THR:HG22  | 10       | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2930) | 1:71:A:ILE:HD13 | 1:91:A:THR:HG23 | 10       | 0.11          |
| (1,2911) | 1:89:A:PHE:HB2  | 1:97:A:ASP:HB2  | 10       | 0.11          |
| (1,2911) | 1:89:A:PHE:HB2  | 1:97:A:ASP:HB2  | 13       | 0.11          |
| (1,2889) | 1:87:A:ASP:HB2  | 1:103:A:MET:HB2 | 14       | 0.11          |
| (1,2889) | 1:87:A:ASP:HB2  | 1:103:A:MET:HB2 | 17       | 0.11          |
| (1,2667) | 1:70:A:THR:H    | 1:71:A:ILE:HD11 | 1        | 0.11          |
| (1,2667) | 1:70:A:THR:H    | 1:71:A:ILE:HD12 | 1        | 0.11          |
| (1,2667) | 1:70:A:THR:H    | 1:71:A:ILE:HD13 | 1        | 0.11          |
| (1,2529) | 1:100:A:MET:HG3 | 1:101:A:PRO:HD3 | 17       | 0.11          |
| (1,2134) | 1:36:A:TRP:HH2  | 1:37:A:PHE:HA   | 5        | 0.11          |
| (1,2134) | 1:36:A:TRP:HH2  | 1:37:A:PHE:HA   | 10       | 0.11          |
| (1,2042) | 1:31:A:GLU:HG3  | 1:32:A:LEU:HA   | 5        | 0.11          |
| (1,1972) | 1:27:A:TYR:HB3  | 1:28:A:THR:HG21 | 3        | 0.11          |
| (1,1972) | 1:27:A:TYR:HB3  | 1:28:A:THR:HG22 | 3        | 0.11          |
| (1,1972) | 1:27:A:TYR:HB3  | 1:28:A:THR:HG23 | 3        | 0.11          |
| (1,1832) | 1:35:A:GLN:HB3  | 1:152:A:LEU:HA  | 15       | 0.11          |
| (1,1804) | 1:20:A:ILE:HG21 | 1:23:A:VAL:H    | 5        | 0.11          |
| (1,1804) | 1:20:A:ILE:HG22 | 1:23:A:VAL:H    | 5        | 0.11          |
| (1,1804) | 1:20:A:ILE:HG23 | 1:23:A:VAL:H    | 5        | 0.11          |
| (1,1804) | 1:20:A:ILE:HG21 | 1:23:A:VAL:H    | 7        | 0.11          |
| (1,1804) | 1:20:A:ILE:HG22 | 1:23:A:VAL:H    | 7        | 0.11          |
| (1,1804) | 1:20:A:ILE:HG23 | 1:23:A:VAL:H    | 7        | 0.11          |
| (1,1772) | 1:18:A:ALA:HB1  | 1:22:A:LYS:HB3  | 2        | 0.11          |
| (1,1772) | 1:18:A:ALA:HB2  | 1:22:A:LYS:HB3  | 2        | 0.11          |
| (1,1772) | 1:18:A:ALA:HB3  | 1:22:A:LYS:HB3  | 2        | 0.11          |
| (1,1772) | 1:18:A:ALA:HB1  | 1:22:A:LYS:HB3  | 12       | 0.11          |
| (1,1772) | 1:18:A:ALA:HB2  | 1:22:A:LYS:HB3  | 12       | 0.11          |
| (1,1772) | 1:18:A:ALA:HB3  | 1:22:A:LYS:HB3  | 12       | 0.11          |
| (1,1676) | 1:13:A:THR:HG21 | 1:14:A:ARG:HB2  | 12       | 0.11          |
| (1,1676) | 1:13:A:THR:HG22 | 1:14:A:ARG:HB2  | 12       | 0.11          |
| (1,1676) | 1:13:A:THR:HG23 | 1:14:A:ARG:HB2  | 12       | 0.11          |
| (1,1675) | 1:53:A:LYS:HD2  | 1:77:A:VAL:HG11 | 11       | 0.11          |
| (1,1675) | 1:53:A:LYS:HD2  | 1:77:A:VAL:HG12 | 11       | 0.11          |
| (1,1675) | 1:53:A:LYS:HD2  | 1:77:A:VAL:HG13 | 11       | 0.11          |
| (1,1675) | 1:53:A:LYS:HD3  | 1:77:A:VAL:HG11 | 11       | 0.11          |
| (1,1675) | 1:53:A:LYS:HD3  | 1:77:A:VAL:HG12 | 11       | 0.11          |
| (1,1675) | 1:53:A:LYS:HD3  | 1:77:A:VAL:HG13 | 11       | 0.11          |
| (1,1636) | 1:3:A:ILE:HA    | 1:12:A:PHE:HA   | 11       | 0.11          |
| (1,1554) | 1:6:A:LYS:HE2   | 1:9:A:LYS:HD3   | 18       | 0.11          |
| (1,1554) | 1:6:A:LYS:HE3   | 1:9:A:LYS:HD3   | 18       | 0.11          |
| (1,1546) | 1:22:A:LYS:HG3  | 1:23:A:VAL:HB   | 17       | 0.11          |
| (1,1542) | 1:6:A:LYS:HG2   | 1:9:A:LYS:HE2   | 13       | 0.11          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1542) | 1:6:A:LYS:HG2    | 1:9:A:LYS:HE3    | 13       | 0.11          |
| (1,1542) | 1:6:A:LYS:HG3    | 1:9:A:LYS:HE2    | 13       | 0.11          |
| (1,1542) | 1:6:A:LYS:HG3    | 1:9:A:LYS:HE3    | 13       | 0.11          |
| (1,1542) | 1:6:A:LYS:HG2    | 1:9:A:LYS:HE2    | 17       | 0.11          |
| (1,1542) | 1:6:A:LYS:HG2    | 1:9:A:LYS:HE3    | 17       | 0.11          |
| (1,1542) | 1:6:A:LYS:HG3    | 1:9:A:LYS:HE2    | 17       | 0.11          |
| (1,1542) | 1:6:A:LYS:HG3    | 1:9:A:LYS:HE3    | 17       | 0.11          |
| (1,1399) | 1:20:A:ILE:HD11  | 1:81:A:TYR:HD1   | 5        | 0.11          |
| (1,1399) | 1:20:A:ILE:HD11  | 1:81:A:TYR:HD2   | 5        | 0.11          |
| (1,1399) | 1:20:A:ILE:HD12  | 1:81:A:TYR:HD1   | 5        | 0.11          |
| (1,1399) | 1:20:A:ILE:HD12  | 1:81:A:TYR:HD2   | 5        | 0.11          |
| (1,1399) | 1:20:A:ILE:HD13  | 1:81:A:TYR:HD1   | 5        | 0.11          |
| (1,1399) | 1:20:A:ILE:HD13  | 1:81:A:TYR:HD2   | 5        | 0.11          |
| (1,1394) | 1:3:A:ILE:HG21   | 1:4:A:GLU:HA     | 16       | 0.11          |
| (1,1394) | 1:3:A:ILE:HG22   | 1:4:A:GLU:HA     | 16       | 0.11          |
| (1,1394) | 1:3:A:ILE:HG23   | 1:4:A:GLU:HA     | 16       | 0.11          |
| (1,1382) | 1:117:A:THR:HG21 | 1:119:A:THR:H    | 18       | 0.11          |
| (1,1382) | 1:117:A:THR:HG22 | 1:119:A:THR:H    | 18       | 0.11          |
| (1,1382) | 1:117:A:THR:HG23 | 1:119:A:THR:H    | 18       | 0.11          |
| (1,1382) | 1:117:A:THR:HG21 | 1:119:A:THR:H    | 19       | 0.11          |
| (1,1382) | 1:117:A:THR:HG22 | 1:119:A:THR:H    | 19       | 0.11          |
| (1,1382) | 1:117:A:THR:HG23 | 1:119:A:THR:H    | 19       | 0.11          |
| (1,1257) | 1:126:A:THR:H    | 1:129:A:ALA:HB1  | 16       | 0.11          |
| (1,1257) | 1:126:A:THR:H    | 1:129:A:ALA:HB2  | 16       | 0.11          |
| (1,1257) | 1:126:A:THR:H    | 1:129:A:ALA:HB3  | 16       | 0.11          |
| (1,1163) | 1:149:A:LEU:H    | 1:153:A:LEU:HD11 | 7        | 0.11          |
| (1,1163) | 1:149:A:LEU:H    | 1:153:A:LEU:HD12 | 7        | 0.11          |
| (1,1163) | 1:149:A:LEU:H    | 1:153:A:LEU:HD13 | 7        | 0.11          |
| (1,1163) | 1:149:A:LEU:H    | 1:153:A:LEU:HD11 | 10       | 0.11          |
| (1,1163) | 1:149:A:LEU:H    | 1:153:A:LEU:HD12 | 10       | 0.11          |
| (1,1163) | 1:149:A:LEU:H    | 1:153:A:LEU:HD13 | 10       | 0.11          |
| (1,1023) | 1:131:A:GLN:H    | 1:134:A:ILE:HG12 | 13       | 0.11          |
| (1,1019) | 1:124:A:PHE:HB2  | 1:131:A:GLN:H    | 17       | 0.11          |
| (1,999)  | 1:126:A:THR:HA   | 1:130:A:ALA:H    | 3        | 0.11          |
| (1,937)  | 1:117:A:THR:H    | 1:118:A:VAL:HB   | 6        | 0.11          |
| (1,908)  | 1:114:A:GLY:H    | 1:115:A:LYS:HB2  | 16       | 0.11          |
| (1,703)  | 1:79:A:ALA:HA    | 1:81:A:TYR:H     | 6        | 0.11          |
| (1,506)  | 1:52:A:THR:HG21  | 1:56:A:SER:H     | 7        | 0.11          |
| (1,506)  | 1:52:A:THR:HG22  | 1:56:A:SER:H     | 7        | 0.11          |
| (1,506)  | 1:52:A:THR:HG23  | 1:56:A:SER:H     | 7        | 0.11          |
| (1,486)  | 1:53:A:LYS:HD2   | 1:54:A:GLY:H     | 20       | 0.11          |
| (1,486)  | 1:53:A:LYS:HD3   | 1:54:A:GLY:H     | 20       | 0.11          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,378)  | 1:39:A:PRO:HG2   | 1:43:A:SER:H     | 10       | 0.11          |
| (1,378)  | 1:39:A:PRO:HG3   | 1:43:A:SER:H     | 10       | 0.11          |
| (1,289)  | 1:34:A:GLU:H     | 1:49:A:PHE:HE1   | 7        | 0.11          |
| (1,289)  | 1:34:A:GLU:H     | 1:49:A:PHE:HE2   | 7        | 0.11          |
| (1,289)  | 1:34:A:GLU:H     | 1:49:A:PHE:HE1   | 13       | 0.11          |
| (1,289)  | 1:34:A:GLU:H     | 1:49:A:PHE:HE2   | 13       | 0.11          |
| (1,226)  | 1:27:A:TYR:H     | 1:28:A:THR:HG21  | 19       | 0.11          |
| (1,226)  | 1:27:A:TYR:H     | 1:28:A:THR:HG22  | 19       | 0.11          |
| (1,226)  | 1:27:A:TYR:H     | 1:28:A:THR:HG23  | 19       | 0.11          |
| (1,195)  | 1:108:A:ASN:H    | 1:118:A:VAL:HG21 | 17       | 0.11          |
| (1,195)  | 1:108:A:ASN:H    | 1:118:A:VAL:HG22 | 17       | 0.11          |
| (1,195)  | 1:108:A:ASN:H    | 1:118:A:VAL:HG23 | 17       | 0.11          |
| (1,150)  | 1:21:A:ASN:H     | 1:23:A:VAL:HB    | 10       | 0.11          |
| (1,150)  | 1:21:A:ASN:H     | 1:23:A:VAL:HB    | 11       | 0.11          |
| (1,150)  | 1:21:A:ASN:H     | 1:23:A:VAL:HB    | 16       | 0.11          |
| (2,273)  | 1:11:A:ILE:HB    | 1:13:A:THR:HG21  | 12       | 0.1           |
| (2,273)  | 1:11:A:ILE:HB    | 1:13:A:THR:HG22  | 12       | 0.1           |
| (2,273)  | 1:11:A:ILE:HB    | 1:13:A:THR:HG23  | 12       | 0.1           |
| (1,4362) | 1:68:A:SER:HA    | 1:69:A:TYR:HE1   | 4        | 0.1           |
| (1,4362) | 1:68:A:SER:HA    | 1:69:A:TYR:HE2   | 4        | 0.1           |
| (1,4202) | 1:125:A:PRO:HB3  | 1:126:A:THR:HG21 | 13       | 0.1           |
| (1,4202) | 1:125:A:PRO:HB3  | 1:126:A:THR:HG22 | 13       | 0.1           |
| (1,4202) | 1:125:A:PRO:HB3  | 1:126:A:THR:HG23 | 13       | 0.1           |
| (1,4112) | 1:67:A:ILE:H     | 1:68:A:SER:HA    | 20       | 0.1           |
| (1,3962) | 1:4:A:GLU:HA     | 1:5:A:LYS:HB3    | 5        | 0.1           |
| (1,3272) | 1:107:A:LEU:HB3  | 1:120:A:SER:HB2  | 7        | 0.1           |
| (1,3249) | 1:118:A:VAL:HG11 | 1:119:A:THR:HB   | 4        | 0.1           |
| (1,3249) | 1:118:A:VAL:HG12 | 1:119:A:THR:HB   | 4        | 0.1           |
| (1,3249) | 1:118:A:VAL:HG13 | 1:119:A:THR:HB   | 4        | 0.1           |
| (1,3155) | 1:83:A:ILE:HG21  | 1:106:A:THR:HG21 | 10       | 0.1           |
| (1,3155) | 1:83:A:ILE:HG21  | 1:106:A:THR:HG22 | 10       | 0.1           |
| (1,3155) | 1:83:A:ILE:HG21  | 1:106:A:THR:HG23 | 10       | 0.1           |
| (1,3155) | 1:83:A:ILE:HG22  | 1:106:A:THR:HG21 | 10       | 0.1           |
| (1,3155) | 1:83:A:ILE:HG22  | 1:106:A:THR:HG22 | 10       | 0.1           |
| (1,3155) | 1:83:A:ILE:HG22  | 1:106:A:THR:HG23 | 10       | 0.1           |
| (1,3155) | 1:83:A:ILE:HG23  | 1:106:A:THR:HG21 | 10       | 0.1           |
| (1,3155) | 1:83:A:ILE:HG23  | 1:106:A:THR:HG22 | 10       | 0.1           |
| (1,3155) | 1:83:A:ILE:HG23  | 1:106:A:THR:HG23 | 10       | 0.1           |
| (1,3075) | 1:103:A:MET:HG2  | 1:105:A:ILE:HG13 | 12       | 0.1           |
| (1,3053) | 1:10:A:ILE:HD11  | 1:142:A:MET:HE1  | 19       | 0.1           |
| (1,3053) | 1:10:A:ILE:HD11  | 1:142:A:MET:HE2  | 19       | 0.1           |
| (1,3053) | 1:10:A:ILE:HD11  | 1:142:A:MET:HE3  | 19       | 0.1           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3053) | 1:10:A:ILE:HD12 | 1:142:A:MET:HE1 | 19       | 0.1           |
| (1,3053) | 1:10:A:ILE:HD12 | 1:142:A:MET:HE2 | 19       | 0.1           |
| (1,3053) | 1:10:A:ILE:HD12 | 1:142:A:MET:HE3 | 19       | 0.1           |
| (1,3053) | 1:10:A:ILE:HD13 | 1:142:A:MET:HE1 | 19       | 0.1           |
| (1,3053) | 1:10:A:ILE:HD13 | 1:142:A:MET:HE2 | 19       | 0.1           |
| (1,3053) | 1:10:A:ILE:HD13 | 1:142:A:MET:HE3 | 19       | 0.1           |
| (1,3008) | 1:95:A:GLU:HB2  | 1:96:A:LYS:HB2  | 17       | 0.1           |
| (1,3008) | 1:95:A:GLU:HB2  | 1:96:A:LYS:HB3  | 17       | 0.1           |
| (1,2999) | 1:88:A:TYR:HE1  | 1:96:A:LYS:HE2  | 5        | 0.1           |
| (1,2999) | 1:88:A:TYR:HE2  | 1:96:A:LYS:HE2  | 5        | 0.1           |
| (1,2930) | 1:71:A:ILE:HD11 | 1:91:A:THR:HG21 | 9        | 0.1           |
| (1,2930) | 1:71:A:ILE:HD11 | 1:91:A:THR:HG22 | 9        | 0.1           |
| (1,2930) | 1:71:A:ILE:HD11 | 1:91:A:THR:HG23 | 9        | 0.1           |
| (1,2930) | 1:71:A:ILE:HD12 | 1:91:A:THR:HG21 | 9        | 0.1           |
| (1,2930) | 1:71:A:ILE:HD12 | 1:91:A:THR:HG22 | 9        | 0.1           |
| (1,2930) | 1:71:A:ILE:HD12 | 1:91:A:THR:HG23 | 9        | 0.1           |
| (1,2930) | 1:71:A:ILE:HD13 | 1:91:A:THR:HG21 | 9        | 0.1           |
| (1,2930) | 1:71:A:ILE:HD13 | 1:91:A:THR:HG22 | 9        | 0.1           |
| (1,2930) | 1:71:A:ILE:HD13 | 1:91:A:THR:HG23 | 9        | 0.1           |
| (1,2739) | 1:53:A:LYS:HD2  | 1:76:A:GLN:HG3  | 13       | 0.1           |
| (1,2739) | 1:53:A:LYS:HD3  | 1:76:A:GLN:HG3  | 13       | 0.1           |
| (1,2667) | 1:70:A:THR:H    | 1:71:A:ILE:HD11 | 17       | 0.1           |
| (1,2667) | 1:70:A:THR:H    | 1:71:A:ILE:HD12 | 17       | 0.1           |
| (1,2667) | 1:70:A:THR:H    | 1:71:A:ILE:HD13 | 17       | 0.1           |
| (1,2489) | 1:117:A:THR:HA  | 1:118:A:VAL:HB  | 18       | 0.1           |
| (1,2486) | 1:62:A:GLN:HG3  | 1:63:A:ALA:H    | 7        | 0.1           |
| (1,2134) | 1:36:A:TRP:HH2  | 1:37:A:PHE:HA   | 1        | 0.1           |
| (1,2083) | 1:128:A:SER:HB2 | 1:131:A:GLN:HG2 | 19       | 0.1           |
| (1,1979) | 1:28:A:THR:HA   | 1:74:A:TYR:HD1  | 13       | 0.1           |
| (1,1979) | 1:28:A:THR:HA   | 1:74:A:TYR:HD2  | 13       | 0.1           |
| (1,1972) | 1:27:A:TYR:HB3  | 1:28:A:THR:HG21 | 6        | 0.1           |
| (1,1972) | 1:27:A:TYR:HB3  | 1:28:A:THR:HG22 | 6        | 0.1           |
| (1,1972) | 1:27:A:TYR:HB3  | 1:28:A:THR:HG23 | 6        | 0.1           |
| (1,1808) | 1:20:A:ILE:HD11 | 1:80:A:PRO:HB3  | 12       | 0.1           |
| (1,1808) | 1:20:A:ILE:HD12 | 1:80:A:PRO:HB3  | 12       | 0.1           |
| (1,1808) | 1:20:A:ILE:HD13 | 1:80:A:PRO:HB3  | 12       | 0.1           |
| (1,1782) | 1:62:A:GLN:HB2  | 1:67:A:ILE:HG21 | 6        | 0.1           |
| (1,1782) | 1:62:A:GLN:HB2  | 1:67:A:ILE:HG22 | 6        | 0.1           |
| (1,1782) | 1:62:A:GLN:HB2  | 1:67:A:ILE:HG23 | 6        | 0.1           |
| (1,1402) | 1:3:A:ILE:HG12  | 1:139:A:GLU:HA  | 8        | 0.1           |
| (1,1264) | 1:8:A:ASN:HD22  | 1:124:A:PHE:H   | 11       | 0.1           |
| (1,1247) | 1:128:A:SER:HA  | 1:132:A:GLN:H   | 10       | 0.1           |

