



# Full wwPDB NMR Structure Validation Report ⓘ

Aug 11, 2025 – 04:11 pm BST

PDB ID : 9HDI / pdb\_00009hdi  
BMRB ID : 50124  
Title : N-terminally truncated CanA from *Pyrodicticum abyssi* - K1-CanA  
Authors : Munte, C.E.; Kalbitzer, H.R.; Kreitner, R.R.; Stetter, K.O.  
Deposited on : 2024-11-12

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0rc1  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
wwPDB-RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
wwPDB-ShiftChecker : v1.2  
BMRB Restraints Analysis : v1.2  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.45.1

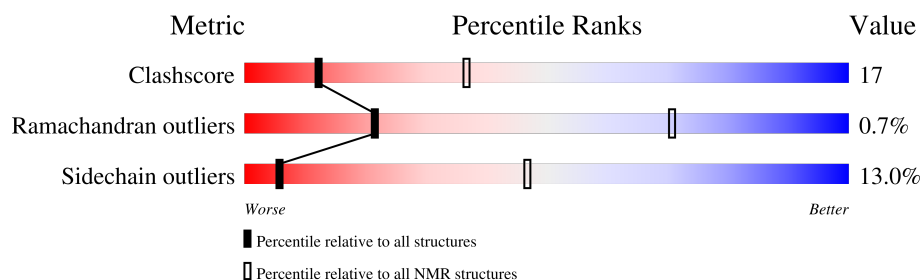
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 95%.

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



| Metric                | Whole archive<br>(#Entries) | NMR archive<br>(#Entries) |
|-----------------------|-----------------------------|---------------------------|
| Clashscore            | 210492                      | 14027                     |
| Ramachandran outliers | 207382                      | 12486                     |
| Sidechain outliers    | 206894                      | 12463                     |

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

| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 1   | A     | 183    | <div> <div style="width: 54%; background-color: green;"></div> <div style="width: 19%; background-color: yellow;"></div> <div style="width: 1%; background-color: orange;"></div> <div style="width: 19%; background-color: cyan;"></div> <div style="width: 6%; background-color: grey;"></div> </div> <div>54% 19% • 19% 6%</div> |

## 2 Ensemble composition and analysis

This entry contains 10 models. Model 4 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

| Well-defined (core) protein residues |   |                   |              |
|--------------------------------------|---|-------------------|--------------|
| Well-defined core                    | Residue range (total)                                     | Backbone RMSD (Å) | Medoid model |
| 1                                    | A:23-A:33, A:39-A:87,<br>A:95-A:119, A:131-A:183<br>(138) | 0.70              | 4            |

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

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

The models can be grouped into 2 clusters and 4 single-model clusters were found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2638 atoms, of which 1317 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Cannulae forming protein.

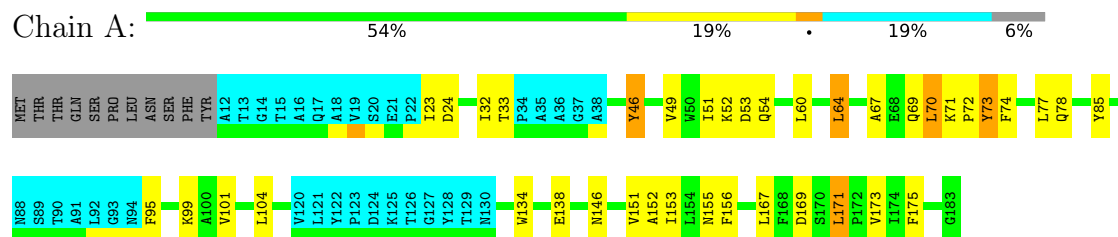
| Mol | Chain | Residues | Atoms |     |      |     |     |   | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|-------|
| 1   | A     | 172      | Total | C   | H    | N   | O   | S | 0     |
|     |       |          | 2638  | 854 | 1317 | 205 | 261 | 1 |       |

## 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: Cannulae forming protein

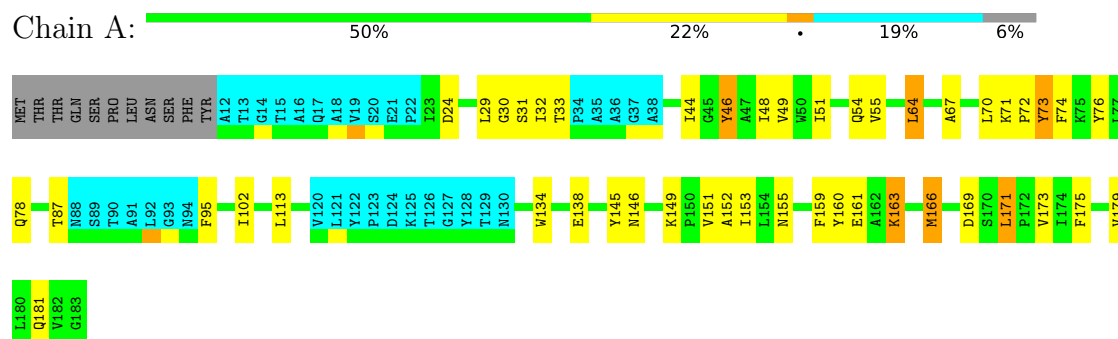


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

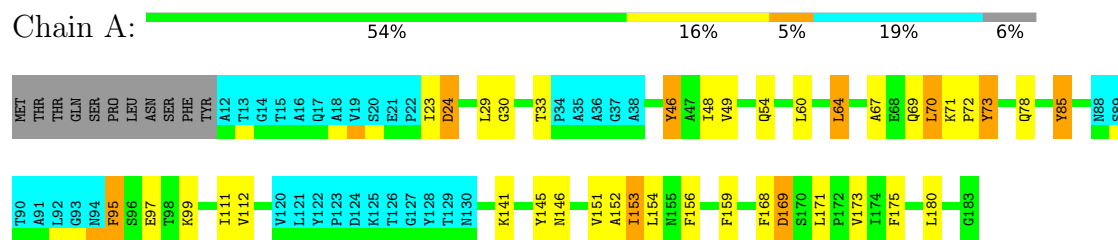
#### 4.2.1 Score per residue for model 1

- Molecule 1: Cannulae forming protein



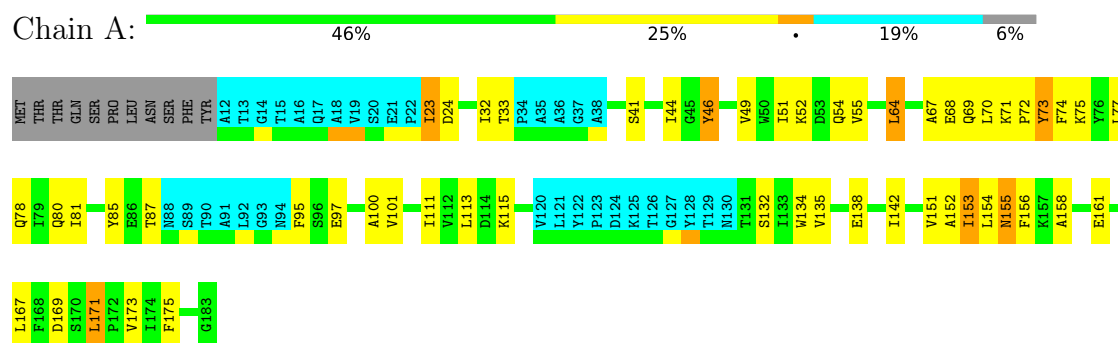
#### 4.2.2 Score per residue for model 2

- Molecule 1: Cannulae forming protein



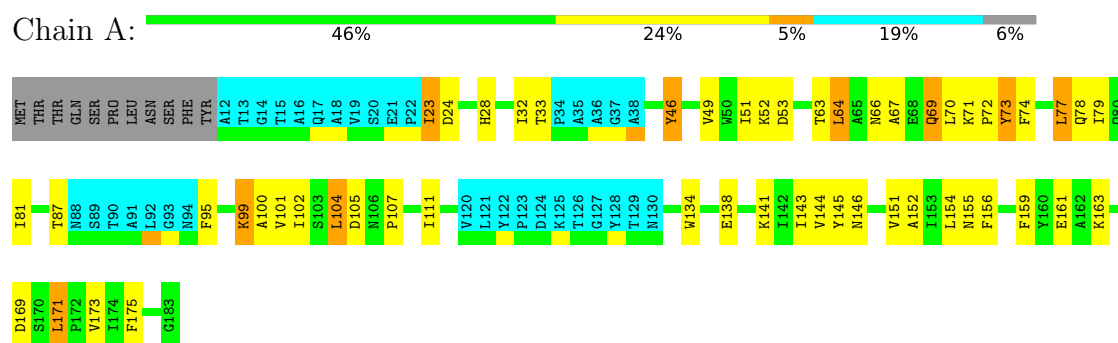
#### 4.2.3 Score per residue for model 3

- Molecule 1: Cannulae forming protein



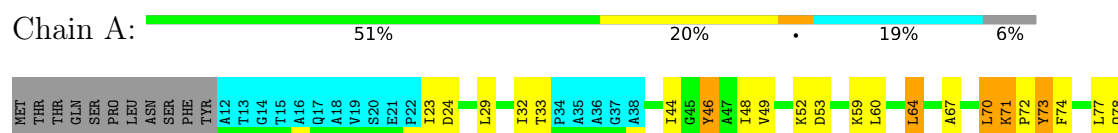
#### 4.2.4 Score per residue for model 4 (medoid)

- Molecule 1: Cannulae forming protein



#### 4.2.5 Score per residue for model 5

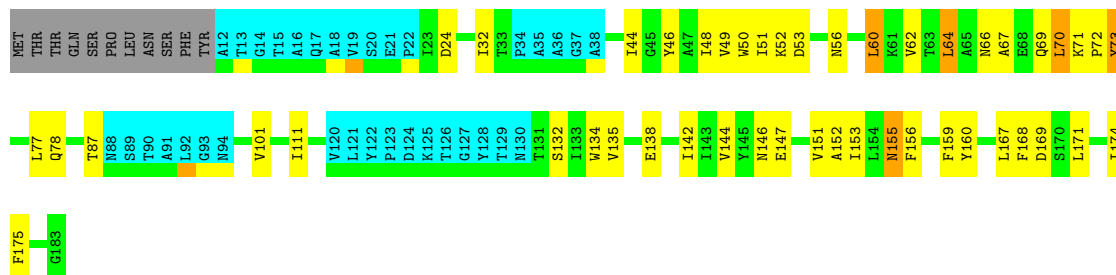
- Molecule 1: Cannulae forming protein





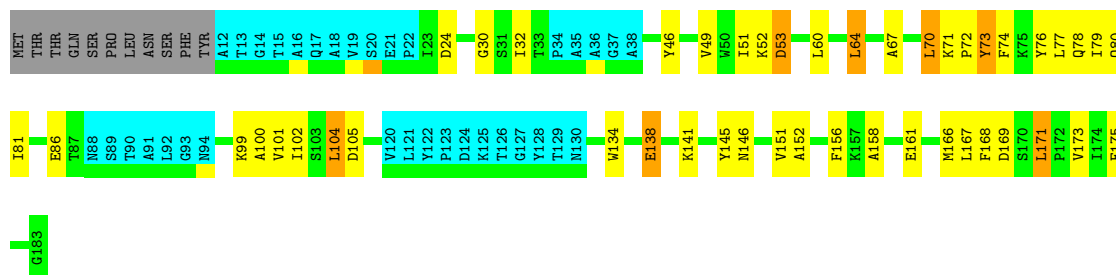
#### 4.2.6 Score per residue for model 6

- Molecule 1: Cannulae forming protein



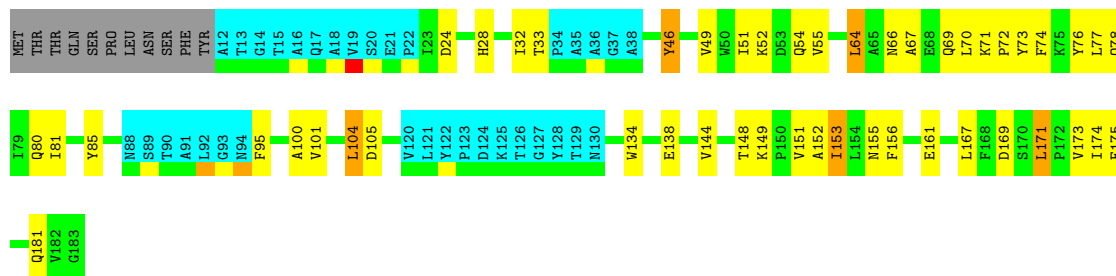
#### 4.2.7 Score per residue for model 7

- Molecule 1: Cannulae forming protein



#### 4.2.8 Score per residue for model 8

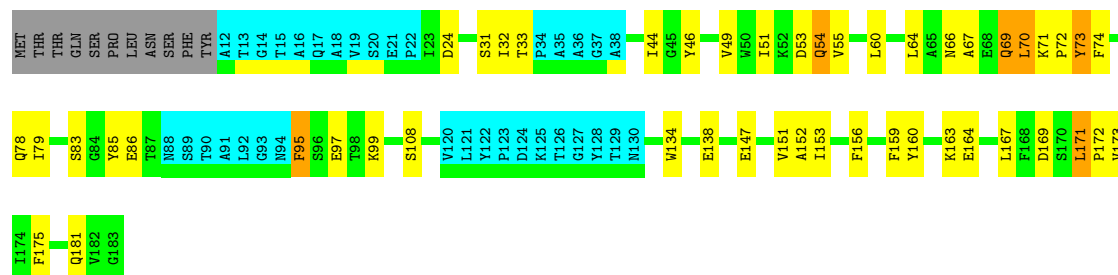
- Molecule 1: Cannulae forming protein



### 4.2.9 Score per residue for model 9

- Molecule 1: Cannulae forming protein

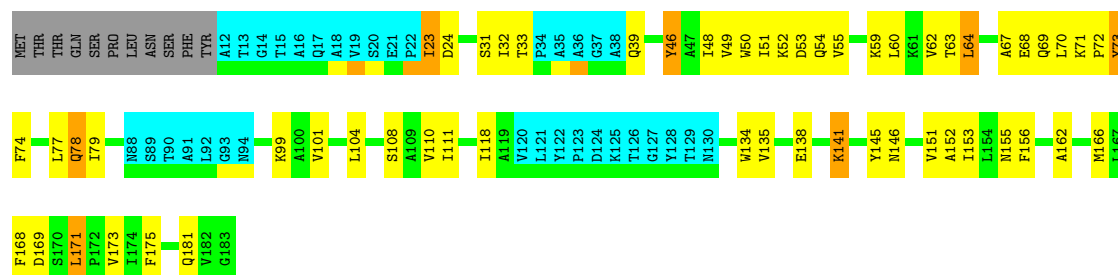
Chain A: 



### 4.2.10 Score per residue for model 10

- Molecule 1: Cannulae forming protein

Chain A: 





## 5 Refinement protocol and experimental data overview

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

Of the 1000 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy*.