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| Key      | Atom-1         | Atom-2           | Model ID | Violation (Å) |
|----------|----------------|------------------|----------|---------------|
| (1,1163) | 1:149:A:LEU:H  | 1:153:A:LEU:HD11 | 2        | 0.1           |
| (1,1163) | 1:149:A:LEU:H  | 1:153:A:LEU:HD12 | 2        | 0.1           |
| (1,1163) | 1:149:A:LEU:H  | 1:153:A:LEU:HD13 | 2        | 0.1           |
| (1,1163) | 1:149:A:LEU:H  | 1:153:A:LEU:HD11 | 5        | 0.1           |
| (1,1163) | 1:149:A:LEU:H  | 1:153:A:LEU:HD12 | 5        | 0.1           |
| (1,1163) | 1:149:A:LEU:H  | 1:153:A:LEU:HD13 | 5        | 0.1           |
| (1,463)  | 1:52:A:THR:H   | 1:74:A:TYR:HD1   | 5        | 0.1           |
| (1,463)  | 1:52:A:THR:H   | 1:74:A:TYR:HD2   | 5        | 0.1           |
| (1,395)  | 1:53:A:LYS:HB2 | 1:77:A:VAL:H     | 17       | 0.1           |
| (1,289)  | 1:34:A:GLU:H   | 1:49:A:PHE:HE1   | 6        | 0.1           |
| (1,289)  | 1:34:A:GLU:H   | 1:49:A:PHE:HE2   | 6        | 0.1           |
| (1,270)  | 1:31:A:GLU:HG3 | 1:32:A:LEU:H     | 14       | 0.1           |
| (1,165)  | 1:22:A:LYS:H   | 1:23:A:VAL:HB    | 16       | 0.1           |
| (1,150)  | 1:21:A:ASN:H   | 1:23:A:VAL:HB    | 13       | 0.1           |
| (1,124)  | 1:14:A:ARG:HG3 | 1:15:A:THR:H     | 20       | 0.1           |



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

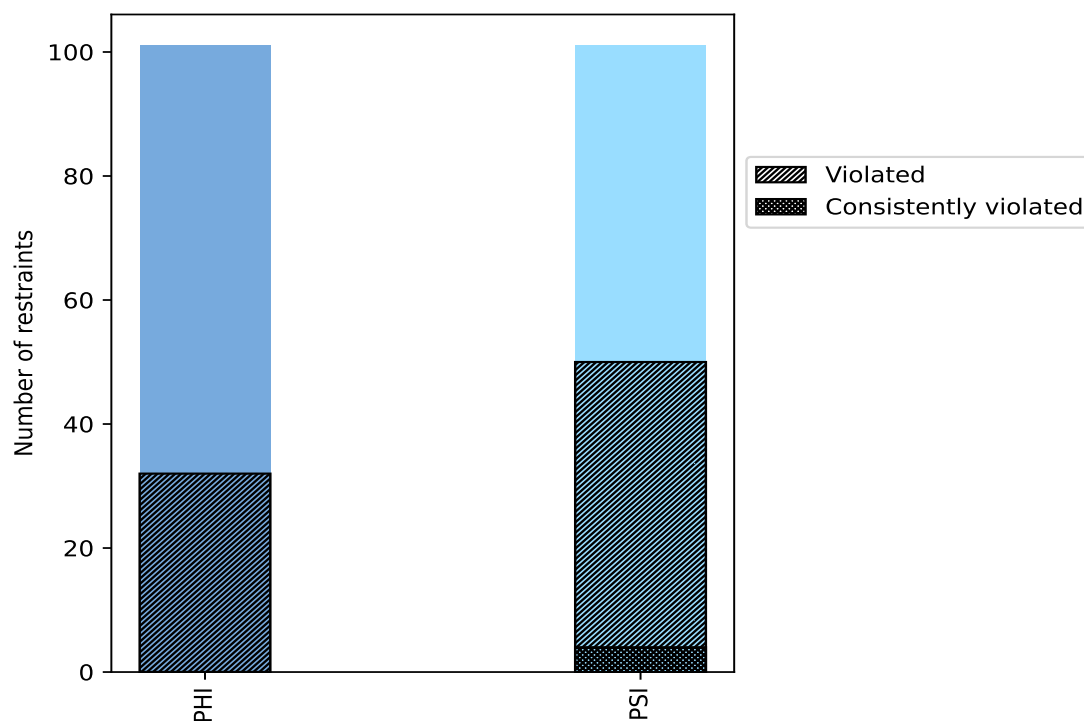
### 10.1 Summary of dihedral-angle violations [i](#)

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

| Angle type | Count | % <sup>1</sup> | Violated <sup>3</sup> |                |                | Consistently Violated <sup>4</sup> |                |                |
|------------|-------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
|            |       |                | Count                 | % <sup>2</sup> | % <sup>1</sup> | Count                              | % <sup>2</sup> | % <sup>1</sup> |
| PHI        | 101   | 50.0           | 32                    | 31.7           | 15.8           | 0                                  | 0.0            | 0.0            |
| PSI        | 101   | 50.0           | 50                    | 49.5           | 24.8           | 4                                  | 4.0            | 2.0            |
| Total      | 202   | 100.0          | 82                    | 40.6           | 40.6           | 4                                  | 2.0            | 2.0            |

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

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



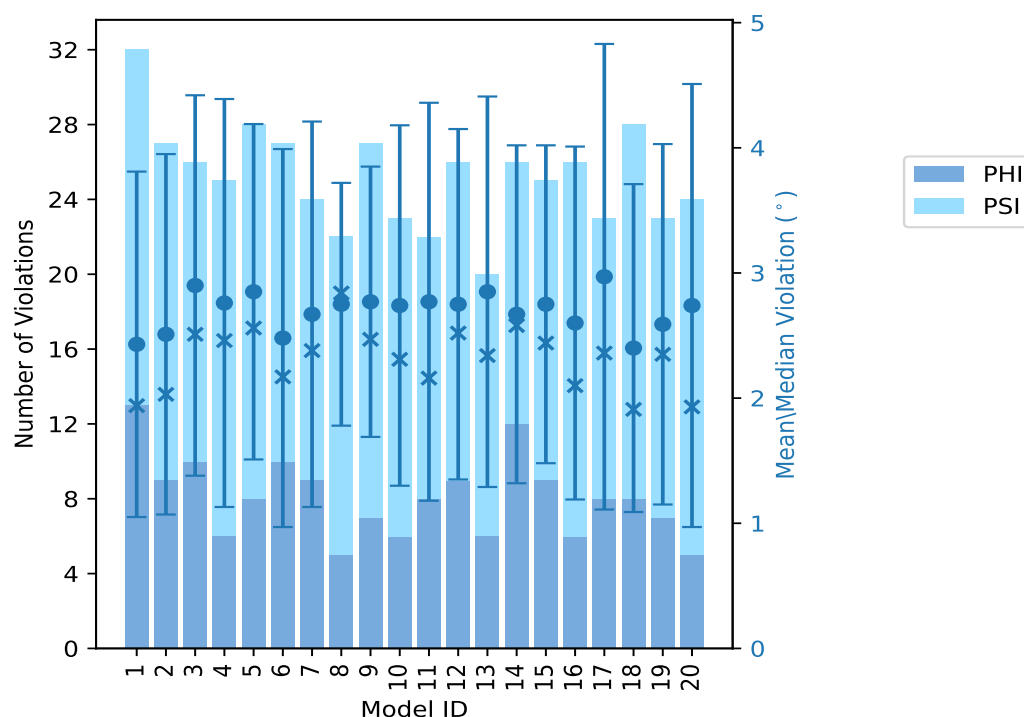
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

## 10.2 Dihedral-angle violation statistics for each model

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

| Model ID | Number of violations |     |       | Mean (°) | Max (°) | SD (°) | Median (°) |
|----------|----------------------|-----|-------|----------|---------|--------|------------|
|          | PHI                  | PSI | Total |          |         |        |            |
| 1        | 13                   | 19  | 32    | 2.43     | 7.32    | 1.38   | 1.94       |
| 2        | 9                    | 18  | 27    | 2.51     | 7.03    | 1.44   | 2.03       |
| 3        | 10                   | 16  | 26    | 2.9      | 6.82    | 1.52   | 2.51       |
| 4        | 6                    | 19  | 25    | 2.76     | 7.03    | 1.63   | 2.46       |
| 5        | 8                    | 20  | 28    | 2.85     | 6.18    | 1.34   | 2.56       |
| 6        | 10                   | 17  | 27    | 2.48     | 8.15    | 1.51   | 2.17       |
| 7        | 9                    | 15  | 24    | 2.67     | 7.86    | 1.54   | 2.38       |
| 8        | 5                    | 17  | 22    | 2.75     | 4.57    | 0.97   | 2.84       |
| 9        | 7                    | 20  | 27    | 2.77     | 5.05    | 1.08   | 2.47       |
| 10       | 6                    | 17  | 23    | 2.74     | 6.43    | 1.44   | 2.31       |
| 11       | 8                    | 14  | 22    | 2.77     | 6.6     | 1.59   | 2.16       |
| 12       | 9                    | 17  | 26    | 2.75     | 6.36    | 1.4    | 2.52       |
| 13       | 6                    | 14  | 20    | 2.85     | 7.31    | 1.56   | 2.34       |
| 14       | 12                   | 14  | 26    | 2.67     | 5.91    | 1.35   | 2.58       |
| 15       | 9                    | 16  | 25    | 2.75     | 6.24    | 1.27   | 2.44       |
| 16       | 6                    | 20  | 26    | 2.6      | 6.74    | 1.41   | 2.1        |
| 17       | 8                    | 15  | 23    | 2.97     | 7.38    | 1.86   | 2.36       |
| 18       | 8                    | 20  | 28    | 2.4      | 6.33    | 1.31   | 1.91       |
| 19       | 7                    | 16  | 23    | 2.59     | 6.56    | 1.44   | 2.35       |
| 20       | 5                    | 19  | 24    | 2.74     | 7.07    | 1.77   | 1.93       |

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



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

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

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

| Number of violated restraints |     |       | Fraction of the ensemble |      |
|-------------------------------|-----|-------|--------------------------|------|
| PHI                           | PSI | Total | Count <sup>1</sup>       | %    |
| 9                             | 11  | 20    | 1                        | 5.0  |
| 2                             | 6   | 8     | 2                        | 10.0 |
| 2                             | 5   | 7     | 3                        | 15.0 |
| 4                             | 4   | 8     | 4                        | 20.0 |
| 2                             | 1   | 3     | 5                        | 25.0 |
| 4                             | 4   | 8     | 6                        | 30.0 |
| 2                             | 2   | 4     | 7                        | 35.0 |
| 1                             | 2   | 3     | 8                        | 40.0 |
| 0                             | 1   | 1     | 9                        | 45.0 |
| 1                             | 1   | 2     | 10                       | 50.0 |
| 3                             | 1   | 4     | 11                       | 55.0 |

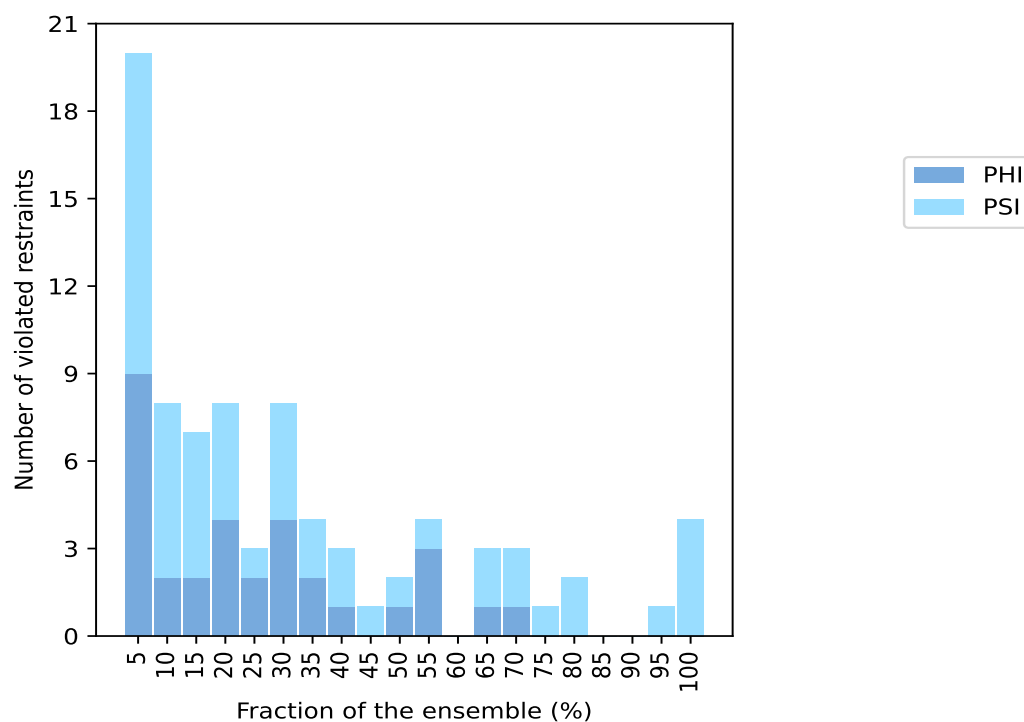
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| Number of violated restraints |     |       | Fraction of the ensemble |       |
|-------------------------------|-----|-------|--------------------------|-------|
| PHI                           | PSI | Total | Count <sup>1</sup>       | %     |
| 0                             | 0   | 0     | 12                       | 60.0  |
| 1                             | 2   | 3     | 13                       | 65.0  |
| 1                             | 2   | 3     | 14                       | 70.0  |
| 0                             | 1   | 1     | 15                       | 75.0  |
| 0                             | 2   | 2     | 16                       | 80.0  |
| 0                             | 0   | 0     | 17                       | 85.0  |
| 0                             | 0   | 0     | 18                       | 90.0  |
| 0                             | 1   | 1     | 19                       | 95.0  |
| 0                             | 4   | 4     | 20                       | 100.0 |

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

### 10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble ⓘ

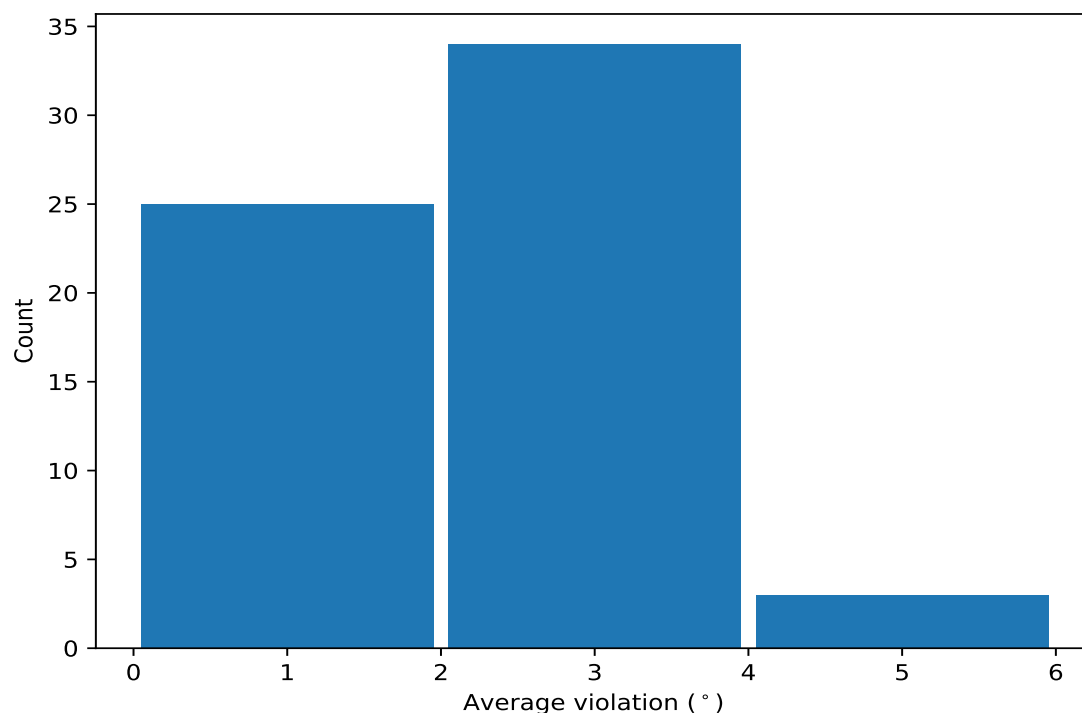


## 10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

### 10.4.1 Histogram : Distribution of mean dihedral-angle violations ⓘ

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

in the ensemble



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

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

| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Models <sup>1</sup> | Mean | SD <sup>2</sup> | Median |
|---------|---------------|----------------|----------------|---------------|---------------------|------|-----------------|--------|
| (1,96)  | 1:73:A:GLU:N  | 1:73:A:GLU:CA  | 1:73:A:GLU:C   | 1:74:A:TYR:N  | 20                  | 5.93 | 1.21            | 6.26   |
| (1,24)  | 1:17:A:SER:N  | 1:17:A:SER:CA  | 1:17:A:SER:C   | 1:18:A:ALA:N  | 20                  | 5.12 | 1.5             | 4.77   |
| (1,94)  | 1:72:A:ALA:N  | 1:72:A:ALA:CA  | 1:72:A:ALA:C   | 1:73:A:GLU:N  | 20                  | 4.23 | 1.0             | 4.22   |
| (1,186) | 1:146:A:LEU:N | 1:146:A:LEU:CA | 1:146:A:LEU:C  | 1:147:A:ASN:N | 20                  | 3.77 | 1.12            | 3.87   |
| (1,146) | 1:120:A:SER:N | 1:120:A:SER:CA | 1:120:A:SER:C  | 1:121:A:THR:N | 19                  | 3.01 | 1.23            | 3.37   |
| (1,80)  | 1:62:A:GLN:N  | 1:62:A:GLN:CA  | 1:62:A:GLN:C   | 1:63:A:ALA:N  | 16                  | 2.71 | 1.15            | 2.4    |
| (1,128) | 1:106:A:THR:N | 1:106:A:THR:CA | 1:106:A:THR:C  | 1:107:A:LEU:N | 16                  | 2.58 | 0.98            | 2.21   |
| (1,116) | 1:87:A:ASP:N  | 1:87:A:ASP:CA  | 1:87:A:ASP:C   | 1:88:A:TYR:N  | 15                  | 3.29 | 1.96            | 2.45   |
| (1,54)  | 1:43:A:SER:N  | 1:43:A:SER:CA  | 1:43:A:SER:C   | 1:44:A:VAL:N  | 14                  | 3.0  | 0.9             | 2.9    |
| (1,12)  | 1:11:A:ILE:N  | 1:11:A:ILE:CA  | 1:11:A:ILE:C   | 1:12:A:PHE:N  | 14                  | 2.44 | 0.78            | 2.42   |
| (1,129) | 1:106:A:THR:C | 1:107:A:LEU:N  | 1:107:A:LEU:CA | 1:107:A:LEU:C | 14                  | 2.36 | 0.95            | 2.3    |
| (1,100) | 1:76:A:GLN:N  | 1:76:A:GLN:CA  | 1:76:A:GLN:C   | 1:77:A:VAL:N  | 13                  | 3.74 | 1.53            | 2.86   |
| (1,114) | 1:86:A:LEU:N  | 1:86:A:LEU:CA  | 1:86:A:LEU:C   | 1:87:A:ASP:N  | 13                  | 2.43 | 0.78            | 2.25   |
| (1,93)  | 1:71:A:ILE:C  | 1:72:A:ALA:N   | 1:72:A:ALA:CA  | 1:72:A:ALA:C  | 13                  | 2.24 | 0.52            | 2.25   |
| (1,77)  | 1:60:A:ALA:C  | 1:61:A:ILE:N   | 1:61:A:ILE:CA  | 1:61:A:ILE:C  | 11                  | 2.42 | 0.72            | 2.28   |
| (1,9)   | 1:9:A:LYS:C   | 1:10:A:ILE:N   | 1:10:A:ILE:CA  | 1:10:A:ILE:C  | 11                  | 2.37 | 0.78            | 2.0    |
| (1,150) | 1:122:A:SER:N | 1:122:A:SER:CA | 1:122:A:SER:C  | 1:123:A:THR:N | 11                  | 2.31 | 0.72            | 2.57   |
| (1,115) | 1:86:A:LEU:C  | 1:87:A:ASP:N   | 1:87:A:ASP:CA  | 1:87:A:ASP:C  | 11                  | 2.26 | 0.74            | 2.29   |
| (1,102) | 1:77:A:VAL:N  | 1:77:A:VAL:CA  | 1:77:A:VAL:C   | 1:78:A:ASP:N  | 10                  | 2.81 | 1.5             | 2.48   |
| (1,109) | 1:83:A:ILE:C  | 1:84:A:GLU:N   | 1:84:A:GLU:CA  | 1:84:A:GLU:C  | 10                  | 1.98 | 0.7             | 1.81   |

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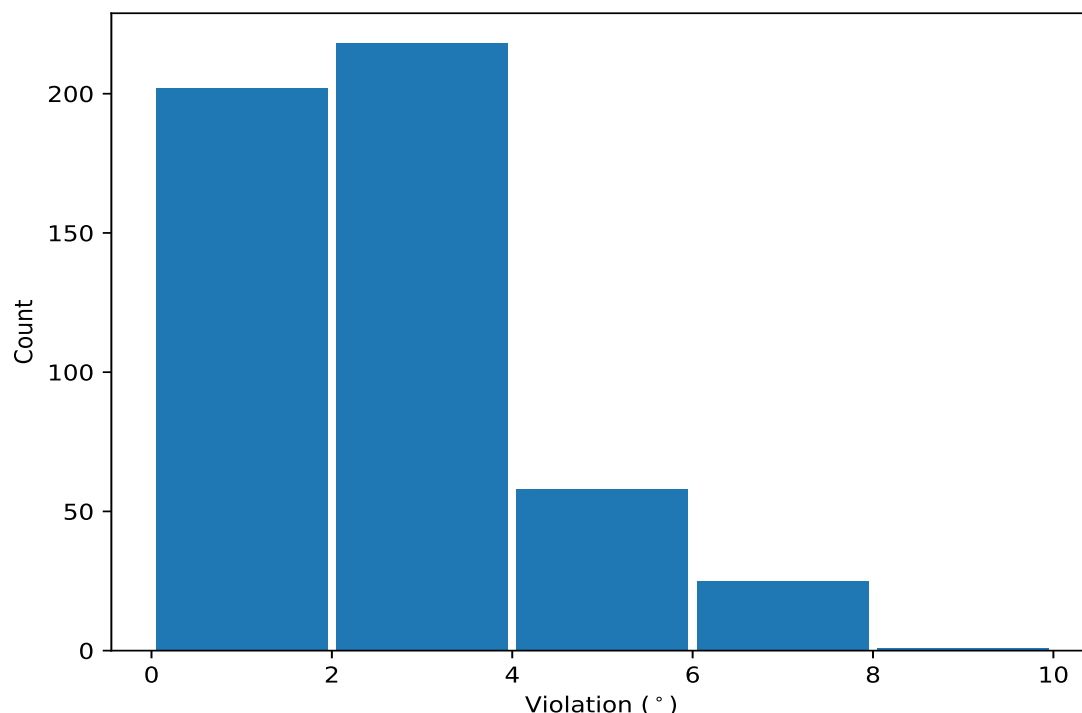
| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Models <sup>1</sup> | Mean | SD <sup>2</sup> | Median |
|---------|---------------|----------------|----------------|---------------|---------------------|------|-----------------|--------|
| (1,66)  | 1:50:A:ASN:N  | 1:50:A:ASN:CA  | 1:50:A:ASN:C   | 1:51:A:ALA:N  | 9                   | 1.68 | 0.49            | 1.41   |
| (1,118) | 1:88:A:TYR:N  | 1:88:A:TYR:CA  | 1:88:A:TYR:C   | 1:89:A:PHE:N  | 8                   | 1.9  | 0.54            | 1.77   |
| (1,88)  | 1:69:A:TYR:N  | 1:69:A:TYR:CA  | 1:69:A:TYR:C   | 1:70:A:THR:N  | 8                   | 1.84 | 0.28            | 1.78   |
| (1,185) | 1:145:A:THR:C | 1:146:A:LEU:N  | 1:146:A:LEU:CA | 1:146:A:LEU:C | 8                   | 1.48 | 0.53            | 1.13   |
| (1,99)  | 1:75:A:LEU:C  | 1:76:A:GLN:N   | 1:76:A:GLN:CA  | 1:76:A:GLN:C  | 7                   | 3.35 | 1.69            | 2.6    |
| (1,148) | 1:121:A:THR:N | 1:121:A:THR:CA | 1:121:A:THR:C  | 1:122:A:SER:N | 7                   | 2.34 | 1.1             | 1.66   |
| (1,84)  | 1:67:A:ILE:N  | 1:67:A:ILE:CA  | 1:67:A:ILE:C   | 1:68:A:SER:N  | 7                   | 2.01 | 0.35            | 2.0    |
| (1,13)  | 1:11:A:ILE:C  | 1:12:A:PHE:N   | 1:12:A:PHE:CA  | 1:12:A:PHE:C  | 7                   | 1.69 | 0.58            | 1.5    |
| (1,130) | 1:107:A:LEU:N | 1:107:A:LEU:CA | 1:107:A:LEU:C  | 1:108:A:ASN:N | 6                   | 2.39 | 0.89            | 2.26   |
| (1,7)   | 1:8:A:ASN:C   | 1:9:A:LYS:N    | 1:9:A:LYS:CA   | 1:9:A:LYS:C   | 6                   | 2.3  | 0.77            | 2.49   |
| (1,201) | 1:153:A:LEU:C | 1:154:A:ASN:N  | 1:154:A:ASN:CA | 1:154:A:ASN:C | 6                   | 2.08 | 0.74            | 2.02   |
| (1,15)  | 1:12:A:PHE:C  | 1:13:A:THR:N   | 1:13:A:THR:CA  | 1:13:A:THR:C  | 6                   | 2.04 | 0.57            | 1.83   |
| (1,1)   | 1:3:A:ILE:C   | 1:4:A:GLU:N    | 1:4:A:GLU:CA   | 1:4:A:GLU:C   | 6                   | 2.0  | 0.92            | 1.6    |
| (1,40)  | 1:28:A:THR:N  | 1:28:A:THR:CA  | 1:28:A:THR:C   | 1:29:A:LYS:N  | 6                   | 1.89 | 0.66            | 1.78   |
| (1,172) | 1:139:A:GLU:N | 1:139:A:GLU:CA | 1:139:A:GLU:C  | 1:140:A:THR:N | 6                   | 1.86 | 0.43            | 1.77   |
| (1,140) | 1:117:A:THR:N | 1:117:A:THR:CA | 1:117:A:THR:C  | 1:118:A:VAL:N | 6                   | 1.75 | 0.42            | 1.71   |
| (1,21)  | 1:15:A:THR:C  | 1:16:A:PHE:N   | 1:16:A:PHE:CA  | 1:16:A:PHE:C  | 5                   | 2.17 | 0.5             | 2.18   |
| (1,121) | 1:89:A:PHE:C  | 1:90:A:ALA:N   | 1:90:A:ALA:CA  | 1:90:A:ALA:C  | 5                   | 2.14 | 0.95            | 1.87   |
| (1,26)  | 1:20:A:ILE:N  | 1:20:A:ILE:CA  | 1:20:A:ILE:C   | 1:21:A:ASN:N  | 5                   | 1.79 | 0.23            | 1.93   |
| (1,61)  | 1:47:A:TYR:C  | 1:48:A:ASP:N   | 1:48:A:ASP:CA  | 1:48:A:ASP:C  | 4                   | 2.02 | 0.79            | 1.85   |
| (1,45)  | 1:30:A:ARG:C  | 1:31:A:GLU:N   | 1:31:A:GLU:CA  | 1:31:A:GLU:C  | 4                   | 1.9  | 0.51            | 2.0    |
| (1,98)  | 1:74:A:TYR:N  | 1:74:A:TYR:CA  | 1:74:A:TYR:C   | 1:75:A:LEU:N  | 4                   | 1.74 | 0.77            | 1.4    |
| (1,168) | 1:136:A:MET:N | 1:136:A:MET:CA | 1:136:A:MET:C  | 1:137:A:GLY:N | 4                   | 1.72 | 0.18            | 1.73   |
| (1,122) | 1:90:A:ALA:N  | 1:90:A:ALA:CA  | 1:90:A:ALA:C   | 1:91:A:THR:N  | 4                   | 1.52 | 0.33            | 1.46   |
| (1,71)  | 1:57:A:ALA:C  | 1:58:A:PHE:N   | 1:58:A:PHE:CA  | 1:58:A:PHE:C  | 4                   | 1.49 | 0.69            | 1.13   |
| (1,55)  | 1:43:A:SER:C  | 1:44:A:VAL:N   | 1:44:A:VAL:CA  | 1:44:A:VAL:C  | 4                   | 1.44 | 0.34            | 1.4    |
| (1,124) | 1:104:A:HIS:N | 1:104:A:HIS:CA | 1:104:A:HIS:C  | 1:105:A:ILE:N | 4                   | 1.2  | 0.15            | 1.17   |
| (1,20)  | 1:15:A:THR:N  | 1:15:A:THR:CA  | 1:15:A:THR:C   | 1:16:A:PHE:N  | 3                   | 2.88 | 1.22            | 2.76   |
| (1,136) | 1:115:A:LYS:N | 1:115:A:LYS:CA | 1:115:A:LYS:C  | 1:116:A:THR:N | 3                   | 2.29 | 0.69            | 2.21   |
| (1,152) | 1:123:A:THR:N | 1:123:A:THR:CA | 1:123:A:THR:C  | 1:124:A:PHE:N | 3                   | 1.66 | 0.56            | 1.52   |
| (1,180) | 1:143:A:ASN:N | 1:143:A:ASN:CA | 1:143:A:ASN:C  | 1:144:A:SER:N | 3                   | 1.62 | 0.22            | 1.5    |
| (1,113) | 1:85:A:TYR:C  | 1:86:A:LEU:N   | 1:86:A:LEU:CA  | 1:86:A:LEU:C  | 3                   | 1.51 | 0.08            | 1.47   |
| (1,65)  | 1:49:A:PHE:C  | 1:50:A:ASN:N   | 1:50:A:ASN:CA  | 1:50:A:ASN:C  | 3                   | 1.36 | 0.22            | 1.32   |
| (1,176) | 1:141:A:GLY:N | 1:141:A:GLY:CA | 1:141:A:GLY:C  | 1:142:A:MET:N | 3                   | 1.35 | 0.28            | 1.35   |
| (1,28)  | 1:21:A:ASN:N  | 1:21:A:ASN:CA  | 1:21:A:ASN:C   | 1:22:A:LYS:N  | 2                   | 3.67 | 0.78            | 3.67   |
| (1,82)  | 1:66:A:MET:N  | 1:66:A:MET:CA  | 1:66:A:MET:C   | 1:67:A:ILE:N  | 2                   | 3.02 | 0.15            | 3.02   |
| (1,29)  | 1:21:A:ASN:C  | 1:22:A:LYS:N   | 1:22:A:LYS:CA  | 1:22:A:LYS:C  | 2                   | 2.92 | 0.44            | 2.92   |
| (1,138) | 1:116:A:THR:N | 1:116:A:THR:CA | 1:116:A:THR:C  | 1:117:A:THR:N | 2                   | 2.63 | 0.14            | 2.63   |
| (1,41)  | 1:28:A:THR:C  | 1:29:A:LYS:N   | 1:29:A:LYS:CA  | 1:29:A:LYS:C  | 2                   | 2.06 | 0.42            | 2.06   |
| (1,178) | 1:142:A:MET:N | 1:142:A:MET:CA | 1:142:A:MET:C  | 1:143:A:ASN:N | 2                   | 1.86 | 0.47            | 1.86   |
| (1,174) | 1:140:A:THR:N | 1:140:A:THR:CA | 1:140:A:THR:C  | 1:141:A:GLY:N | 2                   | 1.38 | 0.32            | 1.38   |
| (1,50)  | 1:33:A:PHE:N  | 1:33:A:PHE:CA  | 1:33:A:PHE:C   | 1:34:A:GLU:N  | 2                   | 1.33 | 0.23            | 1.33   |