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

| Software name | Classification        | Version |
|---------------|-----------------------|---------|
| CNS           | structure calculation |         |
| 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                       | 2170           |
| Number of shifts mapped to atoms             | 2170           |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 95%            |

## 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     | 0.50±0.01    | 0±0/1112 ( 0.0± 0.0%) | 0.80±0.01   | 0±0/1515 ( 0.0± 0.0%) |
| All | All   | 0.50         | 1/11120 ( 0.0%)       | 0.80        | 0/15150 ( 0.0%)       |

All unique bond outliers are listed below.

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) | Models |       |
|-----|-------|-----|------|-------|-------|-------------|----------|--------|-------|
|     |       |     |      |       |       |             |          | Worst  | Total |
| 1   | A     | 138 | GLU  | N-CA  | -5.53 | 1.41        | 1.46     | 7      | 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     | 1089  | 1097     | 1096     | 37±7    |
| All | All   | 10890 | 10970    | 10960    | 366     |

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 17.

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

| Atom-1          | Atom-2         | Clash(Å) | Distance(Å) | Models |       |
|-----------------|----------------|----------|-------------|--------|-------|
|                 |                |          |             | Worst  | Total |
| 1:A:64:LEU:HD23 | 1:A:67:ALA:HB2 | 1.04     | 1.22        | 2      | 10    |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:135:VAL:HG22 | 1:A:153:ILE:HG21 | 0.83     | 1.51        | 10     | 3     |
| 1:A:64:LEU:HD23  | 1:A:67:ALA:CB    | 0.80     | 2.06        | 2      | 10    |
| 1:A:51:ILE:HG23  | 1:A:55:VAL:HG13  | 0.80     | 1.53        | 9      | 5     |
| 1:A:163:LYS:O    | 1:A:166:MET:HE2  | 0.78     | 1.78        | 1      | 1     |
| 1:A:70:LEU:HD22  | 1:A:171:LEU:CD1  | 0.75     | 2.11        | 4      | 2     |
| 1:A:51:ILE:CG2   | 1:A:55:VAL:HG13  | 0.72     | 2.14        | 9      | 3     |
| 1:A:143:ILE:HG22 | 1:A:144:VAL:HG23 | 0.71     | 1.62        | 5      | 2     |
| 1:A:30:GLY:O     | 1:A:173:VAL:HG12 | 0.70     | 1.86        | 1      | 3     |
| 1:A:85:TYR:CE1   | 1:A:153:ILE:HD13 | 0.70     | 2.21        | 3      | 3     |
| 1:A:85:TYR:CD1   | 1:A:153:ILE:HD13 | 0.69     | 2.22        | 2      | 1     |
| 1:A:166:MET:HE1  | 1:A:168:PHE:CE2  | 0.69     | 2.23        | 10     | 1     |
| 1:A:49:VAL:HB    | 1:A:152:ALA:HB3  | 0.68     | 1.65        | 10     | 9     |
| 1:A:77:LEU:HD22  | 1:A:78:GLN:N     | 0.67     | 2.05        | 4      | 2     |
| 1:A:104:LEU:HD12 | 1:A:105:ASP:N    | 0.67     | 2.05        | 4      | 3     |
| 1:A:29:LEU:HD13  | 1:A:173:VAL:O    | 0.67     | 1.89        | 1      | 3     |
| 1:A:73:TYR:OH    | 1:A:171:LEU:HD11 | 0.65     | 1.92        | 10     | 1     |
| 1:A:32:ILE:HG21  | 1:A:74:PHE:CZ    | 0.64     | 2.27        | 5      | 8     |
| 1:A:85:TYR:CZ    | 1:A:153:ILE:HD13 | 0.64     | 2.27        | 3      | 2     |
| 1:A:153:ILE:HD12 | 1:A:153:ILE:N    | 0.64     | 2.08        | 2      | 3     |
| 1:A:70:LEU:HD22  | 1:A:171:LEU:HD11 | 0.63     | 1.71        | 4      | 2     |
| 1:A:180:LEU:HD22 | 1:A:181:GLN:N    | 0.63     | 2.07        | 5      | 1     |
| 1:A:64:LEU:CD2   | 1:A:67:ALA:HB2   | 0.62     | 2.19        | 4      | 5     |
| 1:A:73:TYR:CE1   | 1:A:74:PHE:CE2   | 0.62     | 2.88        | 8      | 1     |
| 1:A:166:MET:O    | 1:A:166:MET:HE3  | 0.61     | 1.95        | 1      | 1     |
| 1:A:69:GLN:NE2   | 1:A:70:LEU:HD23  | 0.61     | 2.11        | 4      | 1     |
| 1:A:49:VAL:O     | 1:A:151:VAL:HG23 | 0.61     | 1.95        | 3      | 8     |
| 1:A:63:THR:HG23  | 1:A:107:PRO:O    | 0.60     | 1.96        | 4      | 1     |
| 1:A:99:LYS:CE    | 1:A:154:LEU:HD22 | 0.60     | 2.26        | 4      | 1     |
| 1:A:100:ALA:HB3  | 1:A:111:ILE:CD1  | 0.59     | 2.28        | 3      | 2     |
| 1:A:64:LEU:HD11  | 1:A:173:VAL:CG2  | 0.59     | 2.28        | 4      | 5     |
| 1:A:64:LEU:HD12  | 1:A:175:PHE:CE2  | 0.58     | 2.33        | 8      | 5     |
| 1:A:64:LEU:HD23  | 1:A:67:ALA:CA    | 0.58     | 2.28        | 8      | 6     |
| 1:A:70:LEU:HD23  | 1:A:171:LEU:CD1  | 0.58     | 2.28        | 5      | 1     |
| 1:A:152:ALA:C    | 1:A:153:ILE:HD12 | 0.58     | 2.23        | 3      | 2     |
| 1:A:64:LEU:HD12  | 1:A:175:PHE:CE1  | 0.58     | 2.34        | 9      | 4     |
| 1:A:23:ILE:HD12  | 1:A:23:ILE:N     | 0.57     | 2.15        | 4      | 2     |
| 1:A:44:ILE:HD11  | 1:A:156:PHE:HB3  | 0.57     | 1.76        | 9      | 2     |
| 1:A:73:TYR:O     | 1:A:166:MET:HE2  | 0.57     | 1.99        | 10     | 1     |
| 1:A:74:PHE:CE2   | 1:A:171:LEU:HD23 | 0.57     | 2.35        | 1      | 1     |
| 1:A:51:ILE:HG22  | 1:A:53:ASP:O     | 0.57     | 1.99        | 4      | 3     |
| 1:A:73:TYR:CE2   | 1:A:171:LEU:HD11 | 0.57     | 2.35        | 8      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:154:LEU:N    | 1:A:154:LEU:HD12 | 0.56     | 2.14        | 2      | 1     |
| 1:A:51:ILE:HD12  | 1:A:55:VAL:HG11  | 0.56     | 1.76        | 8      | 1     |
| 1:A:99:LYS:HE3   | 1:A:154:LEU:HD22 | 0.55     | 1.78        | 4      | 1     |
| 1:A:79:ILE:O     | 1:A:101:VAL:HG23 | 0.54     | 2.03        | 4      | 1     |
| 1:A:49:VAL:C     | 1:A:151:VAL:HG23 | 0.54     | 2.27        | 5      | 8     |
| 1:A:80:GLN:HG3   | 1:A:101:VAL:HG22 | 0.54     | 1.79        | 3      | 3     |
| 1:A:77:LEU:C     | 1:A:77:LEU:HD13  | 0.54     | 2.27        | 4      | 2     |
| 1:A:48:ILE:HG21  | 1:A:50:TRP:CZ2   | 0.54     | 2.38        | 6      | 2     |
| 1:A:73:TYR:CZ    | 1:A:171:LEU:HD11 | 0.54     | 2.38        | 9      | 2     |
| 1:A:73:TYR:N     | 1:A:73:TYR:CD1   | 0.54     | 2.76        | 10     | 1     |
| 1:A:51:ILE:HG23  | 1:A:55:VAL:CG1   | 0.53     | 2.31        | 9      | 2     |
| 1:A:48:ILE:HD13  | 1:A:153:ILE:HD12 | 0.53     | 1.79        | 5      | 1     |
| 1:A:77:LEU:HD23  | 1:A:78:GLN:N     | 0.53     | 2.19        | 3      | 5     |
| 1:A:70:LEU:O     | 1:A:73:TYR:CE2   | 0.53     | 2.62        | 3      | 5     |
| 1:A:51:ILE:CD1   | 1:A:118:ILE:HD12 | 0.53     | 2.34        | 10     | 1     |
| 1:A:73:TYR:CE1   | 1:A:74:PHE:CZ    | 0.52     | 2.97        | 8      | 1     |
| 1:A:70:LEU:O     | 1:A:73:TYR:CE1   | 0.52     | 2.63        | 5      | 5     |
| 1:A:44:ILE:C     | 1:A:44:ILE:HD12  | 0.52     | 2.30        | 3      | 1     |
| 1:A:132:SER:OG   | 1:A:142:ILE:HG23 | 0.52     | 2.04        | 3      | 2     |
| 1:A:73:TYR:OH    | 1:A:171:LEU:CD2  | 0.51     | 2.58        | 8      | 1     |
| 1:A:44:ILE:HD11  | 1:A:156:PHE:CB   | 0.51     | 2.36        | 3      | 1     |
| 1:A:73:TYR:CE2   | 1:A:74:PHE:CE1   | 0.51     | 2.99        | 10     | 1     |
| 1:A:69:GLN:HE21  | 1:A:70:LEU:HD23  | 0.51     | 1.64        | 4      | 2     |
| 1:A:63:THR:HG23  | 1:A:108:SER:HB3  | 0.50     | 1.82        | 10     | 1     |
| 1:A:73:TYR:CZ    | 1:A:74:PHE:CZ    | 0.50     | 3.00        | 8      | 1     |
| 1:A:81:ILE:HD12  | 1:A:100:ALA:O    | 0.50     | 2.06        | 7      | 4     |
| 1:A:156:PHE:N    | 1:A:156:PHE:CD1  | 0.49     | 2.79        | 7      | 6     |
| 1:A:156:PHE:CD2  | 1:A:156:PHE:N    | 0.49     | 2.80        | 9      | 3     |
| 1:A:70:LEU:HA    | 1:A:73:TYR:OH    | 0.49     | 2.07        | 10     | 1     |
| 1:A:167:LEU:C    | 1:A:167:LEU:HD23 | 0.49     | 2.33        | 3      | 4     |
| 1:A:180:LEU:C    | 1:A:180:LEU:HD23 | 0.49     | 2.32        | 2      | 1     |
| 1:A:64:LEU:CD1   | 1:A:175:PHE:CZ   | 0.48     | 2.96        | 8      | 9     |
| 1:A:153:ILE:N    | 1:A:153:ILE:CD1  | 0.48     | 2.76        | 3      | 2     |
| 1:A:167:LEU:C    | 1:A:167:LEU:HD13 | 0.48     | 2.33        | 8      | 1     |
| 1:A:59:LYS:CE    | 1:A:110:VAL:HG13 | 0.48     | 2.38        | 10     | 1     |
| 1:A:73:TYR:CE2   | 1:A:171:LEU:CD1  | 0.48     | 2.97        | 8      | 1     |
| 1:A:32:ILE:HG23  | 1:A:160:TYR:CZ   | 0.47     | 2.44        | 6      | 3     |
| 1:A:143:ILE:HD13 | 1:A:153:ILE:HG13 | 0.47     | 1.85        | 5      | 1     |
| 1:A:32:ILE:HG21  | 1:A:74:PHE:HZ    | 0.47     | 1.68        | 8      | 1     |
| 1:A:73:TYR:OH    | 1:A:74:PHE:CZ    | 0.47     | 2.67        | 8      | 1     |
| 1:A:64:LEU:CD1   | 1:A:175:PHE:CE2  | 0.47     | 2.98        | 1      | 5     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:73:TYR:OH    | 1:A:171:LEU:CD1  | 0.47     | 2.61        | 10     | 3     |
| 1:A:113:LEU:HD21 | 1:A:154:LEU:HD21 | 0.47     | 1.86        | 3      | 2     |
| 1:A:180:LEU:HD22 | 1:A:180:LEU:C    | 0.47     | 2.34        | 5      | 1     |
| 1:A:100:ALA:HB3  | 1:A:111:ILE:HD13 | 0.46     | 1.87        | 3      | 1     |
| 1:A:144:VAL:HG11 | 1:A:148:THR:OG1  | 0.46     | 2.11        | 8      | 1     |
| 1:A:79:ILE:C     | 1:A:101:VAL:HG23 | 0.46     | 2.36        | 5      | 1     |
| 1:A:62:VAL:CG1   | 1:A:175:PHE:CD2  | 0.46     | 2.99        | 6      | 1     |
| 1:A:85:TYR:CE1   | 1:A:153:ILE:CG1  | 0.46     | 2.99        | 9      | 1     |
| 1:A:46:TYR:CD1   | 1:A:46:TYR:N     | 0.46     | 2.83        | 1      | 3     |
| 1:A:85:TYR:OH    | 1:A:153:ILE:HD13 | 0.46     | 2.10        | 3      | 1     |
| 1:A:71:LYS:N     | 1:A:72:PRO:CD    | 0.46     | 2.79        | 7      | 8     |
| 1:A:74:PHE:CZ    | 1:A:171:LEU:HD23 | 0.46     | 2.46        | 1      | 1     |
| 1:A:64:LEU:HD21  | 1:A:70:LEU:HD12  | 0.46     | 1.88        | 8      | 1     |
| 1:A:64:LEU:CD1   | 1:A:175:PHE:CE1  | 0.45     | 2.99        | 2      | 5     |
| 1:A:46:TYR:N     | 1:A:46:TYR:CD2   | 0.45     | 2.85        | 3      | 2     |
| 1:A:95:PHE:CE2   | 1:A:97:GLU:CG    | 0.45     | 2.99        | 3      | 1     |
| 1:A:79:ILE:HD13  | 1:A:175:PHE:HZ   | 0.45     | 1.71        | 10     | 1     |
| 1:A:95:PHE:CD2   | 1:A:95:PHE:O     | 0.45     | 2.69        | 9      | 3     |
| 1:A:145:TYR:CE2  | 1:A:146:ASN:ND2  | 0.45     | 2.85        | 2      | 1     |
| 1:A:78:GLN:O     | 1:A:159:PHE:N    | 0.45     | 2.47        | 6      | 4     |
| 1:A:173:VAL:HG21 | 1:A:175:PHE:CE2  | 0.45     | 2.47        | 9      | 1     |
| 1:A:48:ILE:HG12  | 1:A:153:ILE:HD12 | 0.45     | 1.88        | 1      | 1     |
| 1:A:101:VAL:O    | 1:A:101:VAL:HG23 | 0.45     | 2.12        | 10     | 2     |
| 1:A:44:ILE:HG21  | 1:A:158:ALA:HB2  | 0.45     | 1.88        | 5      | 2     |
| 1:A:69:GLN:NE2   | 1:A:70:LEU:CD1   | 0.45     | 2.79        | 9      | 1     |
| 1:A:134:TRP:CD1  | 1:A:138:GLU:O    | 0.45     | 2.70        | 7      | 8     |
| 1:A:48:ILE:CD1   | 1:A:153:ILE:HD12 | 0.45     | 2.41        | 5      | 1     |
| 1:A:151:VAL:HG12 | 1:A:152:ALA:N    | 0.45     | 2.27        | 10     | 2     |
| 1:A:76:TYR:CE2   | 1:A:161:GLU:CB   | 0.45     | 3.00        | 8      | 1     |
| 1:A:167:LEU:HD13 | 1:A:168:PHE:N    | 0.45     | 2.25        | 7      | 1     |
| 1:A:66:ASN:ND2   | 1:A:172:PRO:O    | 0.45     | 2.50        | 9      | 1     |
| 1:A:180:LEU:H    | 1:A:180:LEU:HD13 | 0.45     | 1.71        | 5      | 1     |
| 1:A:167:LEU:HD13 | 1:A:167:LEU:C    | 0.44     | 2.37        | 7      | 1     |
| 1:A:145:TYR:CD1  | 1:A:146:ASN:N    | 0.44     | 2.85        | 10     | 1     |
| 1:A:81:ILE:HG22  | 1:A:99:LYS:NZ    | 0.44     | 2.27        | 4      | 1     |
| 1:A:99:LYS:HD2   | 1:A:111:ILE:HG23 | 0.44     | 1.90        | 2      | 1     |
| 1:A:112:VAL:HG13 | 1:A:112:VAL:O    | 0.44     | 2.13        | 2      | 1     |
| 1:A:70:LEU:HD23  | 1:A:73:TYR:OH    | 0.44     | 2.13        | 10     | 1     |
| 1:A:74:PHE:CE1   | 1:A:171:LEU:HD23 | 0.44     | 2.47        | 9      | 1     |
| 1:A:71:LYS:N     | 1:A:72:PRO:HD2   | 0.43     | 2.28        | 8      | 2     |
| 1:A:44:ILE:HD11  | 1:A:79:ILE:HG23  | 0.43     | 1.89        | 9      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:59:LYS:HE2   | 1:A:110:VAL:HG13 | 0.43     | 1.90        | 10     | 1     |
| 1:A:70:LEU:HD22  | 1:A:171:LEU:HD21 | 0.43     | 1.90        | 8      | 1     |
| 1:A:69:GLN:NE2   | 1:A:70:LEU:HD12  | 0.43     | 2.28        | 9      | 1     |
| 1:A:113:LEU:HD23 | 1:A:152:ALA:HB1  | 0.43     | 1.90        | 1      | 1     |
| 1:A:76:TYR:CE1   | 1:A:161:GLU:CB   | 0.43     | 3.01        | 7      | 1     |
| 1:A:70:LEU:HD23  | 1:A:171:LEU:HD11 | 0.43     | 1.90        | 10     | 1     |
| 1:A:151:VAL:CG1  | 1:A:152:ALA:N    | 0.43     | 2.82        | 6      | 2     |
| 1:A:28:HIS:CB    | 1:A:46:TYR:CD2   | 0.43     | 3.02        | 4      | 2     |
| 1:A:66:ASN:OD1   | 1:A:69:GLN:HB3   | 0.42     | 2.13        | 4      | 1     |
| 1:A:71:LYS:HG2   | 1:A:104:LEU:HD22 | 0.42     | 1.91        | 10     | 1     |
| 1:A:70:LEU:HD13  | 1:A:77:LEU:CD1   | 0.42     | 2.44        | 7      | 1     |
| 1:A:66:ASN:CB    | 1:A:174:ILE:HB   | 0.42     | 2.44        | 8      | 1     |
| 1:A:155:ASN:C    | 1:A:156:PHE:CD1  | 0.42     | 2.98        | 6      | 3     |
| 1:A:62:VAL:HG12  | 1:A:175:PHE:CD2  | 0.42     | 2.49        | 6      | 1     |
| 1:A:64:LEU:HD12  | 1:A:175:PHE:CD2  | 0.42     | 2.48        | 8      | 1     |
| 1:A:73:TYR:OH    | 1:A:171:LEU:HD21 | 0.42     | 2.14        | 8      | 1     |
| 1:A:79:ILE:HG21  | 1:A:175:PHE:CZ   | 0.42     | 2.50        | 10     | 1     |
| 1:A:66:ASN:HB2   | 1:A:174:ILE:HB   | 0.42     | 1.91        | 8      | 2     |
| 1:A:151:VAL:HG11 | 1:A:153:ILE:HD11 | 0.42     | 1.92        | 6      | 1     |
| 1:A:95:PHE:C     | 1:A:95:PHE:CD1   | 0.42     | 2.97        | 8      | 1     |
| 1:A:60:LEU:CD2   | 1:A:111:ILE:HD11 | 0.42     | 2.45        | 6      | 1     |
| 1:A:53:ASP:O     | 1:A:54:GLN:O     | 0.42     | 2.38        | 9      | 1     |
| 1:A:73:TYR:HH    | 1:A:171:LEU:HD11 | 0.42     | 1.72        | 10     | 1     |
| 1:A:95:PHE:CD2   | 1:A:95:PHE:C     | 0.41     | 2.98        | 2      | 3     |
| 1:A:74:PHE:CE2   | 1:A:171:LEU:CD2  | 0.41     | 3.03        | 1      | 1     |
| 1:A:44:ILE:CG2   | 1:A:158:ALA:HB2  | 0.41     | 2.45        | 3      | 1     |
| 1:A:145:TYR:CD1  | 1:A:146:ASN:OD1  | 0.41     | 2.74        | 4      | 1     |
| 1:A:166:MET:CE   | 1:A:168:PHE:CE2  | 0.41     | 2.99        | 10     | 1     |
| 1:A:48:ILE:CG2   | 1:A:151:VAL:HG21 | 0.41     | 2.45        | 2      | 2     |
| 1:A:145:TYR:CE2  | 1:A:146:ASN:OD1  | 0.41     | 2.74        | 1      | 1     |
| 1:A:179:VAL:O    | 1:A:179:VAL:HG13 | 0.41     | 2.16        | 1      | 1     |
| 1:A:78:GLN:O     | 1:A:158:ALA:HA   | 0.41     | 2.16        | 7      | 2     |
| 1:A:70:LEU:O     | 1:A:73:TYR:CD2   | 0.41     | 2.74        | 3      | 1     |
| 1:A:144:VAL:CG1  | 1:A:147:GLU:CG   | 0.41     | 2.99        | 6      | 1     |
| 1:A:162:ALA:HB1  | 1:A:166:MET:CE   | 0.41     | 2.46        | 10     | 1     |
| 1:A:48:ILE:CG2   | 1:A:151:VAL:CG2  | 0.41     | 2.99        | 2      | 1     |
| 1:A:95:PHE:O     | 1:A:95:PHE:CD2   | 0.41     | 2.74        | 4      | 1     |
| 1:A:60:LEU:C     | 1:A:60:LEU:HD12  | 0.41     | 2.41        | 5      | 1     |
| 1:A:95:PHE:CD1   | 1:A:95:PHE:O     | 0.41     | 2.74        | 1      | 2     |
| 1:A:70:LEU:HD11  | 1:A:171:LEU:HB3  | 0.41     | 1.92        | 9      | 1     |
| 1:A:62:VAL:CG2   | 1:A:111:ILE:CD1  | 0.41     | 2.99        | 10     | 1     |