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

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

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

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



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

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

| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,24)  | 1:17:A:SER:N | 1:17:A:SER:CA | 1:17:A:SER:C  | 1:18:A:ALA:N | 6        | 8.15          |
| (1,96)  | 1:73:A:GLU:N | 1:73:A:GLU:CA | 1:73:A:GLU:C  | 1:74:A:TYR:N | 7        | 7.86          |
| (1,116) | 1:87:A:ASP:N | 1:87:A:ASP:CA | 1:87:A:ASP:C  | 1:88:A:TYR:N | 17       | 7.38          |
| (1,96)  | 1:73:A:GLU:N | 1:73:A:GLU:CA | 1:73:A:GLU:C  | 1:74:A:TYR:N | 1        | 7.32          |
| (1,24)  | 1:17:A:SER:N | 1:17:A:SER:CA | 1:17:A:SER:C  | 1:18:A:ALA:N | 13       | 7.31          |
| (1,96)  | 1:73:A:GLU:N | 1:73:A:GLU:CA | 1:73:A:GLU:C  | 1:74:A:TYR:N | 17       | 7.14          |
| (1,96)  | 1:73:A:GLU:N | 1:73:A:GLU:CA | 1:73:A:GLU:C  | 1:74:A:TYR:N | 20       | 7.07          |
| (1,96)  | 1:73:A:GLU:N | 1:73:A:GLU:CA | 1:73:A:GLU:C  | 1:74:A:TYR:N | 4        | 7.03          |
| (1,24)  | 1:17:A:SER:N | 1:17:A:SER:CA | 1:17:A:SER:C  | 1:18:A:ALA:N | 2        | 7.03          |
| (1,99)  | 1:75:A:LEU:C | 1:76:A:GLN:N  | 1:76:A:GLN:CA | 1:76:A:GLN:C | 3        | 6.82          |
| (1,116) | 1:87:A:ASP:N | 1:87:A:ASP:CA | 1:87:A:ASP:C  | 1:88:A:TYR:N | 16       | 6.74          |
| (1,100) | 1:76:A:GLN:N | 1:76:A:GLN:CA | 1:76:A:GLN:C  | 1:77:A:VAL:N | 4        | 6.64          |
| (1,96)  | 1:73:A:GLU:N | 1:73:A:GLU:CA | 1:73:A:GLU:C  | 1:74:A:TYR:N | 11       | 6.6           |
| (1,96)  | 1:73:A:GLU:N | 1:73:A:GLU:CA | 1:73:A:GLU:C  | 1:74:A:TYR:N | 19       | 6.56          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,24)  | 1:17:A:SER:N  | 1:17:A:SER:CA  | 1:17:A:SER:C   | 1:18:A:ALA:N  | 20       | 6.56          |
| (1,96)  | 1:73:A:GLU:N  | 1:73:A:GLU:CA  | 1:73:A:GLU:C   | 1:74:A:TYR:N  | 10       | 6.43          |
| (1,96)  | 1:73:A:GLU:N  | 1:73:A:GLU:CA  | 1:73:A:GLU:C   | 1:74:A:TYR:N  | 12       | 6.36          |
| (1,24)  | 1:17:A:SER:N  | 1:17:A:SER:CA  | 1:17:A:SER:C   | 1:18:A:ALA:N  | 11       | 6.36          |
| (1,96)  | 1:73:A:GLU:N  | 1:73:A:GLU:CA  | 1:73:A:GLU:C   | 1:74:A:TYR:N  | 18       | 6.33          |
| (1,24)  | 1:17:A:SER:N  | 1:17:A:SER:CA  | 1:17:A:SER:C   | 1:18:A:ALA:N  | 15       | 6.24          |
| (1,96)  | 1:73:A:GLU:N  | 1:73:A:GLU:CA  | 1:73:A:GLU:C   | 1:74:A:TYR:N  | 5        | 6.18          |
| (1,100) | 1:76:A:GLN:N  | 1:76:A:GLN:CA  | 1:76:A:GLN:C   | 1:77:A:VAL:N  | 16       | 6.09          |
| (1,96)  | 1:73:A:GLU:N  | 1:73:A:GLU:CA  | 1:73:A:GLU:C   | 1:74:A:TYR:N  | 3        | 6.07          |
| (1,186) | 1:146:A:LEU:N | 1:146:A:LEU:CA | 1:146:A:LEU:C  | 1:147:A:ASN:N | 7        | 6.04          |
| (1,94)  | 1:72:A:ALA:N  | 1:72:A:ALA:CA  | 1:72:A:ALA:C   | 1:73:A:GLU:N  | 20       | 6.03          |
| (1,24)  | 1:17:A:SER:N  | 1:17:A:SER:CA  | 1:17:A:SER:C   | 1:18:A:ALA:N  | 17       | 6.03          |
| (1,94)  | 1:72:A:ALA:N  | 1:72:A:ALA:CA  | 1:72:A:ALA:C   | 1:73:A:GLU:N  | 14       | 5.91          |
| (1,116) | 1:87:A:ASP:N  | 1:87:A:ASP:CA  | 1:87:A:ASP:C   | 1:88:A:TYR:N  | 14       | 5.84          |
| (1,24)  | 1:17:A:SER:N  | 1:17:A:SER:CA  | 1:17:A:SER:C   | 1:18:A:ALA:N  | 5        | 5.75          |
| (1,96)  | 1:73:A:GLU:N  | 1:73:A:GLU:CA  | 1:73:A:GLU:C   | 1:74:A:TYR:N  | 6        | 5.71          |
| (1,102) | 1:77:A:VAL:N  | 1:77:A:VAL:CA  | 1:77:A:VAL:C   | 1:78:A:ASP:N  | 17       | 5.55          |
| (1,94)  | 1:72:A:ALA:N  | 1:72:A:ALA:CA  | 1:72:A:ALA:C   | 1:73:A:GLU:N  | 12       | 5.5           |
| (1,96)  | 1:73:A:GLU:N  | 1:73:A:GLU:CA  | 1:73:A:GLU:C   | 1:74:A:TYR:N  | 2        | 5.41          |
| (1,24)  | 1:17:A:SER:N  | 1:17:A:SER:CA  | 1:17:A:SER:C   | 1:18:A:ALA:N  | 10       | 5.4           |
| (1,146) | 1:120:A:SER:N | 1:120:A:SER:CA | 1:120:A:SER:C  | 1:121:A:THR:N | 13       | 5.3           |
| (1,80)  | 1:62:A:GLN:N  | 1:62:A:GLN:CA  | 1:62:A:GLN:C   | 1:63:A:ALA:N  | 14       | 5.26          |
| (1,100) | 1:76:A:GLN:N  | 1:76:A:GLN:CA  | 1:76:A:GLN:C   | 1:77:A:VAL:N  | 1        | 5.2           |
| (1,96)  | 1:73:A:GLU:N  | 1:73:A:GLU:CA  | 1:73:A:GLU:C   | 1:74:A:TYR:N  | 16       | 5.2           |
| (1,94)  | 1:72:A:ALA:N  | 1:72:A:ALA:CA  | 1:72:A:ALA:C   | 1:73:A:GLU:N  | 10       | 5.08          |
| (1,80)  | 1:62:A:GLN:N  | 1:62:A:GLN:CA  | 1:62:A:GLN:C   | 1:63:A:ALA:N  | 18       | 5.07          |
| (1,186) | 1:146:A:LEU:N | 1:146:A:LEU:CA | 1:146:A:LEU:C  | 1:147:A:ASN:N | 19       | 5.05          |
| (1,96)  | 1:73:A:GLU:N  | 1:73:A:GLU:CA  | 1:73:A:GLU:C   | 1:74:A:TYR:N  | 9        | 5.05          |
| (1,100) | 1:76:A:GLN:N  | 1:76:A:GLN:CA  | 1:76:A:GLN:C   | 1:77:A:VAL:N  | 3        | 5.01          |
| (1,129) | 1:106:A:THR:C | 1:107:A:LEU:N  | 1:107:A:LEU:CA | 1:107:A:LEU:C | 4        | 4.97          |
| (1,186) | 1:146:A:LEU:N | 1:146:A:LEU:CA | 1:146:A:LEU:C  | 1:147:A:ASN:N | 20       | 4.95          |
| (1,186) | 1:146:A:LEU:N | 1:146:A:LEU:CA | 1:146:A:LEU:C  | 1:147:A:ASN:N | 2        | 4.91          |
| (1,100) | 1:76:A:GLN:N  | 1:76:A:GLN:CA  | 1:76:A:GLN:C   | 1:77:A:VAL:N  | 12       | 4.89          |
| (1,94)  | 1:72:A:ALA:N  | 1:72:A:ALA:CA  | 1:72:A:ALA:C   | 1:73:A:GLU:N  | 5        | 4.88          |
| (1,96)  | 1:73:A:GLU:N  | 1:73:A:GLU:CA  | 1:73:A:GLU:C   | 1:74:A:TYR:N  | 13       | 4.85          |
| (1,94)  | 1:72:A:ALA:N  | 1:72:A:ALA:CA  | 1:72:A:ALA:C   | 1:73:A:GLU:N  | 11       | 4.84          |
| (1,24)  | 1:17:A:SER:N  | 1:17:A:SER:CA  | 1:17:A:SER:C   | 1:18:A:ALA:N  | 4        | 4.8           |
| (1,146) | 1:120:A:SER:N | 1:120:A:SER:CA | 1:120:A:SER:C  | 1:121:A:THR:N | 12       | 4.79          |
| (1,186) | 1:146:A:LEU:N | 1:146:A:LEU:CA | 1:146:A:LEU:C  | 1:147:A:ASN:N | 6        | 4.77          |
| (1,186) | 1:146:A:LEU:N | 1:146:A:LEU:CA | 1:146:A:LEU:C  | 1:147:A:ASN:N | 11       | 4.77          |
| (1,94)  | 1:72:A:ALA:N  | 1:72:A:ALA:CA  | 1:72:A:ALA:C   | 1:73:A:GLU:N  | 9        | 4.77          |
| (1,24)  | 1:17:A:SER:N  | 1:17:A:SER:CA  | 1:17:A:SER:C   | 1:18:A:ALA:N  | 3        | 4.73          |
| (1,54)  | 1:43:A:SER:N  | 1:43:A:SER:CA  | 1:43:A:SER:C   | 1:44:A:VAL:N  | 19       | 4.62          |
| (1,146) | 1:120:A:SER:N | 1:120:A:SER:CA | 1:120:A:SER:C  | 1:121:A:THR:N | 9        | 4.61          |
| (1,24)  | 1:17:A:SER:N  | 1:17:A:SER:CA  | 1:17:A:SER:C   | 1:18:A:ALA:N  | 19       | 4.61          |
| (1,94)  | 1:72:A:ALA:N  | 1:72:A:ALA:CA  | 1:72:A:ALA:C   | 1:73:A:GLU:N  | 3        | 4.6           |
| (1,96)  | 1:73:A:GLU:N  | 1:73:A:GLU:CA  | 1:73:A:GLU:C   | 1:74:A:TYR:N  | 8        | 4.57          |
| (1,24)  | 1:17:A:SER:N  | 1:17:A:SER:CA  | 1:17:A:SER:C   | 1:18:A:ALA:N  | 9        | 4.51          |
| (1,116) | 1:87:A:ASP:N  | 1:87:A:ASP:CA  | 1:87:A:ASP:C   | 1:88:A:TYR:N  | 5        | 4.5           |
| (1,28)  | 1:21:A:ASN:N  | 1:21:A:ASN:CA  | 1:21:A:ASN:C   | 1:22:A:LYS:N  | 5        | 4.45          |
| (1,94)  | 1:72:A:ALA:N  | 1:72:A:ALA:CA  | 1:72:A:ALA:C   | 1:73:A:GLU:N  | 18       | 4.44          |