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| Atom-1           | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|------------------|-----------------|----------|-------------|--------|-------|
|                  |                 |          |             | Worst  | Total |
| 1:A:95:PHE:CD1   | 1:A:95:PHE:C    | 0.40     | 2.99        | 1      | 1     |
| 1:A:23:ILE:HG22  | 1:A:24:ASP:N    | 0.40     | 2.30        | 2      | 1     |
| 1:A:95:PHE:CD1   | 1:A:97:GLU:OE2  | 0.40     | 2.74        | 2      | 1     |
| 1:A:70:LEU:CD1   | 1:A:77:LEU:CD1  | 0.40     | 2.99        | 7      | 1     |
| 1:A:46:TYR:CE2   | 1:A:141:LYS:HD3 | 0.40     | 2.52        | 10     | 1     |
| 1:A:70:LEU:HA    | 1:A:73:TYR:CE1  | 0.40     | 2.51        | 1      | 1     |
| 1:A:166:MET:O    | 1:A:166:MET:CE  | 0.40     | 2.66        | 1      | 1     |
| 1:A:167:LEU:HD23 | 1:A:168:PHE:N   | 0.40     | 2.31        | 6      | 1     |
| 1:A:145:TYR:CE2  | 1:A:146:ASN:CG  | 0.40     | 3.00        | 7      | 1     |
| 1:A:76:TYR:CE2   | 1:A:161:GLU:CD  | 0.40     | 3.00        | 1      | 1     |
| 1:A:78:GLN:CB    | 1:A:159:PHE:HB2 | 0.40     | 2.46        | 4      | 1     |
| 1:A:70:LEU:CD2   | 1:A:171:LEU:CD1 | 0.40     | 3.00        | 5      | 1     |
| 1:A:79:ILE:O     | 1:A:102:ILE:N   | 0.40     | 2.54        | 7      | 1     |
| 1:A:64:LEU:HD23  | 1:A:67:ALA:HA   | 0.40     | 1.92        | 8      | 1     |

## 6.3 Torsion angles

### 6.3.1 Protein backbone

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

| Mol | Chain | Analysed        | Favoured      | Allowed    | Outliers   | Percentiles |    |
|-----|-------|-----------------|---------------|------------|------------|-------------|----|
| 1   | A     | 137/183 (75%)   | 134±1 (97±1%) | 2±1 (2±1%) | 1±1 (1±0%) | 21          | 71 |
| All | All   | 1370/1830 (75%) | 1335 (97%)    | 25 (2%)    | 10 (1%)    | 21          | 71 |

All 5 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 54  | GLN  | 6              |
| 1   | A     | 169 | ASP  | 1              |
| 1   | A     | 53  | ASP  | 1              |
| 1   | A     | 146 | ASN  | 1              |
| 1   | A     | 39  | GLN  | 1              |

### 6.3.2 Protein sidechains ⓘ

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

| Mol | Chain | Analysed        | Rotameric     | Outliers     | Percentiles |    |
|-----|-------|-----------------|---------------|--------------|-------------|----|
| 1   | A     | 122/156 (78%)   | 106±2 (87±2%) | 16±2 (13±2%) | 6           | 47 |
| All | All   | 1220/1560 (78%) | 1061 (87%)    | 159 (13%)    | 6           | 47 |

All 45 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     | 24  | ASP  | 10             |
| 1   | A     | 46  | TYR  | 10             |
| 1   | A     | 169 | ASP  | 10             |
| 1   | A     | 171 | LEU  | 10             |
| 1   | A     | 64  | LEU  | 9              |
| 1   | A     | 73  | TYR  | 9              |
| 1   | A     | 33  | THR  | 8              |
| 1   | A     | 155 | ASN  | 7              |
| 1   | A     | 52  | LYS  | 7              |
| 1   | A     | 69  | GLN  | 6              |
| 1   | A     | 60  | LEU  | 5              |
| 1   | A     | 70  | LEU  | 5              |
| 1   | A     | 181 | GLN  | 4              |
| 1   | A     | 141 | LYS  | 4              |
| 1   | A     | 23  | ILE  | 4              |
| 1   | A     | 99  | LYS  | 4              |
| 1   | A     | 31  | SER  | 3              |
| 1   | A     | 163 | LYS  | 3              |
| 1   | A     | 166 | MET  | 3              |
| 1   | A     | 153 | ILE  | 3              |
| 1   | A     | 104 | LEU  | 3              |
| 1   | A     | 102 | ILE  | 2              |
| 1   | A     | 149 | LYS  | 2              |
| 1   | A     | 85  | TYR  | 2              |
| 1   | A     | 95  | PHE  | 2              |
| 1   | A     | 68  | GLU  | 2              |
| 1   | A     | 161 | GLU  | 2              |
| 1   | A     | 53  | ASP  | 2              |
| 1   | A     | 86  | GLU  | 2              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 44  | ILE  | 1              |
| 1   | A     | 168 | PHE  | 1              |
| 1   | A     | 41  | SER  | 1              |
| 1   | A     | 75  | LYS  | 1              |
| 1   | A     | 115 | LYS  | 1              |
| 1   | A     | 77  | LEU  | 1              |
| 1   | A     | 59  | LYS  | 1              |
| 1   | A     | 71  | LYS  | 1              |
| 1   | A     | 180 | LEU  | 1              |
| 1   | A     | 56  | ASN  | 1              |
| 1   | A     | 83  | SER  | 1              |
| 1   | A     | 97  | GLU  | 1              |
| 1   | A     | 108 | SER  | 1              |
| 1   | A     | 147 | GLU  | 1              |
| 1   | A     | 164 | GLU  | 1              |
| 1   | A     | 78  | GLN  | 1              |

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 6.7 Other polymers [i](#)

There are no such molecules in this entry.