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| Key     | Atom-1        | Atom-2         | Atom-3        | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|---------------|---------------|----------|---------------|
| (1,20)  | 1:15:A:THR:N  | 1:15:A:THR:CA  | 1:15:A:THR:C  | 1:16:A:PHE:N  | 10       | 4.44          |
| (1,128) | 1:106:A:THR:N | 1:106:A:THR:CA | 1:106:A:THR:C | 1:107:A:LEU:N | 15       | 4.43          |
| (1,24)  | 1:17:A:SER:N  | 1:17:A:SER:CA  | 1:17:A:SER:C  | 1:18:A:ALA:N  | 1        | 4.42          |
| (1,186) | 1:146:A:LEU:N | 1:146:A:LEU:CA | 1:146:A:LEU:C | 1:147:A:ASN:N | 15       | 4.38          |
| (1,102) | 1:77:A:VAL:N  | 1:77:A:VAL:CA  | 1:77:A:VAL:C  | 1:78:A:ASP:N  | 15       | 4.36          |
| (1,99)  | 1:75:A:LEU:C  | 1:76:A:GLN:N   | 1:76:A:GLN:CA | 1:76:A:GLN:C  | 5        | 4.36          |
| (1,54)  | 1:43:A:SER:N  | 1:43:A:SER:CA  | 1:43:A:SER:C  | 1:44:A:VAL:N  | 11       | 4.34          |
| (1,54)  | 1:43:A:SER:N  | 1:43:A:SER:CA  | 1:43:A:SER:C  | 1:44:A:VAL:N  | 13       | 4.31          |
| (1,94)  | 1:72:A:ALA:N  | 1:72:A:ALA:CA  | 1:72:A:ALA:C  | 1:73:A:GLU:N  | 8        | 4.23          |
| (1,94)  | 1:72:A:ALA:N  | 1:72:A:ALA:CA  | 1:72:A:ALA:C  | 1:73:A:GLU:N  | 2        | 4.21          |
| (1,12)  | 1:11:A:ILE:N  | 1:11:A:ILE:CA  | 1:11:A:ILE:C  | 1:12:A:PHE:N  | 2        | 4.21          |
| (1,186) | 1:146:A:LEU:N | 1:146:A:LEU:CA | 1:146:A:LEU:C | 1:147:A:ASN:N | 1        | 4.18          |
| (1,94)  | 1:72:A:ALA:N  | 1:72:A:ALA:CA  | 1:72:A:ALA:C  | 1:73:A:GLU:N  | 1        | 4.17          |
| (1,186) | 1:146:A:LEU:N | 1:146:A:LEU:CA | 1:146:A:LEU:C | 1:147:A:ASN:N | 3        | 4.15          |
| (1,146) | 1:120:A:SER:N | 1:120:A:SER:CA | 1:120:A:SER:C | 1:121:A:THR:N | 20       | 4.12          |
| (1,96)  | 1:73:A:GLU:N  | 1:73:A:GLU:CA  | 1:73:A:GLU:C  | 1:74:A:TYR:N  | 15       | 4.12          |
| (1,102) | 1:77:A:VAL:N  | 1:77:A:VAL:CA  | 1:77:A:VAL:C  | 1:78:A:ASP:N  | 12       | 4.06          |
| (1,24)  | 1:17:A:SER:N  | 1:17:A:SER:CA  | 1:17:A:SER:C  | 1:18:A:ALA:N  | 8        | 4.06          |
| (1,24)  | 1:17:A:SER:N  | 1:17:A:SER:CA  | 1:17:A:SER:C  | 1:18:A:ALA:N  | 14       | 4.03          |
| (1,102) | 1:77:A:VAL:N  | 1:77:A:VAL:CA  | 1:77:A:VAL:C  | 1:78:A:ASP:N  | 8        | 3.98          |
| (1,186) | 1:146:A:LEU:N | 1:146:A:LEU:CA | 1:146:A:LEU:C | 1:147:A:ASN:N | 17       | 3.97          |
| (1,121) | 1:89:A:PHE:C  | 1:90:A:ALA:N   | 1:90:A:ALA:CA | 1:90:A:ALA:C  | 15       | 3.95          |
| (1,114) | 1:86:A:LEU:N  | 1:86:A:LEU:CA  | 1:86:A:LEU:C  | 1:87:A:ASP:N  | 18       | 3.95          |
| (1,1)   | 1:3:A:ILE:C   | 1:4:A:GLU:N    | 1:4:A:GLU:CA  | 1:4:A:GLU:C   | 1        | 3.94          |
| (1,146) | 1:120:A:SER:N | 1:120:A:SER:CA | 1:120:A:SER:C | 1:121:A:THR:N | 3        | 3.9           |
| (1,128) | 1:106:A:THR:N | 1:106:A:THR:CA | 1:106:A:THR:C | 1:107:A:LEU:N | 12       | 3.89          |
| (1,116) | 1:87:A:ASP:N  | 1:87:A:ASP:CA  | 1:87:A:ASP:C  | 1:88:A:TYR:N  | 20       | 3.88          |
| (1,77)  | 1:60:A:ALA:C  | 1:61:A:ILE:N   | 1:61:A:ILE:CA | 1:61:A:ILE:C  | 14       | 3.87          |
| (1,128) | 1:106:A:THR:N | 1:106:A:THR:CA | 1:106:A:THR:C | 1:107:A:LEU:N | 9        | 3.83          |
| (1,99)  | 1:75:A:LEU:C  | 1:76:A:GLN:N   | 1:76:A:GLN:CA | 1:76:A:GLN:C  | 15       | 3.83          |
| (1,186) | 1:146:A:LEU:N | 1:146:A:LEU:CA | 1:146:A:LEU:C | 1:147:A:ASN:N | 4        | 3.77          |
| (1,150) | 1:122:A:SER:N | 1:122:A:SER:CA | 1:122:A:SER:C | 1:123:A:THR:N | 10       | 3.77          |
| (1,94)  | 1:72:A:ALA:N  | 1:72:A:ALA:CA  | 1:72:A:ALA:C  | 1:73:A:GLU:N  | 4        | 3.77          |
| (1,146) | 1:120:A:SER:N | 1:120:A:SER:CA | 1:120:A:SER:C | 1:121:A:THR:N | 18       | 3.75          |
| (1,116) | 1:87:A:ASP:N  | 1:87:A:ASP:CA  | 1:87:A:ASP:C  | 1:88:A:TYR:N  | 12       | 3.73          |
| (1,94)  | 1:72:A:ALA:N  | 1:72:A:ALA:CA  | 1:72:A:ALA:C  | 1:73:A:GLU:N  | 7        | 3.71          |
| (1,94)  | 1:72:A:ALA:N  | 1:72:A:ALA:CA  | 1:72:A:ALA:C  | 1:73:A:GLU:N  | 13       | 3.71          |
| (1,148) | 1:121:A:THR:N | 1:121:A:THR:CA | 1:121:A:THR:C | 1:122:A:SER:N | 7        | 3.68          |
| (1,132) | 1:108:A:ASN:N | 1:108:A:ASN:CA | 1:108:A:ASN:C | 1:109:A:PHE:N | 17       | 3.68          |
| (1,80)  | 1:62:A:GLN:N  | 1:62:A:GLN:CA  | 1:62:A:GLN:C  | 1:63:A:ALA:N  | 8        | 3.68          |
| (1,9)   | 1:9:A:LYS:C   | 1:10:A:ILE:N   | 1:10:A:ILE:CA | 1:10:A:ILE:C  | 16       | 3.66          |
| (1,148) | 1:121:A:THR:N | 1:121:A:THR:CA | 1:121:A:THR:C | 1:122:A:SER:N | 15       | 3.65          |
| (1,128) | 1:106:A:THR:N | 1:106:A:THR:CA | 1:106:A:THR:C | 1:107:A:LEU:N | 19       | 3.63          |
| (1,24)  | 1:17:A:SER:N  | 1:17:A:SER:CA  | 1:17:A:SER:C  | 1:18:A:ALA:N  | 18       | 3.61          |
| (1,130) | 1:107:A:LEU:N | 1:107:A:LEU:CA | 1:107:A:LEU:C | 1:108:A:ASN:N | 9        | 3.59          |
| (1,80)  | 1:62:A:GLN:N  | 1:62:A:GLN:CA  | 1:62:A:GLN:C  | 1:63:A:ALA:N  | 16       | 3.58          |
| (1,186) | 1:146:A:LEU:N | 1:146:A:LEU:CA | 1:146:A:LEU:C | 1:147:A:ASN:N | 8        | 3.56          |
| (1,24)  | 1:17:A:SER:N  | 1:17:A:SER:CA  | 1:17:A:SER:C  | 1:18:A:ALA:N  | 7        | 3.56          |
| (1,94)  | 1:72:A:ALA:N  | 1:72:A:ALA:CA  | 1:72:A:ALA:C  | 1:73:A:GLU:N  | 17       | 3.5           |
| (1,9)   | 1:9:A:LYS:C   | 1:10:A:ILE:N   | 1:10:A:ILE:CA | 1:10:A:ILE:C  | 1        | 3.5           |
| (1,146) | 1:120:A:SER:N | 1:120:A:SER:CA | 1:120:A:SER:C | 1:121:A:THR:N | 8        | 3.49          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,114) | 1:86:A:LEU:N  | 1:86:A:LEU:CA  | 1:86:A:LEU:C   | 1:87:A:ASP:N  | 5        | 3.48          |
| (1,7)   | 1:8:A:ASN:C   | 1:9:A:LYS:N    | 1:9:A:LYS:CA   | 1:9:A:LYS:C   | 10       | 3.48          |
| (1,146) | 1:120:A:SER:N | 1:120:A:SER:CA | 1:120:A:SER:C  | 1:121:A:THR:N | 2        | 3.47          |
| (1,128) | 1:106:A:THR:N | 1:106:A:THR:CA | 1:106:A:THR:C  | 1:107:A:LEU:N | 11       | 3.47          |
| (1,146) | 1:120:A:SER:N | 1:120:A:SER:CA | 1:120:A:SER:C  | 1:121:A:THR:N | 10       | 3.45          |
| (1,77)  | 1:60:A:ALA:C  | 1:61:A:ILE:N   | 1:61:A:ILE:CA  | 1:61:A:ILE:C  | 19       | 3.45          |
| (1,186) | 1:146:A:LEU:N | 1:146:A:LEU:CA | 1:146:A:LEU:C  | 1:147:A:ASN:N | 9        | 3.44          |
| (1,148) | 1:121:A:THR:N | 1:121:A:THR:CA | 1:121:A:THR:C  | 1:122:A:SER:N | 9        | 3.44          |
| (1,115) | 1:86:A:LEU:C  | 1:87:A:ASP:N   | 1:87:A:ASP:CA  | 1:87:A:ASP:C  | 3        | 3.44          |
| (1,146) | 1:120:A:SER:N | 1:120:A:SER:CA | 1:120:A:SER:C  | 1:121:A:THR:N | 5        | 3.37          |
| (1,94)  | 1:72:A:ALA:N  | 1:72:A:ALA:CA  | 1:72:A:ALA:C   | 1:73:A:GLU:N  | 6        | 3.36          |
| (1,54)  | 1:43:A:SER:N  | 1:43:A:SER:CA  | 1:43:A:SER:C   | 1:44:A:VAL:N  | 18       | 3.36          |
| (1,29)  | 1:21:A:ASN:C  | 1:22:A:LYS:N   | 1:22:A:LYS:CA  | 1:22:A:LYS:C  | 17       | 3.36          |
| (1,100) | 1:76:A:GLN:N  | 1:76:A:GLN:CA  | 1:76:A:GLN:C   | 1:77:A:VAL:N  | 20       | 3.35          |
| (1,130) | 1:107:A:LEU:N | 1:107:A:LEU:CA | 1:107:A:LEU:C  | 1:108:A:ASN:N | 4        | 3.33          |
| (1,201) | 1:153:A:LEU:C | 1:154:A:ASN:N  | 1:154:A:ASN:CA | 1:154:A:ASN:C | 20       | 3.32          |
| (1,94)  | 1:72:A:ALA:N  | 1:72:A:ALA:CA  | 1:72:A:ALA:C   | 1:73:A:GLU:N  | 16       | 3.32          |
| (1,54)  | 1:43:A:SER:N  | 1:43:A:SER:CA  | 1:43:A:SER:C   | 1:44:A:VAL:N  | 4        | 3.32          |
| (1,115) | 1:86:A:LEU:C  | 1:87:A:ASP:N   | 1:87:A:ASP:CA  | 1:87:A:ASP:C  | 13       | 3.28          |
| (1,3)   | 1:4:A:GLU:C   | 1:5:A:LYS:N    | 1:5:A:LYS:CA   | 1:5:A:LYS:C   | 12       | 3.27          |
| (1,129) | 1:106:A:THR:C | 1:107:A:LEU:N  | 1:107:A:LEU:CA | 1:107:A:LEU:C | 9        | 3.24          |
| (1,109) | 1:83:A:ILE:C  | 1:84:A:GLU:N   | 1:84:A:GLU:CA  | 1:84:A:GLU:C  | 9        | 3.24          |
| (1,186) | 1:146:A:LEU:N | 1:146:A:LEU:CA | 1:146:A:LEU:C  | 1:147:A:ASN:N | 13       | 3.23          |
| (1,12)  | 1:11:A:ILE:N  | 1:11:A:ILE:CA  | 1:11:A:ILE:C   | 1:12:A:PHE:N  | 4        | 3.22          |
| (1,61)  | 1:47:A:TYR:C  | 1:48:A:ASP:N   | 1:48:A:ASP:CA  | 1:48:A:ASP:C  | 11       | 3.21          |
| (1,54)  | 1:43:A:SER:N  | 1:43:A:SER:CA  | 1:43:A:SER:C   | 1:44:A:VAL:N  | 10       | 3.2           |
| (1,136) | 1:115:A:LYS:N | 1:115:A:LYS:CA | 1:115:A:LYS:C  | 1:116:A:THR:N | 16       | 3.18          |
| (1,128) | 1:106:A:THR:N | 1:106:A:THR:CA | 1:106:A:THR:C  | 1:107:A:LEU:N | 5        | 3.16          |
| (1,82)  | 1:66:A:MET:N  | 1:66:A:MET:CA  | 1:66:A:MET:C   | 1:67:A:ILE:N  | 9        | 3.16          |
| (1,114) | 1:86:A:LEU:N  | 1:86:A:LEU:CA  | 1:86:A:LEU:C   | 1:87:A:ASP:N  | 17       | 3.15          |
| (1,15)  | 1:12:A:PHE:C  | 1:13:A:THR:N   | 1:13:A:THR:CA  | 1:13:A:THR:C  | 7        | 3.14          |
| (1,80)  | 1:62:A:GLN:N  | 1:62:A:GLN:CA  | 1:62:A:GLN:C   | 1:63:A:ALA:N  | 3        | 3.13          |
| (1,9)   | 1:9:A:LYS:C   | 1:10:A:ILE:N   | 1:10:A:ILE:CA  | 1:10:A:ILE:C  | 3        | 3.12          |
| (1,129) | 1:106:A:THR:C | 1:107:A:LEU:N  | 1:107:A:LEU:CA | 1:107:A:LEU:C | 7        | 3.07          |
| (1,93)  | 1:71:A:ILE:C  | 1:72:A:ALA:N   | 1:72:A:ALA:CA  | 1:72:A:ALA:C  | 5        | 3.06          |
| (1,186) | 1:146:A:LEU:N | 1:146:A:LEU:CA | 1:146:A:LEU:C  | 1:147:A:ASN:N | 14       | 3.05          |
| (1,146) | 1:120:A:SER:N | 1:120:A:SER:CA | 1:120:A:SER:C  | 1:121:A:THR:N | 14       | 3.02          |
| (1,98)  | 1:74:A:TYR:N  | 1:74:A:TYR:CA  | 1:74:A:TYR:C   | 1:75:A:LEU:N  | 7        | 3.02          |
| (1,118) | 1:88:A:TYR:N  | 1:88:A:TYR:CA  | 1:88:A:TYR:C   | 1:89:A:PHE:N  | 14       | 2.98          |
| (1,114) | 1:86:A:LEU:N  | 1:86:A:LEU:CA  | 1:86:A:LEU:C   | 1:87:A:ASP:N  | 8        | 2.98          |
| (1,21)  | 1:15:A:THR:C  | 1:16:A:PHE:N   | 1:16:A:PHE:CA  | 1:16:A:PHE:C  | 2        | 2.98          |
| (1,77)  | 1:60:A:ALA:C  | 1:61:A:ILE:N   | 1:61:A:ILE:CA  | 1:61:A:ILE:C  | 8        | 2.97          |
| (1,54)  | 1:43:A:SER:N  | 1:43:A:SER:CA  | 1:43:A:SER:C   | 1:44:A:VAL:N  | 6        | 2.97          |
| (1,12)  | 1:11:A:ILE:N  | 1:11:A:ILE:CA  | 1:11:A:ILE:C   | 1:12:A:PHE:N  | 3        | 2.97          |
| (1,12)  | 1:11:A:ILE:N  | 1:11:A:ILE:CA  | 1:11:A:ILE:C   | 1:12:A:PHE:N  | 19       | 2.97          |
| (1,150) | 1:122:A:SER:N | 1:122:A:SER:CA | 1:122:A:SER:C  | 1:123:A:THR:N | 15       | 2.95          |
| (1,116) | 1:87:A:ASP:N  | 1:87:A:ASP:CA  | 1:87:A:ASP:C   | 1:88:A:TYR:N  | 7        | 2.95          |
| (1,13)  | 1:11:A:ILE:C  | 1:12:A:PHE:N   | 1:12:A:PHE:CA  | 1:12:A:PHE:C  | 14       | 2.95          |
| (1,12)  | 1:11:A:ILE:N  | 1:11:A:ILE:CA  | 1:11:A:ILE:C   | 1:12:A:PHE:N  | 8        | 2.92          |
| (1,93)  | 1:71:A:ILE:C  | 1:72:A:ALA:N   | 1:72:A:ALA:CA  | 1:72:A:ALA:C  | 10       | 2.91          |
| (1,28)  | 1:21:A:ASN:N  | 1:21:A:ASN:CA  | 1:21:A:ASN:C   | 1:22:A:LYS:N  | 8        | 2.89          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,109) | 1:83:A:ILE:C  | 1:84:A:GLU:N   | 1:84:A:GLU:CA  | 1:84:A:GLU:C  | 14       | 2.88          |
| (1,115) | 1:86:A:LEU:C  | 1:87:A:ASP:N   | 1:87:A:ASP:CA  | 1:87:A:ASP:C  | 5        | 2.87          |
| (1,114) | 1:86:A:LEU:N  | 1:86:A:LEU:CA  | 1:86:A:LEU:C   | 1:87:A:ASP:N  | 1        | 2.87          |
| (1,82)  | 1:66:A:MET:N  | 1:66:A:MET:CA  | 1:66:A:MET:C   | 1:67:A:ILE:N  | 3        | 2.87          |
| (1,100) | 1:76:A:GLN:N  | 1:76:A:GLN:CA  | 1:76:A:GLN:C   | 1:77:A:VAL:N  | 5        | 2.86          |
| (1,93)  | 1:71:A:ILE:C  | 1:72:A:ALA:N   | 1:72:A:ALA:CA  | 1:72:A:ALA:C  | 3        | 2.84          |
| (1,54)  | 1:43:A:SER:N  | 1:43:A:SER:CA  | 1:43:A:SER:C   | 1:44:A:VAL:N  | 5        | 2.84          |
| (1,9)   | 1:9:A:LYS:C   | 1:10:A:ILE:N   | 1:10:A:ILE:CA  | 1:10:A:ILE:C  | 13       | 2.84          |
| (1,130) | 1:107:A:LEU:N | 1:107:A:LEU:CA | 1:107:A:LEU:C  | 1:108:A:ASN:N | 6        | 2.79          |
| (1,100) | 1:76:A:GLN:N  | 1:76:A:GLN:CA  | 1:76:A:GLN:C   | 1:77:A:VAL:N  | 18       | 2.79          |
| (1,40)  | 1:28:A:THR:N  | 1:28:A:THR:CA  | 1:28:A:THR:C   | 1:29:A:LYS:N  | 8        | 2.79          |
| (1,12)  | 1:11:A:ILE:N  | 1:11:A:ILE:CA  | 1:11:A:ILE:C   | 1:12:A:PHE:N  | 13       | 2.78          |
| (1,138) | 1:116:A:THR:N | 1:116:A:THR:CA | 1:116:A:THR:C  | 1:117:A:THR:N | 1        | 2.77          |
| (1,150) | 1:122:A:SER:N | 1:122:A:SER:CA | 1:122:A:SER:C  | 1:123:A:THR:N | 5        | 2.76          |
| (1,20)  | 1:15:A:THR:N  | 1:15:A:THR:CA  | 1:15:A:THR:C   | 1:16:A:PHE:N  | 7        | 2.76          |
| (1,129) | 1:106:A:THR:C | 1:107:A:LEU:N  | 1:107:A:LEU:CA | 1:107:A:LEU:C | 10       | 2.73          |
| (1,96)  | 1:73:A:GLU:N  | 1:73:A:GLU:CA  | 1:73:A:GLU:C   | 1:74:A:TYR:N  | 14       | 2.71          |
| (1,7)   | 1:8:A:ASN:C   | 1:9:A:LYS:N    | 1:9:A:LYS:CA   | 1:9:A:LYS:C   | 7        | 2.71          |
| (1,109) | 1:83:A:ILE:C  | 1:84:A:GLU:N   | 1:84:A:GLU:CA  | 1:84:A:GLU:C  | 12       | 2.7           |
| (1,80)  | 1:62:A:GLN:N  | 1:62:A:GLN:CA  | 1:62:A:GLN:C   | 1:63:A:ALA:N  | 17       | 2.7           |
| (1,80)  | 1:62:A:GLN:N  | 1:62:A:GLN:CA  | 1:62:A:GLN:C   | 1:63:A:ALA:N  | 11       | 2.69          |
| (1,71)  | 1:57:A:ALA:C  | 1:58:A:PHE:N   | 1:58:A:PHE:CA  | 1:58:A:PHE:C  | 15       | 2.69          |
| (1,12)  | 1:11:A:ILE:N  | 1:11:A:ILE:CA  | 1:11:A:ILE:C   | 1:12:A:PHE:N  | 16       | 2.68          |
| (1,94)  | 1:72:A:ALA:N  | 1:72:A:ALA:CA  | 1:72:A:ALA:C   | 1:73:A:GLU:N  | 15       | 2.67          |
| (1,172) | 1:139:A:GLU:N | 1:139:A:GLU:CA | 1:139:A:GLU:C  | 1:140:A:THR:N | 4        | 2.66          |
| (1,102) | 1:77:A:VAL:N  | 1:77:A:VAL:CA  | 1:77:A:VAL:C   | 1:78:A:ASP:N  | 19       | 2.66          |
| (1,186) | 1:146:A:LEU:N | 1:146:A:LEU:CA | 1:146:A:LEU:C  | 1:147:A:ASN:N | 12       | 2.65          |
| (1,150) | 1:122:A:SER:N | 1:122:A:SER:CA | 1:122:A:SER:C  | 1:123:A:THR:N | 9        | 2.65          |
| (1,115) | 1:86:A:LEU:C  | 1:87:A:ASP:N   | 1:87:A:ASP:CA  | 1:87:A:ASP:C  | 2        | 2.65          |
| (1,54)  | 1:43:A:SER:N  | 1:43:A:SER:CA  | 1:43:A:SER:C   | 1:44:A:VAL:N  | 12       | 2.63          |
| (1,40)  | 1:28:A:THR:N  | 1:28:A:THR:CA  | 1:28:A:THR:C   | 1:29:A:LYS:N  | 14       | 2.62          |
| (1,150) | 1:122:A:SER:N | 1:122:A:SER:CA | 1:122:A:SER:C  | 1:123:A:THR:N | 19       | 2.61          |
| (1,24)  | 1:17:A:SER:N  | 1:17:A:SER:CA  | 1:17:A:SER:C   | 1:18:A:ALA:N  | 12       | 2.61          |
| (1,140) | 1:117:A:THR:N | 1:117:A:THR:CA | 1:117:A:THR:C  | 1:118:A:VAL:N | 18       | 2.6           |
| (1,99)  | 1:75:A:LEU:C  | 1:76:A:GLN:N   | 1:76:A:GLN:CA  | 1:76:A:GLN:C  | 6        | 2.6           |
| (1,129) | 1:106:A:THR:C | 1:107:A:LEU:N  | 1:107:A:LEU:CA | 1:107:A:LEU:C | 20       | 2.58          |
| (1,24)  | 1:17:A:SER:N  | 1:17:A:SER:CA  | 1:17:A:SER:C   | 1:18:A:ALA:N  | 16       | 2.58          |
| (1,7)   | 1:8:A:ASN:C   | 1:9:A:LYS:N    | 1:9:A:LYS:CA   | 1:9:A:LYS:C   | 14       | 2.58          |
| (1,150) | 1:122:A:SER:N | 1:122:A:SER:CA | 1:122:A:SER:C  | 1:123:A:THR:N | 12       | 2.57          |
| (1,129) | 1:106:A:THR:C | 1:107:A:LEU:N  | 1:107:A:LEU:CA | 1:107:A:LEU:C | 14       | 2.57          |
| (1,100) | 1:76:A:GLN:N  | 1:76:A:GLN:CA  | 1:76:A:GLN:C   | 1:77:A:VAL:N  | 17       | 2.57          |
| (1,77)  | 1:60:A:ALA:C  | 1:61:A:ILE:N   | 1:61:A:ILE:CA  | 1:61:A:ILE:C  | 9        | 2.53          |
| (1,80)  | 1:62:A:GLN:N  | 1:62:A:GLN:CA  | 1:62:A:GLN:C   | 1:63:A:ALA:N  | 1        | 2.52          |
| (1,201) | 1:153:A:LEU:C | 1:154:A:ASN:N  | 1:154:A:ASN:CA | 1:154:A:ASN:C | 7        | 2.51          |
| (1,84)  | 1:67:A:ILE:N  | 1:67:A:ILE:CA  | 1:67:A:ILE:C   | 1:68:A:SER:N  | 10       | 2.51          |
| (1,138) | 1:116:A:THR:N | 1:116:A:THR:CA | 1:116:A:THR:C  | 1:117:A:THR:N | 2        | 2.49          |
| (1,114) | 1:86:A:LEU:N  | 1:86:A:LEU:CA  | 1:86:A:LEU:C   | 1:87:A:ASP:N  | 14       | 2.48          |
| (1,100) | 1:76:A:GLN:N  | 1:76:A:GLN:CA  | 1:76:A:GLN:C   | 1:77:A:VAL:N  | 19       | 2.48          |
| (1,41)  | 1:28:A:THR:C  | 1:29:A:LYS:N   | 1:29:A:LYS:CA  | 1:29:A:LYS:C  | 4        | 2.48          |
| (1,29)  | 1:21:A:ASN:C  | 1:22:A:LYS:N   | 1:22:A:LYS:CA  | 1:22:A:LYS:C  | 4        | 2.48          |
| (1,146) | 1:120:A:SER:N | 1:120:A:SER:CA | 1:120:A:SER:C  | 1:121:A:THR:N | 15       | 2.47          |

Continued on next page...

Continued from previous page...

| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,93)  | 1:71:A:ILE:C  | 1:72:A:ALA:N   | 1:72:A:ALA:CA  | 1:72:A:ALA:C  | 9        | 2.47          |
| (1,45)  | 1:30:A:ARG:C  | 1:31:A:GLU:N   | 1:31:A:GLU:CA  | 1:31:A:GLU:C  | 12       | 2.47          |
| (1,66)  | 1:50:A:ASN:N  | 1:50:A:ASN:CA  | 1:50:A:ASN:C   | 1:51:A:ALA:N  | 4        | 2.46          |
| (1,116) | 1:87:A:ASP:N  | 1:87:A:ASP:CA  | 1:87:A:ASP:C   | 1:88:A:TYR:N  | 8        | 2.45          |
| (1,93)  | 1:71:A:ILE:C  | 1:72:A:ALA:N   | 1:72:A:ALA:CA  | 1:72:A:ALA:C  | 1        | 2.45          |
| (1,128) | 1:106:A:THR:N | 1:106:A:THR:CA | 1:106:A:THR:C  | 1:107:A:LEU:N | 2        | 2.44          |
| (1,104) | 1:78:A:ASP:N  | 1:78:A:ASP:CA  | 1:78:A:ASP:C   | 1:79:A:ALA:N  | 15       | 2.44          |
| (1,100) | 1:76:A:GLN:N  | 1:76:A:GLN:CA  | 1:76:A:GLN:C   | 1:77:A:VAL:N  | 9        | 2.44          |
| (1,99)  | 1:75:A:LEU:C  | 1:76:A:GLN:N   | 1:76:A:GLN:CA  | 1:76:A:GLN:C  | 11       | 2.42          |
| (1,9)   | 1:9:A:LYS:C   | 1:10:A:ILE:N   | 1:10:A:ILE:CA  | 1:10:A:ILE:C  | 19       | 2.42          |
| (1,93)  | 1:71:A:ILE:C  | 1:72:A:ALA:N   | 1:72:A:ALA:CA  | 1:72:A:ALA:C  | 15       | 2.41          |
| (1,152) | 1:123:A:THR:N | 1:123:A:THR:CA | 1:123:A:THR:C  | 1:124:A:PHE:N | 18       | 2.4           |
| (1,66)  | 1:50:A:ASN:N  | 1:50:A:ASN:CA  | 1:50:A:ASN:C   | 1:51:A:ALA:N  | 2        | 2.39          |
| (1,54)  | 1:43:A:SER:N  | 1:43:A:SER:CA  | 1:43:A:SER:C   | 1:44:A:VAL:N  | 8        | 2.39          |
| (1,7)   | 1:8:A:ASN:C   | 1:9:A:LYS:N    | 1:9:A:LYS:CA   | 1:9:A:LYS:C   | 13       | 2.39          |
| (1,116) | 1:87:A:ASP:N  | 1:87:A:ASP:CA  | 1:87:A:ASP:C   | 1:88:A:TYR:N  | 6        | 2.38          |
| (1,115) | 1:86:A:LEU:C  | 1:87:A:ASP:N   | 1:87:A:ASP:CA  | 1:87:A:ASP:C  | 6        | 2.38          |
| (1,201) | 1:153:A:LEU:C | 1:154:A:ASN:N  | 1:154:A:ASN:CA | 1:154:A:ASN:C | 5        | 2.36          |
| (1,15)  | 1:12:A:PHE:C  | 1:13:A:THR:N   | 1:13:A:THR:CA  | 1:13:A:THR:C  | 17       | 2.36          |
| (1,129) | 1:106:A:THR:C | 1:107:A:LEU:N  | 1:107:A:LEU:CA | 1:107:A:LEU:C | 19       | 2.35          |
| (1,21)  | 1:15:A:THR:C  | 1:16:A:PHE:N   | 1:16:A:PHE:CA  | 1:16:A:PHE:C  | 15       | 2.35          |
| (1,178) | 1:142:A:MET:N | 1:142:A:MET:CA | 1:142:A:MET:C  | 1:143:A:ASN:N | 6        | 2.33          |
| (1,116) | 1:87:A:ASP:N  | 1:87:A:ASP:CA  | 1:87:A:ASP:C   | 1:88:A:TYR:N  | 9        | 2.33          |
| (1,186) | 1:146:A:LEU:N | 1:146:A:LEU:CA | 1:146:A:LEU:C  | 1:147:A:ASN:N | 10       | 2.31          |
| (1,88)  | 1:69:A:TYR:N  | 1:69:A:TYR:CA  | 1:69:A:TYR:C   | 1:70:A:THR:N  | 5        | 2.31          |
| (1,118) | 1:88:A:TYR:N  | 1:88:A:TYR:CA  | 1:88:A:TYR:C   | 1:89:A:PHE:N  | 5        | 2.3           |
| (1,115) | 1:86:A:LEU:C  | 1:87:A:ASP:N   | 1:87:A:ASP:CA  | 1:87:A:ASP:C  | 1        | 2.29          |
| (1,102) | 1:77:A:VAL:N  | 1:77:A:VAL:CA  | 1:77:A:VAL:C   | 1:78:A:ASP:N  | 5        | 2.29          |
| (1,77)  | 1:60:A:ALA:C  | 1:61:A:ILE:N   | 1:61:A:ILE:CA  | 1:61:A:ILE:C  | 13       | 2.29          |
| (1,54)  | 1:43:A:SER:N  | 1:43:A:SER:CA  | 1:43:A:SER:C   | 1:44:A:VAL:N  | 9        | 2.29          |
| (1,185) | 1:145:A:THR:C | 1:146:A:LEU:N  | 1:146:A:LEU:CA | 1:146:A:LEU:C | 6        | 2.28          |
| (1,84)  | 1:67:A:ILE:N  | 1:67:A:ILE:CA  | 1:67:A:ILE:C   | 1:68:A:SER:N  | 1        | 2.28          |
| (1,80)  | 1:62:A:GLN:N  | 1:62:A:GLN:CA  | 1:62:A:GLN:C   | 1:63:A:ALA:N  | 9        | 2.28          |
| (1,77)  | 1:60:A:ALA:C  | 1:61:A:ILE:N   | 1:61:A:ILE:CA  | 1:61:A:ILE:C  | 16       | 2.28          |
| (1,61)  | 1:47:A:TYR:C  | 1:48:A:ASP:N   | 1:48:A:ASP:CA  | 1:48:A:ASP:C  | 18       | 2.27          |
| (1,80)  | 1:62:A:GLN:N  | 1:62:A:GLN:CA  | 1:62:A:GLN:C   | 1:63:A:ALA:N  | 13       | 2.26          |
| (1,146) | 1:120:A:SER:N | 1:120:A:SER:CA | 1:120:A:SER:C  | 1:121:A:THR:N | 6        | 2.25          |
| (1,114) | 1:86:A:LEU:N  | 1:86:A:LEU:CA  | 1:86:A:LEU:C   | 1:87:A:ASP:N  | 20       | 2.25          |
| (1,93)  | 1:71:A:ILE:C  | 1:72:A:ALA:N   | 1:72:A:ALA:CA  | 1:72:A:ALA:C  | 12       | 2.25          |
| (1,93)  | 1:71:A:ILE:C  | 1:72:A:ALA:N   | 1:72:A:ALA:CA  | 1:72:A:ALA:C  | 14       | 2.25          |
| (1,54)  | 1:43:A:SER:N  | 1:43:A:SER:CA  | 1:43:A:SER:C   | 1:44:A:VAL:N  | 7        | 2.25          |
| (1,45)  | 1:30:A:ARG:C  | 1:31:A:GLU:N   | 1:31:A:GLU:CA  | 1:31:A:GLU:C  | 18       | 2.25          |
| (1,129) | 1:106:A:THR:C | 1:107:A:LEU:N  | 1:107:A:LEU:CA | 1:107:A:LEU:C | 8        | 2.24          |
| (1,128) | 1:106:A:THR:N | 1:106:A:THR:CA | 1:106:A:THR:C  | 1:107:A:LEU:N | 6        | 2.22          |
| (1,114) | 1:86:A:LEU:N  | 1:86:A:LEU:CA  | 1:86:A:LEU:C   | 1:87:A:ASP:N  | 12       | 2.22          |
| (1,136) | 1:115:A:LYS:N | 1:115:A:LYS:CA | 1:115:A:LYS:C  | 1:116:A:THR:N | 17       | 2.21          |
| (1,128) | 1:106:A:THR:N | 1:106:A:THR:CA | 1:106:A:THR:C  | 1:107:A:LEU:N | 16       | 2.2           |
| (1,118) | 1:88:A:TYR:N  | 1:88:A:TYR:CA  | 1:88:A:TYR:C   | 1:89:A:PHE:N  | 16       | 2.2           |
| (1,80)  | 1:62:A:GLN:N  | 1:62:A:GLN:CA  | 1:62:A:GLN:C   | 1:63:A:ALA:N  | 5        | 2.2           |
| (1,1)   | 1:3:A:ILE:C   | 1:4:A:GLU:N    | 1:4:A:GLU:CA   | 1:4:A:GLU:C   | 11       | 2.2           |
| (1,189) | 1:147:A:ASN:C | 1:148:A:GLN:N  | 1:148:A:GLN:CA | 1:148:A:GLN:C | 3        | 2.18          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,84)  | 1:67:A:ILE:N  | 1:67:A:ILE:CA  | 1:67:A:ILE:C   | 1:68:A:SER:N  | 4        | 2.18          |
| (1,77)  | 1:60:A:ALA:C  | 1:61:A:ILE:N   | 1:61:A:ILE:CA  | 1:61:A:ILE:C  | 18       | 2.18          |
| (1,21)  | 1:15:A:THR:C  | 1:16:A:PHE:N   | 1:16:A:PHE:CA  | 1:16:A:PHE:C  | 11       | 2.18          |
| (1,77)  | 1:60:A:ALA:C  | 1:61:A:ILE:N   | 1:61:A:ILE:CA  | 1:61:A:ILE:C  | 6        | 2.17          |
| (1,12)  | 1:11:A:ILE:N  | 1:11:A:ILE:CA  | 1:11:A:ILE:C   | 1:12:A:PHE:N  | 10       | 2.17          |
| (1,186) | 1:146:A:LEU:N | 1:146:A:LEU:CA | 1:146:A:LEU:C  | 1:147:A:ASN:N | 16       | 2.15          |
| (1,100) | 1:76:A:GLN:N  | 1:76:A:GLN:CA  | 1:76:A:GLN:C   | 1:77:A:VAL:N  | 2        | 2.14          |
| (1,40)  | 1:28:A:THR:N  | 1:28:A:THR:CA  | 1:28:A:THR:C   | 1:29:A:LYS:N  | 11       | 2.14          |
| (1,116) | 1:87:A:ASP:N  | 1:87:A:ASP:CA  | 1:87:A:ASP:C   | 1:88:A:TYR:N  | 1        | 2.13          |
| (1,100) | 1:76:A:GLN:N  | 1:76:A:GLN:CA  | 1:76:A:GLN:C   | 1:77:A:VAL:N  | 6        | 2.13          |
| (1,88)  | 1:69:A:TYR:N  | 1:69:A:TYR:CA  | 1:69:A:TYR:C   | 1:70:A:THR:N  | 3        | 2.13          |
| (1,185) | 1:145:A:THR:C | 1:146:A:LEU:N  | 1:146:A:LEU:CA | 1:146:A:LEU:C | 2        | 2.12          |
| (1,128) | 1:106:A:THR:N | 1:106:A:THR:CA | 1:106:A:THR:C  | 1:107:A:LEU:N | 13       | 2.1           |
| (1,115) | 1:86:A:LEU:C  | 1:87:A:ASP:N   | 1:87:A:ASP:CA  | 1:87:A:ASP:C  | 7        | 2.09          |
| (1,185) | 1:145:A:THR:C | 1:146:A:LEU:N  | 1:146:A:LEU:CA | 1:146:A:LEU:C | 13       | 2.07          |
| (1,93)  | 1:71:A:ILE:C  | 1:72:A:ALA:N   | 1:72:A:ALA:CA  | 1:72:A:ALA:C  | 11       | 2.06          |
| (1,66)  | 1:50:A:ASN:N  | 1:50:A:ASN:CA  | 1:50:A:ASN:C   | 1:51:A:ALA:N  | 12       | 2.06          |
| (1,186) | 1:146:A:LEU:N | 1:146:A:LEU:CA | 1:146:A:LEU:C  | 1:147:A:ASN:N | 18       | 2.05          |
| (1,172) | 1:139:A:GLU:N | 1:139:A:GLU:CA | 1:139:A:GLU:C  | 1:140:A:THR:N | 16       | 2.05          |
| (1,26)  | 1:20:A:ILE:N  | 1:20:A:ILE:CA  | 1:20:A:ILE:C   | 1:21:A:ASN:N  | 6        | 2.05          |
| (1,150) | 1:122:A:SER:N | 1:122:A:SER:CA | 1:122:A:SER:C  | 1:123:A:THR:N | 4        | 2.04          |
| (1,128) | 1:106:A:THR:N | 1:106:A:THR:CA | 1:106:A:THR:C  | 1:107:A:LEU:N | 3        | 2.04          |
| (1,88)  | 1:69:A:TYR:N  | 1:69:A:TYR:CA  | 1:69:A:TYR:C   | 1:70:A:THR:N  | 19       | 2.04          |
| (1,12)  | 1:11:A:ILE:N  | 1:11:A:ILE:CA  | 1:11:A:ILE:C   | 1:12:A:PHE:N  | 5        | 2.04          |
| (1,186) | 1:146:A:LEU:N | 1:146:A:LEU:CA | 1:146:A:LEU:C  | 1:147:A:ASN:N | 5        | 2.03          |
| (1,10)  | 1:10:A:ILE:N  | 1:10:A:ILE:CA  | 1:10:A:ILE:C   | 1:11:A:ILE:N  | 2        | 2.03          |
| (1,109) | 1:83:A:ILE:C  | 1:84:A:GLU:N   | 1:84:A:GLU:CA  | 1:84:A:GLU:C  | 16       | 2.02          |
| (1,122) | 1:90:A:ALA:N  | 1:90:A:ALA:CA  | 1:90:A:ALA:C   | 1:91:A:THR:N  | 3        | 2.01          |
| (1,80)  | 1:62:A:GLN:N  | 1:62:A:GLN:CA  | 1:62:A:GLN:C   | 1:63:A:ALA:N  | 6        | 2.01          |
| (1,128) | 1:106:A:THR:N | 1:106:A:THR:CA | 1:106:A:THR:C  | 1:107:A:LEU:N | 20       | 2.0           |
| (1,84)  | 1:67:A:ILE:N  | 1:67:A:ILE:CA  | 1:67:A:ILE:C   | 1:68:A:SER:N  | 20       | 2.0           |
| (1,54)  | 1:43:A:SER:N  | 1:43:A:SER:CA  | 1:43:A:SER:C   | 1:44:A:VAL:N  | 1        | 2.0           |
| (1,9)   | 1:9:A:LYS:C   | 1:10:A:ILE:N   | 1:10:A:ILE:CA  | 1:10:A:ILE:C  | 8        | 2.0           |
| (1,143) | 1:118:A:VAL:C | 1:119:A:THR:N  | 1:119:A:THR:CA | 1:119:A:THR:C | 6        | 1.99          |
| (1,129) | 1:106:A:THR:C | 1:107:A:LEU:N  | 1:107:A:LEU:CA | 1:107:A:LEU:C | 3        | 1.98          |
| (1,115) | 1:86:A:LEU:C  | 1:87:A:ASP:N   | 1:87:A:ASP:CA  | 1:87:A:ASP:C  | 9        | 1.98          |
| (1,9)   | 1:9:A:LYS:C   | 1:10:A:ILE:N   | 1:10:A:ILE:CA  | 1:10:A:ILE:C  | 17       | 1.98          |
| (1,94)  | 1:72:A:ALA:N  | 1:72:A:ALA:CA  | 1:72:A:ALA:C   | 1:73:A:GLU:N  | 19       | 1.97          |
| (1,172) | 1:139:A:GLU:N | 1:139:A:GLU:CA | 1:139:A:GLU:C  | 1:140:A:THR:N | 6        | 1.96          |
| (1,168) | 1:136:A:MET:N | 1:136:A:MET:CA | 1:136:A:MET:C  | 1:137:A:GLY:N | 16       | 1.95          |
| (1,109) | 1:83:A:ILE:C  | 1:84:A:GLU:N   | 1:84:A:GLU:CA  | 1:84:A:GLU:C  | 1        | 1.95          |
| (1,55)  | 1:43:A:SER:C  | 1:44:A:VAL:N   | 1:44:A:VAL:CA  | 1:44:A:VAL:C  | 15       | 1.94          |
| (1,15)  | 1:12:A:PHE:C  | 1:13:A:THR:N   | 1:13:A:THR:CA  | 1:13:A:THR:C  | 1        | 1.94          |
| (1,13)  | 1:11:A:ILE:C  | 1:12:A:PHE:N   | 1:12:A:PHE:CA  | 1:12:A:PHE:C  | 5        | 1.94          |
| (1,180) | 1:143:A:ASN:N | 1:143:A:ASN:CA | 1:143:A:ASN:C  | 1:144:A:SER:N | 1        | 1.93          |
| (1,26)  | 1:20:A:ILE:N  | 1:20:A:ILE:CA  | 1:20:A:ILE:C   | 1:21:A:ASN:N  | 4        | 1.93          |
| (1,26)  | 1:20:A:ILE:N  | 1:20:A:ILE:CA  | 1:20:A:ILE:C   | 1:21:A:ASN:N  | 11       | 1.93          |
| (1,9)   | 1:9:A:LYS:C   | 1:10:A:ILE:N   | 1:10:A:ILE:CA  | 1:10:A:ILE:C  | 10       | 1.93          |
| (1,121) | 1:89:A:PHE:C  | 1:90:A:ALA:N   | 1:90:A:ALA:CA  | 1:90:A:ALA:C  | 2        | 1.92          |
| (1,84)  | 1:67:A:ILE:N  | 1:67:A:ILE:CA  | 1:67:A:ILE:C   | 1:68:A:SER:N  | 14       | 1.92          |
| (1,12)  | 1:11:A:ILE:N  | 1:11:A:ILE:CA  | 1:11:A:ILE:C   | 1:12:A:PHE:N  | 9        | 1.92          |