## 6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 95% for the well-defined parts and 95% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

Chemical shift list name: *assigned\_chemical\_shifts\_1*

#### 7.1.1 Bookkeeping

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

|   |      |
|---|------|
| Total number of shifts                  | 2170 |
| Number of shifts mapped to atoms        | 2170 |
| Number of unparsed shifts               | 0    |
| Number of shifts with mapping errors    | 0    |
| Number of shifts with mapping warnings  | 0    |
| Number of shift outliers (ShiftChecker) | 3    |

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 172      | $0.11 \pm 0.14$                 | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}_\beta$  | 161      | $-0.06 \pm 0.14$                | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}'$       | 154      | $0.43 \pm 0.13$                 | None needed ( $< 0.5$ ppm) |
| $^{15}\text{N}$        | 169      | $0.32 \pm 0.24$                 | None needed ( $< 0.5$ ppm) |

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 95%, i.e. 1806 atoms were assigned a chemical shift out of a possible 1894. 0 out of 25 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total          | $^1\text{H}$   | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|----------------|----------------|-----------------|-----------------|
| Backbone  | 677/685 (99%)  | 277/277 (100%) | 268/276 (97%)   | 132/132 (100%)  |
| Sidechain | 989/1053 (94%) | 675/690 (98%)  | 302/339 (89%)   | 12/24 (50%)     |

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|          | Total           | <sup>1</sup> H  | <sup>13</sup> C | <sup>15</sup> N |
|----------|-----------------|-----------------|-----------------|-----------------|
| Aromatic | 140/156 (90%)   | 73/75 (97%)     | 65/77 (84%)     | 2/4 (50%)       |
| Overall  | 1806/1894 (95%) | 1025/1042 (98%) | 635/692 (92%)   | 146/160 (91%)   |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 95%, i.e. 2162 atoms were assigned a chemical shift out of a possible 2278. 0 out of 29 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total           | <sup>1</sup> H  | <sup>13</sup> C | <sup>15</sup> N |
|-----------|-----------------|-----------------|-----------------|-----------------|
| Backbone  | 827/853 (97%)   | 339/346 (98%)   | 326/344 (95%)   | 162/163 (99%)   |
| Sidechain | 1179/1251 (94%) | 806/821 (98%)   | 357/401 (89%)   | 16/29 (55%)     |
| Aromatic  | 156/174 (90%)   | 81/83 (98%)     | 73/87 (84%)     | 2/4 (50%)       |
| Overall   | 2162/2278 (95%) | 1226/1250 (98%) | 756/832 (91%)   | 180/196 (92%)   |

#### 7.1.4 Statistically unusual chemical shifts ⓘ

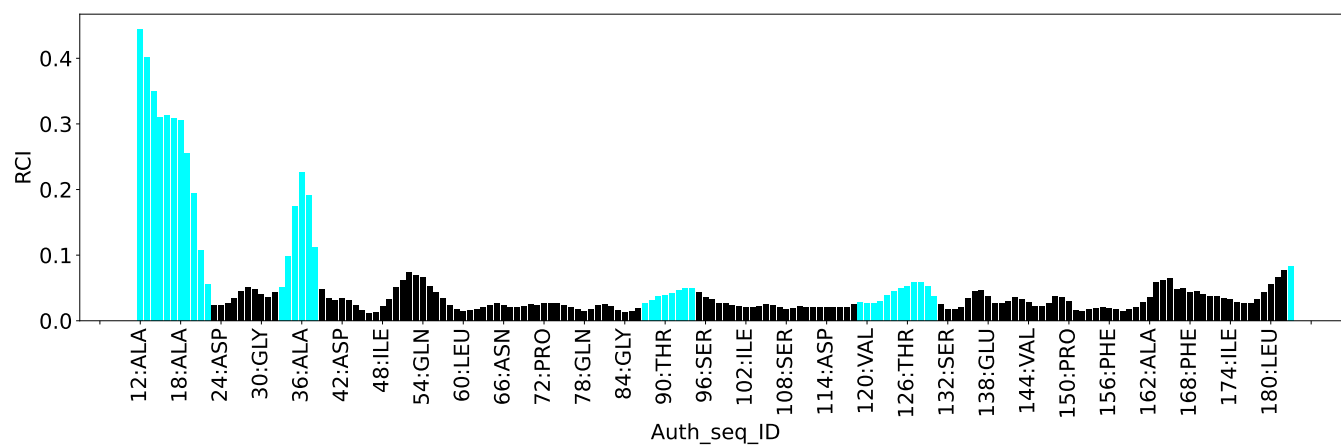
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

| List Id | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|---------|-------|-----|------|------|------------|---------------------|---------|
| 1       | A     | 87  | THR  | HG1  | 5.41       | 0.08 – 2.19         | 20.2    |
| 1       | A     | 86  | GLU  | HB2  | 0.59       | 1.00 – 3.05         | -7.0    |
| 1       | A     | 146 | ASN  | HB3  | 1.09       | 1.12 – 4.38         | -5.1    |

#### 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                                | 3318  |
| Intra-residue ( $ i-j =0$ )                              | 914   |
| Sequential ( $ i-j =1$ )                                 | 736   |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 394   |
| Long range ( $ i-j \geq 5$ )                             | 1220  |
| Inter-chain  | 0     |
| Hydrogen bond restraints                                 | 54    |
| Disulfide bond restraints                                | 0     |
| Total dihedral-angle restraints                          | 284   |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 19.7  |
| Number of long range restraints per residue <sup>1</sup> | 7.0   |

<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)  | 98.3                                   | 0.2     |
| 0.2-0.5 (Medium) | 124.9                                  | 0.5     |
| >0.5 (Large)     | 57.4                                   | 1.18    |

### 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)   | 67.0                                   | 9.99    |
| 10.0-20.0 (Medium) | 1.0                                    | 17.55   |
| >20.0 (Large)      | 4.1                                    | 43.26   |

## 9 Distance violation analysis ⓘ

### 9.1 Summary of distance violations ⓘ

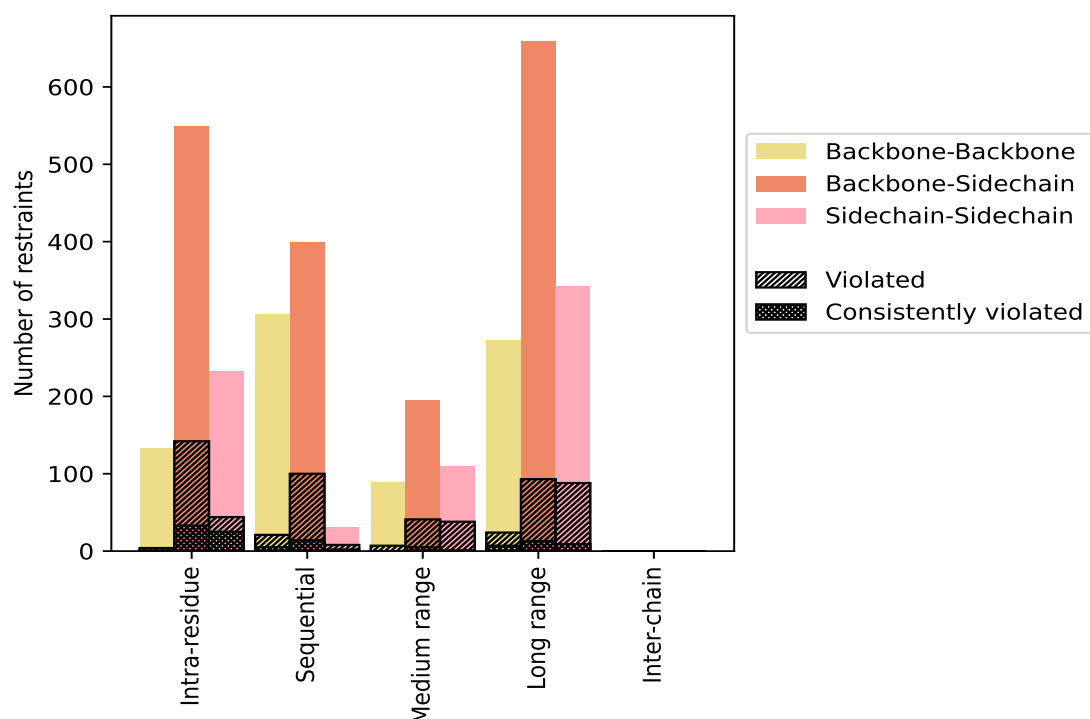
The following table shows the summary of distance violations in different restraint categories based on the sequence separation of the atoms involved. Each category is further sub-divided into three sub-categories based on the atoms involved. Violations less than 0.1 Å are not included in the statistics.

| Restraints type   | Count       | % <sup>1</sup> | Violated <sup>3</sup> |                |                | Consistently Violated <sup>4</sup> |                |                |
|---|-------------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
|   |             |                | Count                 | % <sup>2</sup> | % <sup>1</sup> | Count                              | % <sup>2</sup> | % <sup>1</sup> |
| <b>Intra-residue (<math> i-j =0</math>)</b>                                 | <b>914</b>  | <b>27.5</b>    | <b>190</b>            | <b>20.8</b>    | <b>5.7</b>     | <b>59</b>                          | <b>6.5</b>     | <b>1.8</b>     |
| Backbone-Backbone   | 133         | 4.0            | 4                     | 3.0            | 0.1            | 1                                  | 0.8            | 0.0            |
| Backbone-Sidechain  | 549         | 16.5           | 142                   | 25.9           | 4.3            | 33                                 | 6.0            | 1.0            |
| Sidechain-Sidechain   | 232         | 7.0            | 44                    | 19.0           | 1.3            | 25                                 | 10.8           | 0.8            |
| <b>Sequential (<math> i-j =1</math>)</b>                                    | <b>736</b>  | <b>22.2</b>    | <b>129</b>            | <b>17.5</b>    | <b>3.9</b>     | <b>21</b>                          | <b>2.9</b>     | <b>0.6</b>     |
| Backbone-Backbone   | 306         | 9.2            | 21                    | 6.9            | 0.6            | 5                                  | 1.6            | 0.2            |
| Backbone-Sidechain  | 399         | 12.0           | 100                   | 25.1           | 3.0            | 14                                 | 3.5            | 0.4            |
| Sidechain-Sidechain   | 31          | 0.9            | 8                     | 25.8           | 0.2            | 2                                  | 6.5            | 0.1            |
| <b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b> | <b>394</b>  | <b>11.9</b>    | <b>86</b>             | <b>21.8</b>    | <b>2.6</b>     | <b>6</b>                           | <b>1.5</b>     | <b>0.2</b>     |
| Backbone-Backbone   | 89          | 2.7            | 7                     | 7.9            | 0.2            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain  | 195         | 5.9            | 41                    | 21.0           | 1.2            | 5                                  | 2.6            | 0.2            |
| Sidechain-Sidechain   | 110         | 3.3            | 38                    | 34.5           | 1.1            | 1                                  | 0.9            | 0.0            |
| <b>Long range (<math> i-j \geq 5</math>)</b>                                | <b>1220</b> | <b>36.8</b>    | <b>204</b>            | <b>16.7</b>    | <b>6.1</b>     | <b>29</b>                          | <b>2.4</b>     | <b>0.9</b>     |
| Backbone-Backbone   | 273         | 8.2            | 24                    | 8.8            | 0.7            | 7                                  | 2.6            | 0.2            |
| Backbone-Sidechain  | 605         | 18.2           | 92                    | 15.2           | 2.8            | 13                                 | 2.1            | 0.4            |
| Sidechain-Sidechain   | 342         | 10.3           | 88                    | 25.7           | 2.7            | 9                                  | 2.6            | 0.3            |
| <b>Inter-chain</b>  | <b>0</b>    | <b>0.0</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| Backbone-Backbone   | 0           | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain  | 0           | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain   | 0           | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| <b>Hydrogen bond</b>  | <b>54</b>   | <b>1.6</b>     | <b>1</b>              | <b>1.9</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| <b>Disulfide bond</b>   | <b>0</b>    | <b>0.0</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| <b>Total</b>  | <b>3318</b> | <b>100.0</b>   | <b>610</b>            | <b>18.4</b>    | <b>18.4</b>    | <b>115</b>                         | <b>3.5</b>     | <b>3.5</b>     |
| Backbone-Backbone   | 801         | 24.1           | 56                    | 7.0            | 1.7            | 13                                 | 1.6            | 0.4            |
| Backbone-Sidechain  | 1802        | 54.3           | 376                   | 20.9           | 11.3           | 65                                 | 3.6            | 2.0            |
| Sidechain-Sidechain   | 715         | 21.5           | 178                   | 24.9           | 5.4            | 37                                 | 5.2            | 1.1            |

<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 disulfid bonds are counted in their appropriate category on the x-axis

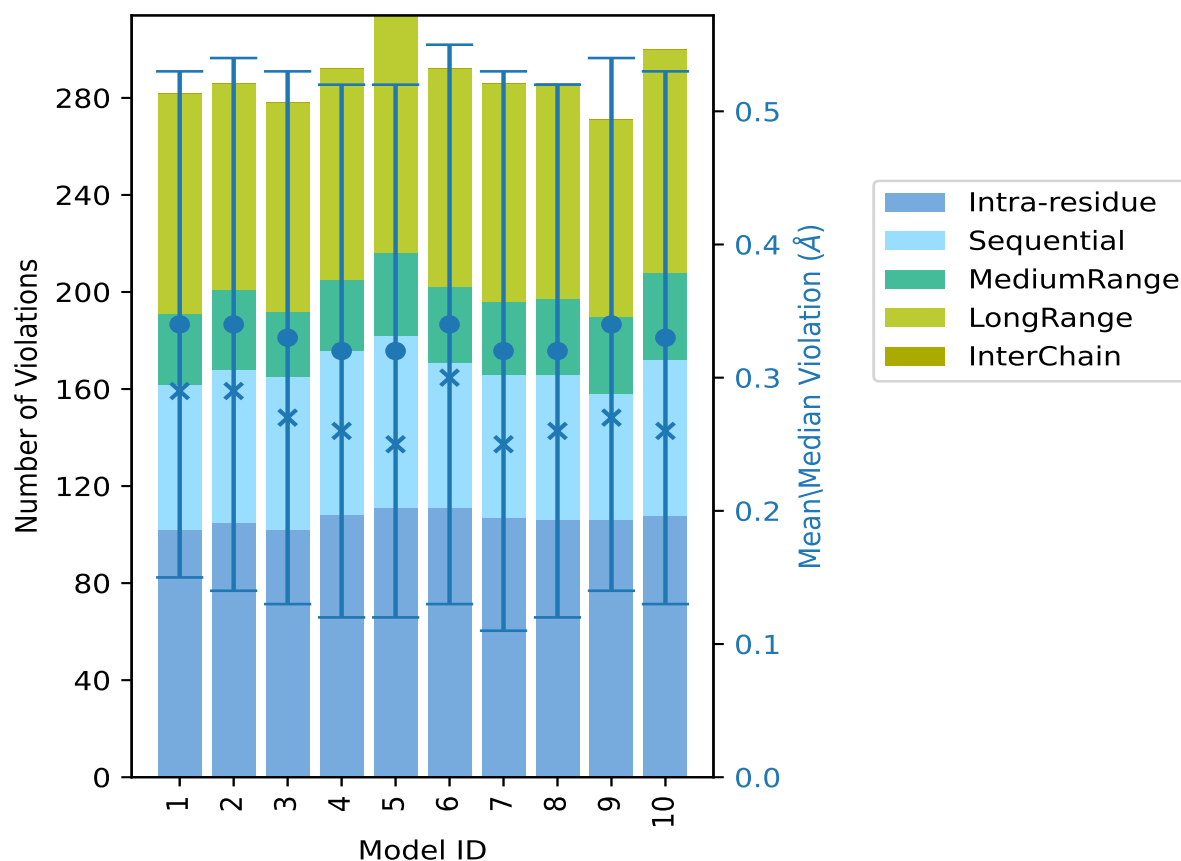
## 9.2 Distance violation statistics for each model [i](#)