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Continued from previous page...

| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,77)  | 1:60:A:ALA:C  | 1:61:A:ILE:N   | 1:61:A:ILE:CA  | 1:61:A:ILE:C  | 3        | 1.91          |
| (1,93)  | 1:71:A:ILE:C  | 1:72:A:ALA:N   | 1:72:A:ALA:CA  | 1:72:A:ALA:C  | 8        | 1.89          |
| (1,121) | 1:89:A:PHE:C  | 1:90:A:ALA:N   | 1:90:A:ALA:CA  | 1:90:A:ALA:C  | 14       | 1.87          |
| (1,66)  | 1:50:A:ASN:N  | 1:50:A:ASN:CA  | 1:50:A:ASN:C   | 1:51:A:ALA:N  | 20       | 1.86          |
| (1,88)  | 1:69:A:TYR:N  | 1:69:A:TYR:CA  | 1:69:A:TYR:C   | 1:70:A:THR:N  | 10       | 1.85          |
| (1,84)  | 1:67:A:ILE:N  | 1:67:A:ILE:CA  | 1:67:A:ILE:C   | 1:68:A:SER:N  | 13       | 1.85          |
| (1,114) | 1:86:A:LEU:N  | 1:86:A:LEU:CA  | 1:86:A:LEU:C   | 1:87:A:ASP:N  | 16       | 1.84          |
| (1,99)  | 1:75:A:LEU:C  | 1:76:A:GLN:N   | 1:76:A:GLN:CA  | 1:76:A:GLN:C  | 14       | 1.84          |
| (1,146) | 1:120:A:SER:N | 1:120:A:SER:CA | 1:120:A:SER:C  | 1:121:A:THR:N | 19       | 1.82          |
| (1,168) | 1:136:A:MET:N | 1:136:A:MET:CA | 1:136:A:MET:C  | 1:137:A:GLY:N | 20       | 1.81          |
| (1,12)  | 1:11:A:ILE:N  | 1:11:A:ILE:CA  | 1:11:A:ILE:C   | 1:12:A:PHE:N  | 11       | 1.81          |
| (1,128) | 1:106:A:THR:N | 1:106:A:THR:CA | 1:106:A:THR:C  | 1:107:A:LEU:N | 17       | 1.8           |
| (1,121) | 1:89:A:PHE:C  | 1:90:A:ALA:N   | 1:90:A:ALA:CA  | 1:90:A:ALA:C  | 7        | 1.8           |
| (1,118) | 1:88:A:TYR:N  | 1:88:A:TYR:CA  | 1:88:A:TYR:C   | 1:89:A:PHE:N  | 15       | 1.8           |
| (1,150) | 1:122:A:SER:N | 1:122:A:SER:CA | 1:122:A:SER:C  | 1:123:A:THR:N | 17       | 1.78          |
| (1,13)  | 1:11:A:ILE:C  | 1:12:A:PHE:N   | 1:12:A:PHE:CA  | 1:12:A:PHE:C  | 18       | 1.77          |
| (1,9)   | 1:9:A:LYS:C   | 1:10:A:ILE:N   | 1:10:A:ILE:CA  | 1:10:A:ILE:C  | 9        | 1.77          |
| (1,9)   | 1:9:A:LYS:C   | 1:10:A:ILE:N   | 1:10:A:ILE:CA  | 1:10:A:ILE:C  | 18       | 1.77          |
| (1,140) | 1:117:A:THR:N | 1:117:A:THR:CA | 1:117:A:THR:C  | 1:118:A:VAL:N | 15       | 1.76          |
| (1,80)  | 1:62:A:GLN:N  | 1:62:A:GLN:CA  | 1:62:A:GLN:C   | 1:63:A:ALA:N  | 7        | 1.76          |
| (1,45)  | 1:30:A:ARG:C  | 1:31:A:GLU:N   | 1:31:A:GLU:CA  | 1:31:A:GLU:C  | 20       | 1.76          |
| (1,21)  | 1:15:A:THR:C  | 1:16:A:PHE:N   | 1:16:A:PHE:CA  | 1:16:A:PHE:C  | 10       | 1.76          |
| (1,140) | 1:117:A:THR:N | 1:117:A:THR:CA | 1:117:A:THR:C  | 1:118:A:VAL:N | 8        | 1.75          |
| (1,1)   | 1:3:A:ILE:C   | 1:4:A:GLU:N    | 1:4:A:GLU:CA   | 1:4:A:GLU:C   | 9        | 1.75          |
| (1,118) | 1:88:A:TYR:N  | 1:88:A:TYR:CA  | 1:88:A:TYR:C   | 1:89:A:PHE:N  | 18       | 1.74          |
| (1,114) | 1:86:A:LEU:N  | 1:86:A:LEU:CA  | 1:86:A:LEU:C   | 1:87:A:ASP:N  | 9        | 1.74          |
| (1,130) | 1:107:A:LEU:N | 1:107:A:LEU:CA | 1:107:A:LEU:C  | 1:108:A:ASN:N | 18       | 1.72          |
| (1,88)  | 1:69:A:TYR:N  | 1:69:A:TYR:CA  | 1:69:A:TYR:C   | 1:70:A:THR:N  | 16       | 1.72          |
| (1,15)  | 1:12:A:PHE:C  | 1:13:A:THR:N   | 1:13:A:THR:CA  | 1:13:A:THR:C  | 16       | 1.72          |
| (1,130) | 1:107:A:LEU:N | 1:107:A:LEU:CA | 1:107:A:LEU:C  | 1:108:A:ASN:N | 8        | 1.71          |
| (1,174) | 1:140:A:THR:N | 1:140:A:THR:CA | 1:140:A:THR:C  | 1:141:A:GLY:N | 5        | 1.7           |
| (1,116) | 1:87:A:ASP:N  | 1:87:A:ASP:CA  | 1:87:A:ASP:C   | 1:88:A:TYR:N  | 13       | 1.7           |
| (1,93)  | 1:71:A:ILE:C  | 1:72:A:ALA:N   | 1:72:A:ALA:CA  | 1:72:A:ALA:C  | 16       | 1.7           |
| (1,201) | 1:153:A:LEU:C | 1:154:A:ASN:N  | 1:154:A:ASN:CA | 1:154:A:ASN:C | 1        | 1.69          |
| (1,176) | 1:141:A:GLY:N | 1:141:A:GLY:CA | 1:141:A:GLY:C  | 1:142:A:MET:N | 20       | 1.69          |
| (1,12)  | 1:11:A:ILE:N  | 1:11:A:ILE:CA  | 1:11:A:ILE:C   | 1:12:A:PHE:N  | 18       | 1.68          |
| (1,140) | 1:117:A:THR:N | 1:117:A:THR:CA | 1:117:A:THR:C  | 1:118:A:VAL:N | 10       | 1.67          |
| (1,114) | 1:86:A:LEU:N  | 1:86:A:LEU:CA  | 1:86:A:LEU:C   | 1:87:A:ASP:N  | 2        | 1.67          |
| (1,114) | 1:86:A:LEU:N  | 1:86:A:LEU:CA  | 1:86:A:LEU:C   | 1:87:A:ASP:N  | 11       | 1.67          |
| (1,109) | 1:83:A:ILE:C  | 1:84:A:GLU:N   | 1:84:A:GLU:CA  | 1:84:A:GLU:C  | 2        | 1.67          |
| (1,148) | 1:121:A:THR:N | 1:121:A:THR:CA | 1:121:A:THR:C  | 1:122:A:SER:N | 11       | 1.66          |
| (1,88)  | 1:69:A:TYR:N  | 1:69:A:TYR:CA  | 1:69:A:TYR:C   | 1:70:A:THR:N  | 15       | 1.66          |
| (1,62)  | 1:48:A:ASP:N  | 1:48:A:ASP:CA  | 1:48:A:ASP:C   | 1:49:A:PHE:N  | 20       | 1.66          |
| (1,168) | 1:136:A:MET:N | 1:136:A:MET:CA | 1:136:A:MET:C  | 1:137:A:GLY:N | 2        | 1.65          |
| (1,148) | 1:121:A:THR:N | 1:121:A:THR:CA | 1:121:A:THR:C  | 1:122:A:SER:N | 19       | 1.65          |
| (1,93)  | 1:71:A:ILE:C  | 1:72:A:ALA:N   | 1:72:A:ALA:CA  | 1:72:A:ALA:C  | 2        | 1.65          |
| (1,65)  | 1:49:A:PHE:C  | 1:50:A:ASN:N   | 1:50:A:ASN:CA  | 1:50:A:ASN:C  | 18       | 1.65          |
| (1,146) | 1:120:A:SER:N | 1:120:A:SER:CA | 1:120:A:SER:C  | 1:121:A:THR:N | 17       | 1.64          |
| (1,98)  | 1:74:A:TYR:N  | 1:74:A:TYR:CA  | 1:74:A:TYR:C   | 1:75:A:LEU:N  | 4        | 1.64          |
| (1,41)  | 1:28:A:THR:C  | 1:29:A:LYS:N   | 1:29:A:LYS:CA  | 1:29:A:LYS:C  | 3        | 1.64          |
| (1,80)  | 1:62:A:GLN:N  | 1:62:A:GLN:CA  | 1:62:A:GLN:C   | 1:63:A:ALA:N  | 15       | 1.63          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,146) | 1:120:A:SER:N | 1:120:A:SER:CA | 1:120:A:SER:C  | 1:121:A:THR:N | 1        | 1.62          |
| (1,122) | 1:90:A:ALA:N  | 1:90:A:ALA:CA  | 1:90:A:ALA:C   | 1:91:A:THR:N  | 15       | 1.62          |
| (1,118) | 1:88:A:TYR:N  | 1:88:A:TYR:CA  | 1:88:A:TYR:C   | 1:89:A:PHE:N  | 9        | 1.62          |
| (1,113) | 1:85:A:TYR:C  | 1:86:A:LEU:N   | 1:86:A:LEU:CA  | 1:86:A:LEU:C  | 16       | 1.62          |
| (1,26)  | 1:20:A:ILE:N  | 1:20:A:ILE:CA  | 1:20:A:ILE:C   | 1:21:A:ASN:N  | 16       | 1.62          |
| (1,129) | 1:106:A:THR:C | 1:107:A:LEU:N  | 1:107:A:LEU:CA | 1:107:A:LEU:C | 15       | 1.61          |
| (1,15)  | 1:12:A:PHE:C  | 1:13:A:THR:N   | 1:13:A:THR:CA  | 1:13:A:THR:C  | 6        | 1.61          |
| (1,99)  | 1:75:A:LEU:C  | 1:76:A:GLN:N   | 1:76:A:GLN:CA  | 1:76:A:GLN:C  | 1        | 1.6           |
| (1,70)  | 1:57:A:ALA:N  | 1:57:A:ALA:CA  | 1:57:A:ALA:C   | 1:58:A:PHE:N  | 7        | 1.6           |
| (1,151) | 1:122:A:SER:C | 1:123:A:THR:N  | 1:123:A:THR:CA | 1:123:A:THR:C | 12       | 1.59          |
| (1,109) | 1:83:A:ILE:C  | 1:84:A:GLU:N   | 1:84:A:GLU:CA  | 1:84:A:GLU:C  | 6        | 1.59          |
| (1,88)  | 1:69:A:TYR:N  | 1:69:A:TYR:CA  | 1:69:A:TYR:C   | 1:70:A:THR:N  | 4        | 1.59          |
| (1,172) | 1:139:A:GLU:N | 1:139:A:GLU:CA | 1:139:A:GLU:C  | 1:140:A:THR:N | 10       | 1.58          |
| (1,12)  | 1:11:A:ILE:N  | 1:11:A:ILE:CA  | 1:11:A:ILE:C   | 1:12:A:PHE:N  | 15       | 1.57          |
| (1,201) | 1:153:A:LEU:C | 1:154:A:ASN:N  | 1:154:A:ASN:CA | 1:154:A:ASN:C | 17       | 1.56          |
| (1,129) | 1:106:A:THR:C | 1:107:A:LEU:N  | 1:107:A:LEU:CA | 1:107:A:LEU:C | 12       | 1.56          |
| (1,50)  | 1:33:A:PHE:N  | 1:33:A:PHE:CA  | 1:33:A:PHE:C   | 1:34:A:GLU:N  | 18       | 1.56          |
| (1,21)  | 1:15:A:THR:C  | 1:16:A:PHE:N   | 1:16:A:PHE:CA  | 1:16:A:PHE:C  | 7        | 1.56          |
| (1,77)  | 1:60:A:ALA:C  | 1:61:A:ILE:N   | 1:61:A:ILE:CA  | 1:61:A:ILE:C  | 5        | 1.54          |
| (1,152) | 1:123:A:THR:N | 1:123:A:THR:CA | 1:123:A:THR:C  | 1:124:A:PHE:N | 2        | 1.52          |
| (1,102) | 1:77:A:VAL:N  | 1:77:A:VAL:CA  | 1:77:A:VAL:C   | 1:78:A:ASP:N  | 4        | 1.51          |
| (1,190) | 1:148:A:GLN:N | 1:148:A:GLN:CA | 1:148:A:GLN:C  | 1:149:A:LEU:N | 1        | 1.5           |
| (1,180) | 1:143:A:ASN:N | 1:143:A:ASN:CA | 1:143:A:ASN:C  | 1:144:A:SER:N | 12       | 1.5           |
| (1,146) | 1:120:A:SER:N | 1:120:A:SER:CA | 1:120:A:SER:C  | 1:121:A:THR:N | 16       | 1.5           |
| (1,55)  | 1:43:A:SER:C  | 1:44:A:VAL:N   | 1:44:A:VAL:CA  | 1:44:A:VAL:C  | 12       | 1.5           |
| (1,13)  | 1:11:A:ILE:C  | 1:12:A:PHE:N   | 1:12:A:PHE:CA  | 1:12:A:PHE:C  | 19       | 1.5           |
| (1,136) | 1:115:A:LYS:N | 1:115:A:LYS:CA | 1:115:A:LYS:C  | 1:116:A:THR:N | 1        | 1.49          |
| (1,128) | 1:106:A:THR:N | 1:106:A:THR:CA | 1:106:A:THR:C  | 1:107:A:LEU:N | 4        | 1.49          |
| (1,128) | 1:106:A:THR:N | 1:106:A:THR:CA | 1:106:A:THR:C  | 1:107:A:LEU:N | 1        | 1.48          |
| (1,58)  | 1:45:A:THR:N  | 1:45:A:THR:CA  | 1:45:A:THR:C   | 1:46:A:VAL:N  | 3        | 1.48          |
| (1,43)  | 1:29:A:LYS:C  | 1:30:A:ARG:N   | 1:30:A:ARG:CA  | 1:30:A:ARG:C  | 3        | 1.48          |
| (1,172) | 1:139:A:GLU:N | 1:139:A:GLU:CA | 1:139:A:GLU:C  | 1:140:A:THR:N | 18       | 1.47          |
| (1,168) | 1:136:A:MET:N | 1:136:A:MET:CA | 1:136:A:MET:C  | 1:137:A:GLY:N | 14       | 1.47          |
| (1,115) | 1:86:A:LEU:C  | 1:87:A:ASP:N   | 1:87:A:ASP:CA  | 1:87:A:ASP:C  | 17       | 1.47          |
| (1,113) | 1:85:A:TYR:C  | 1:86:A:LEU:N   | 1:86:A:LEU:CA  | 1:86:A:LEU:C  | 8        | 1.47          |
| (1,109) | 1:83:A:ILE:C  | 1:84:A:GLU:N   | 1:84:A:GLU:CA  | 1:84:A:GLU:C  | 11       | 1.46          |
| (1,54)  | 1:43:A:SER:N  | 1:43:A:SER:CA  | 1:43:A:SER:C   | 1:44:A:VAL:N  | 2        | 1.46          |
| (1,33)  | 1:23:A:VAL:C  | 1:24:A:PHE:N   | 1:24:A:PHE:CA  | 1:24:A:PHE:C  | 14       | 1.46          |
| (1,15)  | 1:12:A:PHE:C  | 1:13:A:THR:N   | 1:13:A:THR:CA  | 1:13:A:THR:C  | 2        | 1.46          |
| (1,150) | 1:122:A:SER:N | 1:122:A:SER:CA | 1:122:A:SER:C  | 1:123:A:THR:N | 1        | 1.45          |
| (1,140) | 1:117:A:THR:N | 1:117:A:THR:CA | 1:117:A:THR:C  | 1:118:A:VAL:N | 6        | 1.45          |
| (1,20)  | 1:15:A:THR:N  | 1:15:A:THR:CA  | 1:15:A:THR:C   | 1:16:A:PHE:N  | 2        | 1.45          |
| (1,180) | 1:143:A:ASN:N | 1:143:A:ASN:CA | 1:143:A:ASN:C  | 1:144:A:SER:N | 20       | 1.44          |
| (1,150) | 1:122:A:SER:N | 1:122:A:SER:CA | 1:122:A:SER:C  | 1:123:A:THR:N | 7        | 1.44          |
| (1,150) | 1:122:A:SER:N | 1:122:A:SER:CA | 1:122:A:SER:C  | 1:123:A:THR:N | 13       | 1.44          |
| (1,124) | 1:104:A:HIS:N | 1:104:A:HIS:CA | 1:104:A:HIS:C  | 1:105:A:ILE:N | 8        | 1.44          |
| (1,113) | 1:85:A:TYR:C  | 1:86:A:LEU:N   | 1:86:A:LEU:CA  | 1:86:A:LEU:C  | 10       | 1.44          |
| (1,26)  | 1:20:A:ILE:N  | 1:20:A:ILE:CA  | 1:20:A:ILE:C   | 1:21:A:ASN:N  | 10       | 1.44          |
| (1,1)   | 1:3:A:ILE:C   | 1:4:A:GLU:N    | 1:4:A:GLU:CA   | 1:4:A:GLU:C   | 19       | 1.44          |
| (1,172) | 1:139:A:GLU:N | 1:139:A:GLU:CA | 1:139:A:GLU:C  | 1:140:A:THR:N | 12       | 1.43          |
| (1,88)  | 1:69:A:TYR:N  | 1:69:A:TYR:CA  | 1:69:A:TYR:C   | 1:70:A:THR:N  | 1        | 1.43          |

Continued on next page...

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,61)  | 1:47:A:TYR:C  | 1:48:A:ASP:N   | 1:48:A:ASP:CA  | 1:48:A:ASP:C  | 7        | 1.43          |
| (1,129) | 1:106:A:THR:C | 1:107:A:LEU:N  | 1:107:A:LEU:CA | 1:107:A:LEU:C | 1        | 1.42          |
| (1,40)  | 1:28:A:THR:N  | 1:28:A:THR:CA  | 1:28:A:THR:C   | 1:29:A:LYS:N  | 16       | 1.42          |
| (1,16)  | 1:13:A:THR:N  | 1:13:A:THR:CA  | 1:13:A:THR:C   | 1:14:A:ARG:N  | 12       | 1.42          |
| (1,80)  | 1:62:A:GLN:N  | 1:62:A:GLN:CA  | 1:62:A:GLN:C   | 1:63:A:ALA:N  | 20       | 1.41          |
| (1,77)  | 1:60:A:ALA:C  | 1:61:A:ILE:N   | 1:61:A:ILE:CA  | 1:61:A:ILE:C  | 11       | 1.41          |
| (1,66)  | 1:50:A:ASN:N  | 1:50:A:ASN:CA  | 1:50:A:ASN:C   | 1:51:A:ALA:N  | 9        | 1.41          |
| (1,7)   | 1:8:A:ASN:C   | 1:9:A:LYS:N    | 1:9:A:LYS:CA   | 1:9:A:LYS:C   | 2        | 1.41          |
| (1,178) | 1:142:A:MET:N | 1:142:A:MET:CA | 1:142:A:MET:C  | 1:143:A:ASN:N | 5        | 1.39          |
| (1,115) | 1:86:A:LEU:C  | 1:87:A:ASP:N   | 1:87:A:ASP:CA  | 1:87:A:ASP:C  | 12       | 1.38          |
| (1,92)  | 1:71:A:ILE:N  | 1:71:A:ILE:CA  | 1:71:A:ILE:C   | 1:72:A:ALA:N  | 20       | 1.38          |
| (1,66)  | 1:50:A:ASN:N  | 1:50:A:ASN:CA  | 1:50:A:ASN:C   | 1:51:A:ALA:N  | 3        | 1.38          |
| (1,1)   | 1:3:A:ILE:C   | 1:4:A:GLU:N    | 1:4:A:GLU:CA   | 1:4:A:GLU:C   | 7        | 1.38          |
| (1,146) | 1:120:A:SER:N | 1:120:A:SER:CA | 1:120:A:SER:C  | 1:121:A:THR:N | 4        | 1.36          |
| (1,176) | 1:141:A:GLY:N | 1:141:A:GLY:CA | 1:141:A:GLY:C  | 1:142:A:MET:N | 9        | 1.35          |
| (1,129) | 1:106:A:THR:C | 1:107:A:LEU:N  | 1:107:A:LEU:CA | 1:107:A:LEU:C | 18       | 1.35          |
| (1,198) | 1:152:A:LEU:N | 1:152:A:LEU:CA | 1:152:A:LEU:C  | 1:153:A:LEU:N | 16       | 1.34          |
| (1,84)  | 1:67:A:ILE:N  | 1:67:A:ILE:CA  | 1:67:A:ILE:C   | 1:68:A:SER:N  | 7        | 1.34          |
| (1,13)  | 1:11:A:ILE:C  | 1:12:A:PHE:N   | 1:12:A:PHE:CA  | 1:12:A:PHE:C  | 1        | 1.33          |
| (1,102) | 1:77:A:VAL:N  | 1:77:A:VAL:CA  | 1:77:A:VAL:C   | 1:78:A:ASP:N  | 1        | 1.32          |
| (1,65)  | 1:49:A:PHE:C  | 1:50:A:ASN:N   | 1:50:A:ASN:CA  | 1:50:A:ASN:C  | 1        | 1.32          |
| (1,129) | 1:106:A:THR:C | 1:107:A:LEU:N  | 1:107:A:LEU:CA | 1:107:A:LEU:C | 6        | 1.31          |
| (1,122) | 1:90:A:ALA:N  | 1:90:A:ALA:CA  | 1:90:A:ALA:C   | 1:91:A:THR:N  | 16       | 1.31          |
| (1,55)  | 1:43:A:SER:C  | 1:44:A:VAL:N   | 1:44:A:VAL:CA  | 1:44:A:VAL:C  | 17       | 1.3           |
| (1,13)  | 1:11:A:ILE:C  | 1:12:A:PHE:N   | 1:12:A:PHE:CA  | 1:12:A:PHE:C  | 11       | 1.3           |
| (1,1)   | 1:3:A:ILE:C   | 1:4:A:GLU:N    | 1:4:A:GLU:CA   | 1:4:A:GLU:C   | 3        | 1.29          |
| (1,116) | 1:87:A:ASP:N  | 1:87:A:ASP:CA  | 1:87:A:ASP:C   | 1:88:A:TYR:N  | 11       | 1.28          |
| (1,118) | 1:88:A:TYR:N  | 1:88:A:TYR:CA  | 1:88:A:TYR:C   | 1:89:A:PHE:N  | 2        | 1.27          |
| (1,140) | 1:117:A:THR:N | 1:117:A:THR:CA | 1:117:A:THR:C  | 1:118:A:VAL:N | 3        | 1.25          |
| (1,118) | 1:88:A:TYR:N  | 1:88:A:TYR:CA  | 1:88:A:TYR:C   | 1:89:A:PHE:N  | 4        | 1.25          |
| (1,40)  | 1:28:A:THR:N  | 1:28:A:THR:CA  | 1:28:A:THR:C   | 1:29:A:LYS:N  | 9        | 1.25          |
| (1,114) | 1:86:A:LEU:N  | 1:86:A:LEU:CA  | 1:86:A:LEU:C   | 1:87:A:ASP:N  | 19       | 1.23          |
| (1,80)  | 1:62:A:GLN:N  | 1:62:A:GLN:CA  | 1:62:A:GLN:C   | 1:63:A:ALA:N  | 10       | 1.23          |
| (1,66)  | 1:50:A:ASN:N  | 1:50:A:ASN:CA  | 1:50:A:ASN:C   | 1:51:A:ALA:N  | 10       | 1.23          |
| (1,7)   | 1:8:A:ASN:C   | 1:9:A:LYS:N    | 1:9:A:LYS:CA   | 1:9:A:LYS:C   | 15       | 1.23          |
| (1,148) | 1:121:A:THR:N | 1:121:A:THR:CA | 1:121:A:THR:C  | 1:122:A:SER:N | 14       | 1.22          |
| (1,130) | 1:107:A:LEU:N | 1:107:A:LEU:CA | 1:107:A:LEU:C  | 1:108:A:ASN:N | 12       | 1.21          |
| (1,124) | 1:104:A:HIS:N | 1:104:A:HIS:CA | 1:104:A:HIS:C  | 1:105:A:ILE:N | 14       | 1.21          |
| (1,109) | 1:83:A:ILE:C  | 1:84:A:GLU:N   | 1:84:A:GLU:CA  | 1:84:A:GLU:C  | 20       | 1.21          |
| (1,185) | 1:145:A:THR:C | 1:146:A:LEU:N  | 1:146:A:LEU:CA | 1:146:A:LEU:C | 12       | 1.2           |
| (1,102) | 1:77:A:VAL:N  | 1:77:A:VAL:CA  | 1:77:A:VAL:C   | 1:78:A:ASP:N  | 6        | 1.2           |
| (1,66)  | 1:50:A:ASN:N  | 1:50:A:ASN:CA  | 1:50:A:ASN:C   | 1:51:A:ALA:N  | 19       | 1.2           |
| (1,12)  | 1:11:A:ILE:N  | 1:11:A:ILE:CA  | 1:11:A:ILE:C   | 1:12:A:PHE:N  | 7        | 1.2           |
| (1,61)  | 1:47:A:TYR:C  | 1:48:A:ASP:N   | 1:48:A:ASP:CA  | 1:48:A:ASP:C  | 14       | 1.19          |
| (1,146) | 1:120:A:SER:N | 1:120:A:SER:CA | 1:120:A:SER:C  | 1:121:A:THR:N | 7        | 1.18          |
| (1,93)  | 1:71:A:ILE:C  | 1:72:A:ALA:N   | 1:72:A:ALA:CA  | 1:72:A:ALA:C  | 6        | 1.18          |
| (1,137) | 1:115:A:LYS:C | 1:116:A:THR:N  | 1:116:A:THR:CA | 1:116:A:THR:C | 18       | 1.17          |
| (1,98)  | 1:74:A:TYR:N  | 1:74:A:TYR:CA  | 1:74:A:TYR:C   | 1:75:A:LEU:N  | 5        | 1.17          |
| (1,102) | 1:77:A:VAL:N  | 1:77:A:VAL:CA  | 1:77:A:VAL:C   | 1:78:A:ASP:N  | 18       | 1.16          |
| (1,122) | 1:90:A:ALA:N  | 1:90:A:ALA:CA  | 1:90:A:ALA:C   | 1:91:A:THR:N  | 2        | 1.15          |
| (1,40)  | 1:28:A:THR:N  | 1:28:A:THR:CA  | 1:28:A:THR:C   | 1:29:A:LYS:N  | 13       | 1.15          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,155) | 1:129:A:ALA:C | 1:130:A:ALA:N  | 1:130:A:ALA:CA | 1:130:A:ALA:C | 19       | 1.14          |
| (1,121) | 1:89:A:PHE:C  | 1:90:A:ALA:N   | 1:90:A:ALA:CA  | 1:90:A:ALA:C  | 1        | 1.14          |
| (1,71)  | 1:57:A:ALA:C  | 1:58:A:PHE:N   | 1:58:A:PHE:CA  | 1:58:A:PHE:C  | 13       | 1.14          |
| (1,66)  | 1:50:A:ASN:N  | 1:50:A:ASN:CA  | 1:50:A:ASN:C   | 1:51:A:ALA:N  | 17       | 1.14          |
| (1,124) | 1:104:A:HIS:N | 1:104:A:HIS:CA | 1:104:A:HIS:C  | 1:105:A:ILE:N | 20       | 1.13          |
| (1,98)  | 1:74:A:TYR:N  | 1:74:A:TYR:CA  | 1:74:A:TYR:C   | 1:75:A:LEU:N  | 11       | 1.13          |
| (1,45)  | 1:30:A:ARG:C  | 1:31:A:GLU:N   | 1:31:A:GLU:CA  | 1:31:A:GLU:C  | 14       | 1.13          |
| (1,71)  | 1:57:A:ALA:C  | 1:58:A:PHE:N   | 1:58:A:PHE:CA  | 1:58:A:PHE:C  | 14       | 1.12          |
| (1,148) | 1:121:A:THR:N | 1:121:A:THR:CA | 1:121:A:THR:C  | 1:122:A:SER:N | 20       | 1.11          |
| (1,65)  | 1:49:A:PHE:C  | 1:50:A:ASN:N   | 1:50:A:ASN:CA  | 1:50:A:ASN:C  | 2        | 1.11          |
| (1,50)  | 1:33:A:PHE:N  | 1:33:A:PHE:CA  | 1:33:A:PHE:C   | 1:34:A:GLU:N  | 8        | 1.1           |
| (1,116) | 1:87:A:ASP:N  | 1:87:A:ASP:CA  | 1:87:A:ASP:C   | 1:88:A:TYR:N  | 3        | 1.09          |
| (1,13)  | 1:11:A:ILE:C  | 1:12:A:PHE:N   | 1:12:A:PHE:CA  | 1:12:A:PHE:C  | 20       | 1.07          |
| (1,201) | 1:153:A:LEU:C | 1:154:A:ASN:N  | 1:154:A:ASN:CA | 1:154:A:ASN:C | 4        | 1.06          |
| (1,185) | 1:145:A:THR:C | 1:146:A:LEU:N  | 1:146:A:LEU:CA | 1:146:A:LEU:C | 15       | 1.06          |
| (1,185) | 1:145:A:THR:C | 1:146:A:LEU:N  | 1:146:A:LEU:CA | 1:146:A:LEU:C | 5        | 1.05          |
| (1,185) | 1:145:A:THR:C | 1:146:A:LEU:N  | 1:146:A:LEU:CA | 1:146:A:LEU:C | 19       | 1.05          |
| (1,174) | 1:140:A:THR:N | 1:140:A:THR:CA | 1:140:A:THR:C  | 1:141:A:GLY:N | 10       | 1.05          |
| (1,152) | 1:123:A:THR:N | 1:123:A:THR:CA | 1:123:A:THR:C  | 1:124:A:PHE:N | 6        | 1.05          |
| (1,128) | 1:106:A:THR:N | 1:106:A:THR:CA | 1:106:A:THR:C  | 1:107:A:LEU:N | 18       | 1.05          |
| (1,124) | 1:104:A:HIS:N | 1:104:A:HIS:CA | 1:104:A:HIS:C  | 1:105:A:ILE:N | 18       | 1.04          |
| (1,109) | 1:83:A:ILE:C  | 1:84:A:GLU:N   | 1:84:A:GLU:CA  | 1:84:A:GLU:C  | 17       | 1.04          |
| (1,181) | 1:143:A:ASN:C | 1:144:A:SER:N  | 1:144:A:SER:CA | 1:144:A:SER:C | 17       | 1.03          |
| (1,9)   | 1:9:A:LYS:C   | 1:10:A:ILE:N   | 1:10:A:ILE:CA  | 1:10:A:ILE:C  | 5        | 1.03          |
| (1,185) | 1:145:A:THR:C | 1:146:A:LEU:N  | 1:146:A:LEU:CA | 1:146:A:LEU:C | 4        | 1.02          |
| (1,116) | 1:87:A:ASP:N  | 1:87:A:ASP:CA  | 1:87:A:ASP:C   | 1:88:A:TYR:N  | 19       | 1.02          |
| (1,71)  | 1:57:A:ALA:C  | 1:58:A:PHE:N   | 1:58:A:PHE:CA  | 1:58:A:PHE:C  | 6        | 1.02          |
| (1,55)  | 1:43:A:SER:C  | 1:44:A:VAL:N   | 1:44:A:VAL:CA  | 1:44:A:VAL:C  | 1        | 1.02          |
| (1,176) | 1:141:A:GLY:N | 1:141:A:GLY:CA | 1:141:A:GLY:C  | 1:142:A:MET:N | 18       | 1.01          |
| (1,115) | 1:86:A:LEU:C  | 1:87:A:ASP:N   | 1:87:A:ASP:CA  | 1:87:A:ASP:C  | 4        | 1.01          |
| (1,14)  | 1:12:A:PHE:N  | 1:12:A:PHE:CA  | 1:12:A:PHE:C   | 1:13:A:THR:N  | 13       | 1.01          |