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        | 102                  | 60              | 29              | 91              | 0               | 282   | 0.34     | 1.07    | 0.19                | 0.29       |
| 2        | 105                  | 63              | 33              | 85              | 0               | 286   | 0.34     | 1.01    | 0.2                 | 0.29       |
| 3        | 102                  | 63              | 27              | 86              | 0               | 278   | 0.33     | 0.98    | 0.2                 | 0.27       |
| 4        | 108                  | 68              | 29              | 87              | 0               | 292   | 0.32     | 1.08    | 0.2                 | 0.26       |
| 5        | 111                  | 71              | 34              | 98              | 0               | 314   | 0.32     | 1.11    | 0.2                 | 0.25       |
| 6        | 111                  | 60              | 31              | 90              | 0               | 292   | 0.34     | 1.18    | 0.21                | 0.3        |
| 7        | 107                  | 59              | 30              | 90              | 0               | 286   | 0.32     | 1.07    | 0.21                | 0.25       |
| 8        | 106                  | 60              | 31              | 89              | 0               | 286   | 0.32     | 1.06    | 0.2                 | 0.26       |
| 9        | 106                  | 52              | 32              | 81              | 0               | 271   | 0.34     | 1.08    | 0.2                 | 0.27       |
| 10       | 108                  | 64              | 36              | 92              | 0               | 300   | 0.33     | 0.93    | 0.2                 | 0.26       |

<sup>1</sup>Intra-residue restraints, <sup>2</sup>Sequential restraints, <sup>3</sup>Medium range restraints, <sup>4</sup>Long range restraints, <sup>5</sup>Inter-chain restraints, <sup>6</sup>Standard deviation

### 9.2.1 Bar graph : Distance Violation statistics for each model [i](#)



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

### 9.3 Distance violation statistics for the ensemble [i](#)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 2655(IR:724, SQ:607, MR:308, LR:1016, 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>       | %    |
| 48                            | 19              | 33              | 56              | 0               | 156   | 1                        | 10.0 |
| 11                            | 31              | 15              | 33              | 0               | 90    | 2                        | 20.0 |
| 15                            | 8               | 6               | 21              | 0               | 50    | 3                        | 30.0 |

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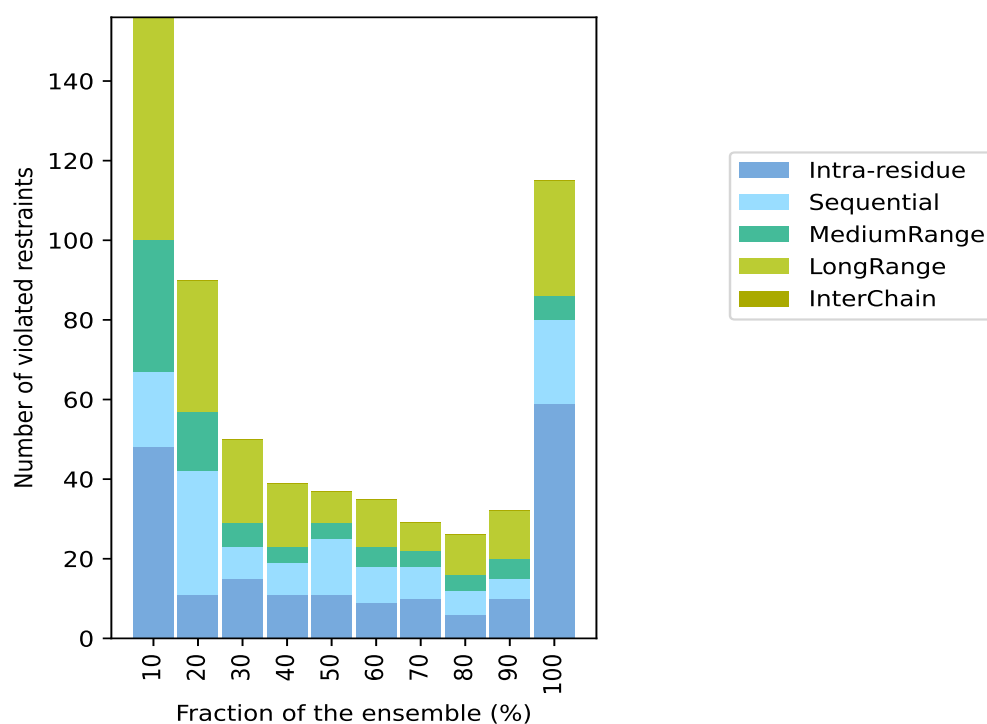
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| Number of violated restraints |                 |                 |                 |                 |       | Fraction of the ensemble |       |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|-------|
| IR <sup>1</sup>               | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total | Count <sup>6</sup>       | %     |
| 11                            | 8               | 4               | 16              | 0               | 39    | 4                        | 40.0  |
| 11                            | 14              | 4               | 8               | 0               | 37    | 5                        | 50.0  |
| 9                             | 9               | 5               | 12              | 0               | 35    | 6                        | 60.0  |
| 10                            | 8               | 4               | 7               | 0               | 29    | 7                        | 70.0  |
| 6                             | 6               | 4               | 10              | 0               | 26    | 8                        | 80.0  |
| 10                            | 5               | 5               | 12              | 0               | 32    | 9                        | 90.0  |
| 59                            | 21              | 6               | 29              | 0               | 115   | 10                       | 100.0 |

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

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

### 9.3.1 Bar graph : Distance violation statistics for the ensemble ⓘ

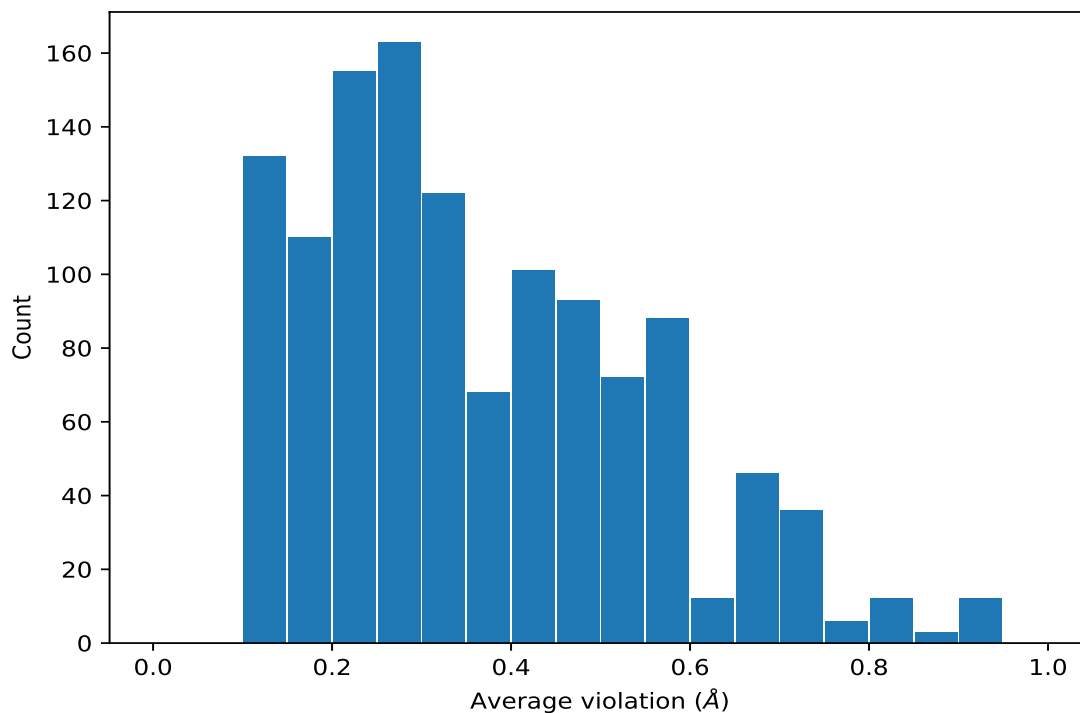


## 9.4 Most violated distance restraints in the ensemble ⓘ

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

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

in the ensemble



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

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

| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,10)   | 1:19:A:VAL:HG11 | 1:19:A:VAL:H    | 10                  | 0.93     | 0.14                | 0.94       |
| (1,10)   | 1:19:A:VAL:HG12 | 1:19:A:VAL:H    | 10                  | 0.93     | 0.14                | 0.94       |
| (1,10)   | 1:19:A:VAL:HG13 | 1:19:A:VAL:H    | 10                  | 0.93     | 0.14                | 0.94       |
| (1,10)   | 1:19:A:VAL:HG21 | 1:19:A:VAL:H    | 10                  | 0.93     | 0.14                | 0.94       |
| (1,10)   | 1:19:A:VAL:HG22 | 1:19:A:VAL:H    | 10                  | 0.93     | 0.14                | 0.94       |
| (1,10)   | 1:19:A:VAL:HG23 | 1:19:A:VAL:H    | 10                  | 0.93     | 0.14                | 0.94       |
| (1,1030) | 1:74:A:PHE:HE1  | 1:162:A:ALA:HB1 | 10                  | 0.9      | 0.27                | 1.02       |
| (1,1030) | 1:74:A:PHE:HE1  | 1:162:A:ALA:HB2 | 10                  | 0.9      | 0.27                | 1.02       |
| (1,1030) | 1:74:A:PHE:HE1  | 1:162:A:ALA:HB3 | 10                  | 0.9      | 0.27                | 1.02       |
| (1,1030) | 1:74:A:PHE:HE2  | 1:162:A:ALA:HB1 | 10                  | 0.9      | 0.27                | 1.02       |
| (1,1030) | 1:74:A:PHE:HE2  | 1:162:A:ALA:HB2 | 10                  | 0.9      | 0.27                | 1.02       |
| (1,1030) | 1:74:A:PHE:HE2  | 1:162:A:ALA:HB3 | 10                  | 0.9      | 0.27                | 1.02       |
| (2,469)  | 1:79:A:ILE:HG21 | 1:157:A:LYS:H   | 10                  | 0.88     | 0.02                | 0.88       |
| (2,469)  | 1:79:A:ILE:HG22 | 1:157:A:LYS:H   | 10                  | 0.88     | 0.02                | 0.88       |
| (2,469)  | 1:79:A:ILE:HG23 | 1:157:A:LYS:H   | 10                  | 0.88     | 0.02                | 0.88       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (2,466)  | 1:79:A:ILE:HG21  | 1:102:A:ILE:H    | 10                  | 0.82     | 0.03                | 0.82       |
| (2,466)  | 1:79:A:ILE:HG22  | 1:102:A:ILE:H    | 10                  | 0.82     | 0.03                | 0.82       |
| (2,466)  | 1:79:A:ILE:HG23  | 1:102:A:ILE:H    | 10                  | 0.82     | 0.03                | 0.82       |
| (1,1940) | 1:135:A:VAL:HG11 | 1:155:A:ASN:HD21 | 10                  | 0.81     | 0.18                | 0.88       |
| (1,1940) | 1:135:A:VAL:HG11 | 1:155:A:ASN:HD22 | 10                  | 0.81     | 0.18                | 0.88       |
| (1,1940) | 1:135:A:VAL:HG12 | 1:155:A:ASN:HD21 | 10                  | 0.81     | 0.18                | 0.88       |
| (1,1940) | 1:135:A:VAL:HG12 | 1:155:A:ASN:HD22 | 10                  | 0.81     | 0.18                | 0.88       |
| (1,1940) | 1:135:A:VAL:HG13 | 1:155:A:ASN:HD21 | 10                  | 0.81     | 0.18                | 0.88       |
| (1,1940) | 1:135:A:VAL:HG13 | 1:155:A:ASN:HD22 | 10                  | 0.81     | 0.18                | 0.88       |
| (2,6)    | 1:16:A:ALA:HB1   | 1:17:A:GLN:H     | 10                  | 0.8      | 0.01                | 0.8        |
| (2,6)    | 1:16:A:ALA:HB2   | 1:17:A:GLN:H     | 10                  | 0.8      | 0.01                | 0.8        |
| (2,6)    | 1:16:A:ALA:HB3   | 1:17:A:GLN:H     | 10                  | 0.8      | 0.01                | 0.8        |
| (1,288)  | 1:36:A:ALA:HB1   | 1:37:A:GLY:H     | 10                  | 0.77     | 0.15                | 0.8        |
| (1,288)  | 1:36:A:ALA:HB2   | 1:37:A:GLY:H     | 10                  | 0.77     | 0.15                | 0.8        |
| (1,288)  | 1:36:A:ALA:HB3   | 1:37:A:GLY:H     | 10                  | 0.77     | 0.15                | 0.8        |
| (2,719)  | 1:142:A:ILE:HG21 | 1:145:A:TYR:HA   | 10                  | 0.74     | 0.11                | 0.78       |
| (2,719)  | 1:142:A:ILE:HG22 | 1:145:A:TYR:HA   | 10                  | 0.74     | 0.11                | 0.78       |
| (2,719)  | 1:142:A:ILE:HG23 | 1:145:A:TYR:HA   | 10                  | 0.74     | 0.11                | 0.78       |
| (1,261)  | 1:33:A:THR:HG21  | 1:34:A:PRO:HD2   | 10                  | 0.73     | 0.04                | 0.74       |
| (1,261)  | 1:33:A:THR:HG22  | 1:34:A:PRO:HD2   | 10                  | 0.73     | 0.04                | 0.74       |
| (1,261)  | 1:33:A:THR:HG23  | 1:34:A:PRO:HD2   | 10                  | 0.73     | 0.04                | 0.74       |
| (2,467)  | 1:79:A:ILE:HG21  | 1:156:A:PHE:HA   | 10                  | 0.72     | 0.08                | 0.76       |
| (2,467)  | 1:79:A:ILE:HG22  | 1:156:A:PHE:HA   | 10                  | 0.72     | 0.08                | 0.76       |
| (2,467)  | 1:79:A:ILE:HG23  | 1:156:A:PHE:HA   | 10                  | 0.72     | 0.08                | 0.76       |
| (1,489)  | 1:48:A:ILE:HG21  | 1:48:A:ILE:HD11  | 10                  | 0.71     | 0.07                | 0.69       |
| (1,489)  | 1:48:A:ILE:HG21  | 1:48:A:ILE:HD12  | 10                  | 0.71     | 0.07                | 0.69       |
| (1,489)  | 1:48:A:ILE:HG21  | 1:48:A:ILE:HD13  | 10                  | 0.71     | 0.07                | 0.69       |
| (1,489)  | 1:48:A:ILE:HG22  | 1:48:A:ILE:HD11  | 10                  | 0.71     | 0.07                | 0.69       |
| (1,489)  | 1:48:A:ILE:HG22  | 1:48:A:ILE:HD12  | 10                  | 0.71     | 0.07                | 0.69       |
| (1,489)  | 1:48:A:ILE:HG22  | 1:48:A:ILE:HD13  | 10                  | 0.71     | 0.07                | 0.69       |
| (1,489)  | 1:48:A:ILE:HG23  | 1:48:A:ILE:HD11  | 10                  | 0.71     | 0.07                | 0.69       |
| (1,489)  | 1:48:A:ILE:HG23  | 1:48:A:ILE:HD12  | 10                  | 0.71     | 0.07                | 0.69       |
| (1,489)  | 1:48:A:ILE:HG23  | 1:48:A:ILE:HD13  | 10                  | 0.71     | 0.07                | 0.69       |
| (2,520)  | 1:84:A:GLY:HA2   | 1:155:A:ASN:HD21 | 10                  | 0.69     | 0.09                | 0.67       |
| (2,520)  | 1:84:A:GLY:HA2   | 1:155:A:ASN:HD22 | 10                  | 0.69     | 0.09                | 0.67       |
| (2,520)  | 1:84:A:GLY:HA3   | 1:155:A:ASN:HD21 | 10                  | 0.69     | 0.09                | 0.67       |
| (2,520)  | 1:84:A:GLY:HA3   | 1:155:A:ASN:HD22 | 10                  | 0.69     | 0.09                | 0.67       |
| (1,6)    | 1:18:A:ALA:HB1   | 1:19:A:VAL:H     | 10                  | 0.66     | 0.09                | 0.7        |
| (1,6)    | 1:18:A:ALA:HB2   | 1:19:A:VAL:H     | 10                  | 0.66     | 0.09                | 0.7        |
| (1,6)    | 1:18:A:ALA:HB3   | 1:19:A:VAL:H     | 10                  | 0.66     | 0.09                | 0.7        |
| (1,756)  | 1:63:A:THR:HG21  | 1:108:A:SER:HB2  | 10                  | 0.66     | 0.03                | 0.68       |
| (1,756)  | 1:63:A:THR:HG21  | 1:108:A:SER:HB3  | 10                  | 0.66     | 0.03                | 0.68       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,756)  | 1:63:A:THR:HG22  | 1:108:A:SER:HB2  | 10                  | 0.66     | 0.03                | 0.68       |
| (1,756)  | 1:63:A:THR:HG22  | 1:108:A:SER:HB3  | 10                  | 0.66     | 0.03                | 0.68       |
| (1,756)  | 1:63:A:THR:HG23  | 1:108:A:SER:HB2  | 10                  | 0.66     | 0.03                | 0.68       |
| (1,756)  | 1:63:A:THR:HG23  | 1:108:A:SER:HB3  | 10                  | 0.66     | 0.03                | 0.68       |
| (1,2078) | 1:151:A:VAL:HG11 | 1:151:A:VAL:HG21 | 10                  | 0.65     | 0.03                | 0.66       |
| (1,2078) | 1:151:A:VAL:HG11 | 1:151:A:VAL:HG22 | 10                  | 0.65     | 0.03                | 0.66       |
| (1,2078) | 1:151:A:VAL:HG11 | 1:151:A:VAL:HG23 | 10                  | 0.65     | 0.03                | 0.66       |
| (1,2078) | 1:151:A:VAL:HG12 | 1:151:A:VAL:HG21 | 10                  | 0.65     | 0.03                | 0.66       |
| (1,2078) | 1:151:A:VAL:HG12 | 1:151:A:VAL:HG22 | 10                  | 0.65     | 0.03                | 0.66       |
| (1,2078) | 1:151:A:VAL:HG12 | 1:151:A:VAL:HG23 | 10                  | 0.65     | 0.03                | 0.66       |
| (1,2078) | 1:151:A:VAL:HG13 | 1:151:A:VAL:HG21 | 10                  | 0.65     | 0.03                | 0.66       |
| (1,2078) | 1:151:A:VAL:HG13 | 1:151:A:VAL:HG22 | 10                  | 0.65     | 0.03                | 0.66       |
| (1,2078) | 1:151:A:VAL:HG13 | 1:151:A:VAL:HG23 | 10                  | 0.65     | 0.03                | 0.66       |
| (1,1206) | 1:81:A:ILE:HA    | 1:81:A:ILE:HG21  | 10                  | 0.59     | 0.01                | 0.59       |
| (1,1206) | 1:81:A:ILE:HA    | 1:81:A:ILE:HG22  | 10                  | 0.59     | 0.01                | 0.59       |
| (1,1206) | 1:81:A:ILE:HA    | 1:81:A:ILE:HG23  | 10                  | 0.59     | 0.01                | 0.59       |
| (1,1215) | 1:81:A:ILE:HD11  | 1:100:A:ALA:HB1  | 10                  | 0.58     | 0.19                | 0.64       |
| (1,1215) | 1:81:A:ILE:HD11  | 1:100:A:ALA:HB2  | 10                  | 0.58     | 0.19                | 0.64       |
| (1,1215) | 1:81:A:ILE:HD11  | 1:100:A:ALA:HB3  | 10                  | 0.58     | 0.19                | 0.64       |
| (1,1215) | 1:81:A:ILE:HD12  | 1:100:A:ALA:HB1  | 10                  | 0.58     | 0.19                | 0.64       |
| (1,1215) | 1:81:A:ILE:HD12  | 1:100:A:ALA:HB2  | 10                  | 0.58     | 0.19                | 0.64       |
| (1,1215) | 1:81:A:ILE:HD12  | 1:100:A:ALA:HB3  | 10                  | 0.58     | 0.19                | 0.64       |
| (1,1215) | 1:81:A:ILE:HD13  | 1:100:A:ALA:HB1  | 10                  | 0.58     | 0.19                | 0.64       |
| (1,1215) | 1:81:A:ILE:HD13  | 1:100:A:ALA:HB2  | 10                  | 0.58     | 0.19                | 0.64       |
| (1,1215) | 1:81:A:ILE:HD13  | 1:100:A:ALA:HB3  | 10                  | 0.58     | 0.19                | 0.64       |
| (1,2032) | 1:143:A:ILE:HG21 | 1:144:A:VAL:H    | 10                  | 0.57     | 0.14                | 0.62       |
| (1,2032) | 1:143:A:ILE:HG22 | 1:144:A:VAL:H    | 10                  | 0.57     | 0.14                | 0.62       |
| (1,2032) | 1:143:A:ILE:HG23 | 1:144:A:VAL:H    | 10                  | 0.57     | 0.14                | 0.62       |
| (2,490)  | 1:81:A:ILE:HD11  | 1:101:A:VAL:H    | 10                  | 0.57     | 0.13                | 0.55       |
| (2,490)  | 1:81:A:ILE:HD12  | 1:101:A:VAL:H    | 10                  | 0.57     | 0.13                | 0.55       |
| (2,490)  | 1:81:A:ILE:HD13  | 1:101:A:VAL:H    | 10                  | 0.57     | 0.13                | 0.55       |
| (1,1758) | 1:119:A:ALA:HB1  | 1:151:A:VAL:H    | 10                  | 0.56     | 0.05                | 0.59       |
| (1,1758) | 1:119:A:ALA:HB2  | 1:151:A:VAL:H    | 10                  | 0.56     | 0.05                | 0.59       |
| (1,1758) | 1:119:A:ALA:HB3  | 1:151:A:VAL:H    | 10                  | 0.56     | 0.05                | 0.59       |
| (2,656)  | 1:125:A:LYS:HB2  | 1:126:A:THR:H    | 10                  | 0.56     | 0.04                | 0.56       |
| (2,656)  | 1:125:A:LYS:HB3  | 1:126:A:THR:H    | 10                  | 0.56     | 0.04                | 0.56       |
| (2,473)  | 1:80:A:GLN:HB2   | 1:101:A:VAL:HA   | 10                  | 0.55     | 0.02                | 0.56       |
| (2,473)  | 1:80:A:GLN:HB3   | 1:101:A:VAL:HA   | 10                  | 0.55     | 0.02                | 0.56       |
| (2,4)    | 1:15:A:THR:HG21  | 1:16:A:ALA:H     | 10                  | 0.55     | 0.2                 | 0.54       |
| (2,4)    | 1:15:A:THR:HG22  | 1:16:A:ALA:H     | 10                  | 0.55     | 0.2                 | 0.54       |
| (2,4)    | 1:15:A:THR:HG23  | 1:16:A:ALA:H     | 10                  | 0.55     | 0.2                 | 0.54       |
| (2,535)  | 1:85:A:TYR:HE1   | 1:153:A:ILE:H    | 10                  | 0.54     | 0.02                | 0.55       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (2,535)  | 1:85:A:TYR:HE2   | 1:153:A:ILE:H    | 10                  | 0.54     | 0.02                | 0.55       |
| (3,8)    | 1:111:A:ILE:HA   | 1:111:A:ILE:HG21 | 10                  | 0.54     | 0.02                | 0.54       |
| (3,8)    | 1:111:A:ILE:HA   | 1:111:A:ILE:HG22 | 10                  | 0.54     | 0.02                | 0.54       |
| (3,8)    | 1:111:A:ILE:HA   | 1:111:A:ILE:HG23 | 10                  | 0.54     | 0.02                | 0.54       |
| (1,287)  | 1:36:A:ALA:HB1   | 1:36:A:ALA:H     | 10                  | 0.53     | 0.15                | 0.55       |
| (1,287)  | 1:36:A:ALA:HB2   | 1:36:A:ALA:H     | 10                  | 0.53     | 0.15                | 0.55       |
| (1,287)  | 1:36:A:ALA:HB3   | 1:36:A:ALA:H     | 10                  | 0.53     | 0.15                | 0.55       |
| (2,239)  | 1:46:A:TYR:HB3   | 1:155:A:ASN:HD21 | 10                  | 0.52     | 0.11                | 0.57       |
| (2,239)  | 1:46:A:TYR:HB3   | 1:155:A:ASN:HD22 | 10                  | 0.52     | 0.11                | 0.57       |
| (1,2460) | 1:182:A:VAL:HG11 | 1:182:A:VAL:HG21 | 10                  | 0.51     | 0.0                 | 0.51       |
| (1,2460) | 1:182:A:VAL:HG11 | 1:182:A:VAL:HG22 | 10                  | 0.51     | 0.0                 | 0.51       |
| (1,2460) | 1:182:A:VAL:HG11 | 1:182:A:VAL:HG23 | 10                  | 0.51     | 0.0                 | 0.51       |
| (1,2460) | 1:182:A:VAL:HG12 | 1:182:A:VAL:HG21 | 10                  | 0.51     | 0.0                 | 0.51       |
| (1,2460) | 1:182:A:VAL:HG12 | 1:182:A:VAL:HG22 | 10                  | 0.51     | 0.0                 | 0.51       |
| (1,2460) | 1:182:A:VAL:HG12 | 1:182:A:VAL:HG23 | 10                  | 0.51     | 0.0                 | 0.51       |
| (1,2460) | 1:182:A:VAL:HG13 | 1:182:A:VAL:HG21 | 10                  | 0.51     | 0.0                 | 0.51       |
| (1,2460) | 1:182:A:VAL:HG13 | 1:182:A:VAL:HG22 | 10                  | 0.51     | 0.0                 | 0.51       |
| (1,2460) | 1:182:A:VAL:HG13 | 1:182:A:VAL:HG23 | 10                  | 0.51     | 0.0                 | 0.51       |
| (1,1213) | 1:81:A:ILE:HD11  | 1:81:A:ILE:H     | 10                  | 0.5      | 0.01                | 0.51       |
| (1,1213) | 1:81:A:ILE:HD12  | 1:81:A:ILE:H     | 10                  | 0.5      | 0.01                | 0.51       |
| (1,1213) | 1:81:A:ILE:HD13  | 1:81:A:ILE:H     | 10                  | 0.5      | 0.01                | 0.51       |
| (2,125)  | 1:28:A:HIS:HE1   | 1:46:A:TYR:HE1   | 10                  | 0.49     | 0.08                | 0.52       |
| (2,125)  | 1:28:A:HIS:HE1   | 1:46:A:TYR:HE2   | 10                  | 0.49     | 0.08                | 0.52       |
| (2,16)   | 1:17:A:GLN:HG2   | 1:18:A:ALA:H     | 10                  | 0.49     | 0.03                | 0.5        |
| (2,16)   | 1:17:A:GLN:HG3   | 1:18:A:ALA:H     | 10                  | 0.49     | 0.03                | 0.5        |
| (2,740)  | 1:162:A:ALA:HA   | 1:168:A:PHE:HE1  | 10                  | 0.48     | 0.1                 | 0.52       |
| (2,740)  | 1:162:A:ALA:HA   | 1:168:A:PHE:HE2  | 10                  | 0.48     | 0.1                 | 0.52       |
| (1,139)  | 1:28:A:HIS:HD2   | 1:46:A:TYR:HE1   | 10                  | 0.48     | 0.16                | 0.55       |
| (1,139)  | 1:28:A:HIS:HD2   | 1:46:A:TYR:HE2   | 10                  | 0.48     | 0.16                | 0.55       |
| (1,294)  | 1:38:A:ALA:HA    | 1:38:A:ALA:HB1   | 10                  | 0.47     | 0.01                | 0.47       |
| (1,294)  | 1:38:A:ALA:HA    | 1:38:A:ALA:HB2   | 10                  | 0.47     | 0.01                | 0.47       |
| (1,294)  | 1:38:A:ALA:HA    | 1:38:A:ALA:HB3   | 10                  | 0.47     | 0.01                | 0.47       |
| (1,580)  | 1:51:A:ILE:HG21  | 1:53:A:ASP:H     | 10                  | 0.46     | 0.03                | 0.47       |
| (1,580)  | 1:51:A:ILE:HG22  | 1:53:A:ASP:H     | 10                  | 0.46     | 0.03                | 0.47       |
| (1,580)  | 1:51:A:ILE:HG23  | 1:53:A:ASP:H     | 10                  | 0.46     | 0.03                | 0.47       |
| (1,581)  | 1:51:A:ILE:HG21  | 1:53:A:ASP:H     | 10                  | 0.46     | 0.03                | 0.47       |
| (1,581)  | 1:51:A:ILE:HG22  | 1:53:A:ASP:H     | 10                  | 0.46     | 0.03                | 0.47       |
| (1,581)  | 1:51:A:ILE:HG23  | 1:53:A:ASP:H     | 10                  | 0.46     | 0.03                | 0.47       |
| (1,1804) | 1:129:A:THR:HB   | 1:129:A:THR:HG21 | 10                  | 0.46     | 0.0                 | 0.46       |
| (1,1804) | 1:129:A:THR:HB   | 1:129:A:THR:HG22 | 10                  | 0.46     | 0.0                 | 0.46       |
| (1,1804) | 1:129:A:THR:HB   | 1:129:A:THR:HG23 | 10                  | 0.46     | 0.0                 | 0.46       |
| (1,1)    | 1:15:A:THR:HB    | 1:15:A:THR:HG21  | 10                  | 0.46     | 0.0                 | 0.46       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1)    | 1:15:A:THR:HB    | 1:15:A:THR:HG22  | 10                  | 0.46     | 0.0                 | 0.46       |
| (1,1)    | 1:15:A:THR:HB    | 1:15:A:THR:HG23  | 10                  | 0.46     | 0.0                 | 0.46       |
| (1,1630) | 1:110:A:VAL:HG21 | 1:110:A:VAL:H    | 10                  | 0.45     | 0.02                | 0.46       |
| (1,1630) | 1:110:A:VAL:HG22 | 1:110:A:VAL:H    | 10                  | 0.45     | 0.02                | 0.46       |
| (1,1630) | 1:110:A:VAL:HG23 | 1:110:A:VAL:H    | 10                  | 0.45     | 0.02                | 0.46       |
| (1,2022) | 1:143:A:ILE:HA   | 1:143:A:ILE:HG21 | 10                  | 0.45     | 0.12                | 0.52       |
| (1,2022) | 1:143:A:ILE:HA   | 1:143:A:ILE:HG22 | 10                  | 0.45     | 0.12                | 0.52       |
| (1,2022) | 1:143:A:ILE:HA   | 1:143:A:ILE:HG23 | 10                  | 0.45     | 0.12                | 0.52       |
| (1,1228) | 1:81:A:ILE:HG21  | 1:82:A:THR:HA    | 10                  | 0.44     | 0.03                | 0.44       |
| (1,1228) | 1:81:A:ILE:HG22  | 1:82:A:THR:HA    | 10                  | 0.44     | 0.03                | 0.44       |
| (1,1228) | 1:81:A:ILE:HG23  | 1:82:A:THR:HA    | 10                  | 0.44     | 0.03                | 0.44       |
| (1,162)  | 1:29:A:LEU:HD11  | 1:29:A:LEU:HD21  | 10                  | 0.43     | 0.01                | 0.42       |
| (1,162)  | 1:29:A:LEU:HD11  | 1:29:A:LEU:HD22  | 10                  | 0.43     | 0.01                | 0.42       |
| (1,162)  | 1:29:A:LEU:HD11  | 1:29:A:LEU:HD23  | 10                  | 0.43     | 0.01                | 0.42       |
| (1,162)  | 1:29:A:LEU:HD12  | 1:29:A:LEU:HD21  | 10                  | 0.43     | 0.01                | 0.42       |
| (1,162)  | 1:29:A:LEU:HD12  | 1:29:A:LEU:HD22  | 10                  | 0.43     | 0.01                | 0.42       |
| (1,162)  | 1:29:A:LEU:HD12  | 1:29:A:LEU:HD23  | 10                  | 0.43     | 0.01                | 0.42       |
| (1,162)  | 1:29:A:LEU:HD13  | 1:29:A:LEU:HD21  | 10                  | 0.43     | 0.01                | 0.42       |
| (1,162)  | 1:29:A:LEU:HD13  | 1:29:A:LEU:HD22  | 10                  | 0.43     | 0.01                | 0.42       |
| (1,162)  | 1:29:A:LEU:HD13  | 1:29:A:LEU:HD23  | 10                  | 0.43     | 0.01                | 0.42       |
| (2,768)  | 1:173:A:VAL:HB   | 1:175:A:PHE:HE1  | 10                  | 0.42     | 0.11                | 0.47       |
| (2,768)  | 1:173:A:VAL:HB   | 1:175:A:PHE:HE2  | 10                  | 0.42     | 0.11                | 0.47       |
| (1,2463) | 1:182:A:VAL:HG21 | 1:182:A:VAL:H    | 10                  | 0.41     | 0.12                | 0.46       |
| (1,2463) | 1:182:A:VAL:HG22 | 1:182:A:VAL:H    | 10                  | 0.41     | 0.12                | 0.46       |
| (1,2463) | 1:182:A:VAL:HG23 | 1:182:A:VAL:H    | 10                  | 0.41     | 0.12                | 0.46       |
| (1,1270) | 1:82:A:THR:HG21  | 1:83:A:SER:HA    | 10                  | 0.4      | 0.02                | 0.41       |
| (1,1270) | 1:82:A:THR:HG22  | 1:83:A:SER:HA    | 10                  | 0.4      | 0.02                | 0.41       |
| (1,1270) | 1:82:A:THR:HG23  | 1:83:A:SER:HA    | 10                  | 0.4      | 0.02                | 0.41       |
| (1,1451) | 1:91:A:ALA:HB1   | 1:91:A:ALA:H     | 10                  | 0.38     | 0.01                | 0.38       |
| (1,1451) | 1:91:A:ALA:HB2   | 1:91:A:ALA:H     | 10                  | 0.38     | 0.01                | 0.38       |
| (1,1451) | 1:91:A:ALA:HB3   | 1:91:A:ALA:H     | 10                  | 0.38     | 0.01                | 0.38       |
| (1,2098) | 1:153:A:ILE:HB   | 1:153:A:ILE:HG21 | 10                  | 0.38     | 0.01                | 0.38       |
| (1,2098) | 1:153:A:ILE:HB   | 1:153:A:ILE:HG22 | 10                  | 0.38     | 0.01                | 0.38       |
| (1,2098) | 1:153:A:ILE:HB   | 1:153:A:ILE:HG23 | 10                  | 0.38     | 0.01                | 0.38       |
| (1,2320) | 1:171:A:LEU:HD11 | 1:171:A:LEU:HD21 | 10                  | 0.38     | 0.05                | 0.37       |
| (1,2320) | 1:171:A:LEU:HD11 | 1:171:A:LEU:HD22 | 10                  | 0.38     | 0.05                | 0.37       |
| (1,2320) | 1:171:A:LEU:HD11 | 1:171:A:LEU:HD23 | 10                  | 0.38     | 0.05                | 0.37       |
| (1,2320) | 1:171:A:LEU:HD12 | 1:171:A:LEU:HD21 | 10                  | 0.38     | 0.05                | 0.37       |
| (1,2320) | 1:171:A:LEU:HD12 | 1:171:A:LEU:HD22 | 10                  | 0.38     | 0.05                | 0.37       |
| (1,2320) | 1:171:A:LEU:HD12 | 1:171:A:LEU:HD23 | 10                  | 0.38     | 0.05                | 0.37       |
| (1,2320) | 1:171:A:LEU:HD13 | 1:171:A:LEU:HD21 | 10                  | 0.38     | 0.05                | 0.37       |
| (1,2320) | 1:171:A:LEU:HD13 | 1:171:A:LEU:HD22 | 10                  | 0.38     | 0.05                | 0.37       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2320) | 1:171:A:LEU:HD13 | 1:171:A:LEU:HD23 | 10                  | 0.38     | 0.05                | 0.37       |
| (1,520)  | 1:49:A:VAL:HB    | 1:152:A:ALA:HB1  | 10                  | 0.38     | 0.02                | 0.37       |
| (1,520)  | 1:49:A:VAL:HB    | 1:152:A:ALA:HB2  | 10                  | 0.38     | 0.02                | 0.37       |
| (1,520)  | 1:49:A:VAL:HB    | 1:152:A:ALA:HB3  | 10                  | 0.38     | 0.02                | 0.37       |
| (2,754)  | 1:167:A:LEU:HD21 | 1:167:A:LEU:H    | 10                  | 0.37     | 0.16                | 0.4        |
| (2,754)  | 1:167:A:LEU:HD22 | 1:167:A:LEU:H    | 10                  | 0.37     | 0.16                | 0.4        |
| (2,754)  | 1:167:A:LEU:HD23 | 1:167:A:LEU:H    | 10                  | 0.37     | 0.16                | 0.4        |
| (2,756)  | 1:167:A:LEU:H    | 1:167:A:LEU:HD21 | 10                  | 0.37     | 0.16                | 0.4        |
| (2,756)  | 1:167:A:LEU:H    | 1:167:A:LEU:HD22 | 10                  | 0.37     | 0.16                | 0.4        |
| (2,756)  | 1:167:A:LEU:H    | 1:167:A:LEU:HD23 | 10                  | 0.37     | 0.16                | 0.4        |
| (1,1816) | 1:131:A:THR:HB   | 1:131:A:THR:HG21 | 10                  | 0.37     | 0.0                 | 0.37       |
| (1,1816) | 1:131:A:THR:HB   | 1:131:A:THR:HG22 | 10                  | 0.37     | 0.0                 | 0.37       |
| (1,1816) | 1:131:A:THR:HB   | 1:131:A:THR:HG23 | 10                  | 0.37     | 0.0                 | 0.37       |
| (1,2067) | 1:148:A:THR:HB   | 1:148:A:THR:HG21 | 10                  | 0.37     | 0.01                | 0.37       |
| (1,2067) | 1:148:A:THR:HB   | 1:148:A:THR:HG22 | 10                  | 0.37     | 0.01                | 0.37       |
| (1,2067) | 1:148:A:THR:HB   | 1:148:A:THR:HG23 | 10                  | 0.37     | 0.01                | 0.37       |
| (1,1447) | 1:90:A:THR:HB    | 1:90:A:THR:HG21  | 10                  | 0.36     | 0.01                | 0.36       |
| (1,1447) | 1:90:A:THR:HB    | 1:90:A:THR:HG22  | 10                  | 0.36     | 0.01                | 0.36       |
| (1,1447) | 1:90:A:THR:HB    | 1:90:A:THR:HG23  | 10                  | 0.36     | 0.01                | 0.36       |
| (1,3)    | 1:16:A:ALA:HB1   | 1:16:A:ALA:H     | 10                  | 0.36     | 0.07                | 0.33       |
| (1,3)    | 1:16:A:ALA:HB2   | 1:16:A:ALA:H     | 10                  | 0.36     | 0.07                | 0.33       |
| (1,3)    | 1:16:A:ALA:HB3   | 1:16:A:ALA:H     | 10                  | 0.36     | 0.07                | 0.33       |
| (1,1941) | 1:135:A:VAL:HG21 | 1:135:A:VAL:H    | 10                  | 0.36     | 0.04                | 0.37       |
| (1,1941) | 1:135:A:VAL:HG22 | 1:135:A:VAL:H    | 10                  | 0.36     | 0.04                | 0.37       |
| (1,1941) | 1:135:A:VAL:HG23 | 1:135:A:VAL:H    | 10                  | 0.36     | 0.04                | 0.37       |
| (1,2038) | 1:144:A:VAL:HG21 | 1:144:A:VAL:H    | 10                  | 0.35     | 0.06                | 0.34       |
| (1,2038) | 1:144:A:VAL:HG22 | 1:144:A:VAL:H    | 10                  | 0.35     | 0.06                | 0.34       |
| (1,2038) | 1:144:A:VAL:HG23 | 1:144:A:VAL:H    | 10                  | 0.35     | 0.06                | 0.34       |
| (1,1236) | 1:81:A:ILE:HG21  | 1:154:A:LEU:HB3  | 10                  | 0.34     | 0.06                | 0.34       |
| (1,1236) | 1:81:A:ILE:HG22  | 1:154:A:LEU:HB3  | 10                  | 0.34     | 0.06                | 0.34       |
| (1,1236) | 1:81:A:ILE:HG23  | 1:154:A:LEU:HB3  | 10                  | 0.34     | 0.06                | 0.34       |
| (1,123)  | 1:27:A:SER:HB2   | 1:27:A:SER:H     | 10                  | 0.34     | 0.03                | 0.34       |
| (1,123)  | 1:27:A:SER:HB3   | 1:27:A:SER:H     | 10                  | 0.34     | 0.03                | 0.34       |
| (1,2015) | 1:142:A:ILE:HG21 | 1:144:A:VAL:H    | 10                  | 0.34     | 0.14                | 0.38       |
| (1,2015) | 1:142:A:ILE:HG22 | 1:144:A:VAL:H    | 10                  | 0.34     | 0.14                | 0.38       |
| (1,2015) | 1:142:A:ILE:HG23 | 1:144:A:VAL:H    | 10                  | 0.34     | 0.14                | 0.38       |
| (1,2093) | 1:153:A:ILE:HA   | 1:153:A:ILE:HG21 | 10                  | 0.32     | 0.07                | 0.34       |
| (1,2093) | 1:153:A:ILE:HA   | 1:153:A:ILE:HG22 | 10                  | 0.32     | 0.07                | 0.34       |
| (1,2093) | 1:153:A:ILE:HA   | 1:153:A:ILE:HG23 | 10                  | 0.32     | 0.07                | 0.34       |
| (1,1938) | 1:135:A:VAL:HG11 | 1:135:A:VAL:HG21 | 10                  | 0.32     | 0.02                | 0.32       |
| (1,1938) | 1:135:A:VAL:HG11 | 1:135:A:VAL:HG22 | 10                  | 0.32     | 0.02                | 0.32       |
| (1,1938) | 1:135:A:VAL:HG11 | 1:135:A:VAL:HG23 | 10                  | 0.32     | 0.02                | 0.32       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1938) | 1:135:A:VAL:HG12 | 1:135:A:VAL:HG21 | 10                  | 0.32     | 0.02                | 0.32       |
| (1,1938) | 1:135:A:VAL:HG12 | 1:135:A:VAL:HG22 | 10                  | 0.32     | 0.02                | 0.32       |
| (1,1938) | 1:135:A:VAL:HG12 | 1:135:A:VAL:HG23 | 10                  | 0.32     | 0.02                | 0.32       |
| (1,1938) | 1:135:A:VAL:HG13 | 1:135:A:VAL:HG21 | 10                  | 0.32     | 0.02                | 0.32       |
| (1,1938) | 1:135:A:VAL:HG13 | 1:135:A:VAL:HG22 | 10                  | 0.32     | 0.02                | 0.32       |
| (1,1938) | 1:135:A:VAL:HG13 | 1:135:A:VAL:HG23 | 10                  | 0.32     | 0.02                | 0.32       |
| (1,1162) | 1:79:A:ILE:HG13  | 1:80:A:GLN:H     | 10                  | 0.32     | 0.04                | 0.32       |
| (1,389)  | 1:44:A:ILE:HG21  | 1:44:A:ILE:H     | 10                  | 0.31     | 0.1                 | 0.32       |
| (1,389)  | 1:44:A:ILE:HG22  | 1:44:A:ILE:H     | 10                  | 0.31     | 0.1                 | 0.32       |
| (1,389)  | 1:44:A:ILE:HG23  | 1:44:A:ILE:H     | 10                  | 0.31     | 0.1                 | 0.32       |
| (1,2352) | 1:173:A:VAL:HG11 | 1:173:A:VAL:HG21 | 10                  | 0.31     | 0.01                | 0.31       |
| (1,2352) | 1:173:A:VAL:HG11 | 1:173:A:VAL:HG22 | 10                  | 0.31     | 0.01                | 0.31       |
| (1,2352) | 1:173:A:VAL:HG11 | 1:173:A:VAL:HG23 | 10                  | 0.31     | 0.01                | 0.31       |
| (1,2352) | 1:173:A:VAL:HG12 | 1:173:A:VAL:HG21 | 10                  | 0.31     | 0.01                | 0.31       |
| (1,2352) | 1:173:A:VAL:HG12 | 1:173:A:VAL:HG22 | 10                  | 0.31     | 0.01                | 0.31       |
| (1,2352) | 1:173:A:VAL:HG12 | 1:173:A:VAL:HG23 | 10                  | 0.31     | 0.01                | 0.31       |
| (1,2352) | 1:173:A:VAL:HG13 | 1:173:A:VAL:HG21 | 10                  | 0.31     | 0.01                | 0.31       |
| (1,2352) | 1:173:A:VAL:HG13 | 1:173:A:VAL:HG22 | 10                  | 0.31     | 0.01                | 0.31       |
| (1,2352) | 1:173:A:VAL:HG13 | 1:173:A:VAL:HG23 | 10                  | 0.31     | 0.01                | 0.31       |
| (1,232)  | 1:32:A:ILE:HG21  | 1:32:A:ILE:HD11  | 10                  | 0.3      | 0.07                | 0.32       |
| (1,232)  | 1:32:A:ILE:HG21  | 1:32:A:ILE:HD12  | 10                  | 0.3      | 0.07                | 0.32       |
| (1,232)  | 1:32:A:ILE:HG21  | 1:32:A:ILE:HD13  | 10                  | 0.3      | 0.07                | 0.32       |
| (1,232)  | 1:32:A:ILE:HG22  | 1:32:A:ILE:HD11  | 10                  | 0.3      | 0.07                | 0.32       |
| (1,232)  | 1:32:A:ILE:HG22  | 1:32:A:ILE:HD12  | 10                  | 0.3      | 0.07                | 0.32       |
| (1,232)  | 1:32:A:ILE:HG22  | 1:32:A:ILE:HD13  | 10                  | 0.3      | 0.07                | 0.32       |
| (1,232)  | 1:32:A:ILE:HG23  | 1:32:A:ILE:HD11  | 10                  | 0.3      | 0.07                | 0.32       |
| (1,232)  | 1:32:A:ILE:HG23  | 1:32:A:ILE:HD12  | 10                  | 0.3      | 0.07                | 0.32       |
| (1,232)  | 1:32:A:ILE:HG23  | 1:32:A:ILE:HD13  | 10                  | 0.3      | 0.07                | 0.32       |
| (1,209)  | 1:32:A:ILE:HA    | 1:32:A:ILE:HG21  | 10                  | 0.3      | 0.12                | 0.37       |
| (1,209)  | 1:32:A:ILE:HA    | 1:32:A:ILE:HG22  | 10                  | 0.3      | 0.12                | 0.37       |
| (1,209)  | 1:32:A:ILE:HA    | 1:32:A:ILE:HG23  | 10                  | 0.3      | 0.12                | 0.37       |
| (1,610)  | 1:55:A:VAL:HA    | 1:55:A:VAL:HG11  | 10                  | 0.3      | 0.03                | 0.29       |
| (1,610)  | 1:55:A:VAL:HA    | 1:55:A:VAL:HG12  | 10                  | 0.3      | 0.03                | 0.29       |
| (1,610)  | 1:55:A:VAL:HA    | 1:55:A:VAL:HG13  | 10                  | 0.3      | 0.03                | 0.29       |
| (2,753)  | 1:167:A:LEU:HD11 | 1:167:A:LEU:H    | 10                  | 0.3      | 0.17                | 0.29       |
| (2,753)  | 1:167:A:LEU:HD12 | 1:167:A:LEU:H    | 10                  | 0.3      | 0.17                | 0.29       |
| (2,753)  | 1:167:A:LEU:HD13 | 1:167:A:LEU:H    | 10                  | 0.3      | 0.17                | 0.29       |
| (2,755)  | 1:167:A:LEU:H    | 1:167:A:LEU:HD11 | 10                  | 0.3      | 0.17                | 0.29       |
| (2,755)  | 1:167:A:LEU:H    | 1:167:A:LEU:HD12 | 10                  | 0.3      | 0.17                | 0.29       |
| (2,755)  | 1:167:A:LEU:H    | 1:167:A:LEU:HD13 | 10                  | 0.3      | 0.17                | 0.29       |
| (1,257)  | 1:33:A:THR:HB    | 1:33:A:THR:HG21  | 10                  | 0.28     | 0.01                | 0.28       |
| (1,257)  | 1:33:A:THR:HB    | 1:33:A:THR:HG22  | 10                  | 0.28     | 0.01                | 0.28       |

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| Key      | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,257)  | 1:33:A:THR:HB   | 1:33:A:THR:HG23  | 10                  | 0.28     | 0.01                | 0.28       |
| (1,1343) | 1:85:A:TYR:HE1  | 1:152:A:ALA:HA   | 10                  | 0.26     | 0.12                | 0.27       |
| (1,1343) | 1:85:A:TYR:HE2  | 1:152:A:ALA:HA   | 10                  | 0.26     | 0.12                | 0.27       |
| (1,2177) | 1:157:A:LYS:H   | 1:158:A:ALA:HA   | 10                  | 0.26     | 0.01                | 0.26       |
| (1,621)  | 1:55:A:VAL:H    | 1:55:A:VAL:HG21  | 10                  | 0.26     | 0.04                | 0.25       |
| (1,621)  | 1:55:A:VAL:H    | 1:55:A:VAL:HG22  | 10                  | 0.26     | 0.04                | 0.25       |
| (1,621)  | 1:55:A:VAL:H    | 1:55:A:VAL:HG23  | 10                  | 0.26     | 0.04                | 0.25       |
| (1,2003) | 1:142:A:ILE:HA  | 1:142:A:ILE:HG21 | 10                  | 0.26     | 0.02                | 0.26       |
| (1,2003) | 1:142:A:ILE:HA  | 1:142:A:ILE:HG22 | 10                  | 0.26     | 0.02                | 0.26       |
| (1,2003) | 1:142:A:ILE:HA  | 1:142:A:ILE:HG23 | 10                  | 0.26     | 0.02                | 0.26       |
| (1,1180) | 1:80:A:GLN:HA   | 1:101:A:VAL:H    | 10                  | 0.25     | 0.04                | 0.26       |
| (1,2066) | 1:148:A:THR:HA  | 1:149:A:LYS:H    | 10                  | 0.25     | 0.01                | 0.25       |
| (1,709)  | 1:62:A:VAL:HA   | 1:62:A:VAL:HG11  | 10                  | 0.24     | 0.02                | 0.25       |
| (1,709)  | 1:62:A:VAL:HA   | 1:62:A:VAL:HG12  | 10                  | 0.24     | 0.02                | 0.25       |
| (1,709)  | 1:62:A:VAL:HA   | 1:62:A:VAL:HG13  | 10                  | 0.24     | 0.02                | 0.25       |
| (1,1173) | 1:79:A:ILE:H    | 1:158:A:ALA:HA   | 10                  | 0.24     | 0.03                | 0.26       |
| (1,1013) | 1:74:A:PHE:HB2  | 1:163:A:LYS:H    | 10                  | 0.24     | 0.03                | 0.24       |
| (2,628)  | 1:122:A:TYR:HB3 | 1:123:A:PRO:HD2  | 10                  | 0.23     | 0.07                | 0.24       |
| (1,1252) | 1:82:A:THR:HA   | 1:82:A:THR:HG21  | 10                  | 0.23     | 0.04                | 0.22       |
| (1,1252) | 1:82:A:THR:HA   | 1:82:A:THR:HG22  | 10                  | 0.23     | 0.04                | 0.22       |
| (1,1252) | 1:82:A:THR:HA   | 1:82:A:THR:HG23  | 10                  | 0.23     | 0.04                | 0.22       |
| (1,109)  | 1:26:A:GLU:H    | 1:47:A:ALA:HA    | 10                  | 0.22     | 0.02                | 0.22       |
| (1,627)  | 1:56:A:ASN:HB2  | 1:56:A:ASN:HD21  | 10                  | 0.22     | 0.02                | 0.23       |
| (1,627)  | 1:56:A:ASN:HB3  | 1:56:A:ASN:HD21  | 10                  | 0.22     | 0.02                | 0.23       |
| (1,1114) | 1:78:A:GLN:HA   | 1:159:A:PHE:HB3  | 10                  | 0.22     | 0.02                | 0.22       |
| (1,1852) | 1:133:A:ILE:HA  | 1:133:A:ILE:HG21 | 10                  | 0.22     | 0.02                | 0.22       |
| (1,1852) | 1:133:A:ILE:HA  | 1:133:A:ILE:HG22 | 10                  | 0.22     | 0.02                | 0.22       |
| (1,1852) | 1:133:A:ILE:HA  | 1:133:A:ILE:HG23 | 10                  | 0.22     | 0.02                | 0.22       |
| (1,1165) | 1:79:A:ILE:HG12 | 1:79:A:ILE:H     | 10                  | 0.22     | 0.02                | 0.21       |
| (1,779)  | 1:64:A:LEU:HD11 | 1:64:A:LEU:HD21  | 10                  | 0.21     | 0.04                | 0.22       |
| (1,779)  | 1:64:A:LEU:HD11 | 1:64:A:LEU:HD22  | 10                  | 0.21     | 0.04                | 0.22       |
| (1,779)  | 1:64:A:LEU:HD11 | 1:64:A:LEU:HD23  | 10                  | 0.21     | 0.04                | 0.22       |
| (1,779)  | 1:64:A:LEU:HD12 | 1:64:A:LEU:HD21  | 10                  | 0.21     | 0.04                | 0.22       |
| (1,779)  | 1:64:A:LEU:HD12 | 1:64:A:LEU:HD22  | 10                  | 0.21     | 0.04                | 0.22       |
| (1,779)  | 1:64:A:LEU:HD12 | 1:64:A:LEU:HD23  | 10                  | 0.21     | 0.04                | 0.22       |
| (1,779)  | 1:64:A:LEU:HD13 | 1:64:A:LEU:HD21  | 10                  | 0.21     | 0.04                | 0.22       |
| (1,779)  | 1:64:A:LEU:HD13 | 1:64:A:LEU:HD22  | 10                  | 0.21     | 0.04                | 0.22       |
| (1,779)  | 1:64:A:LEU:HD13 | 1:64:A:LEU:HD23  | 10                  | 0.21     | 0.04                | 0.22       |
| (1,1502) | 1:97:A:GLU:H    | 1:98:A:THR:HA    | 10                  | 0.2      | 0.01                | 0.19       |
| (1,1785) | 1:123:A:PRO:HD3 | 1:123:A:PRO:HD2  | 10                  | 0.2      | 0.0                 | 0.2        |
| (3,4)    | 1:57:A:ASP:HA   | 1:114:A:ASP:HA   | 10                  | 0.2      | 0.06                | 0.18       |
| (3,12)   | 1:181:A:GLN:HA  | 1:181:A:GLN:HB3  | 10                  | 0.2      | 0.02                | 0.2        |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1116) | 1:78:A:GLN:HB3   | 1:78:A:GLN:H     | 10                  | 0.19     | 0.01                | 0.19       |
| (1,684)  | 1:60:A:LEU:H     | 1:61:A:LYS:H     | 10                  | 0.19     | 0.03                | 0.18       |
| (1,2346) | 1:173:A:VAL:HB   | 1:173:A:VAL:HG11 | 10                  | 0.18     | 0.01                | 0.18       |
| (1,2346) | 1:173:A:VAL:HB   | 1:173:A:VAL:HG12 | 10                  | 0.18     | 0.01                | 0.18       |
| (1,2346) | 1:173:A:VAL:HB   | 1:173:A:VAL:HG13 | 10                  | 0.18     | 0.01                | 0.18       |
| (1,623)  | 1:55:A:VAL:H     | 1:115:A:LYS:HA   | 10                  | 0.18     | 0.04                | 0.18       |
| (3,13)   | 1:181:A:GLN:HA   | 1:181:A:GLN:HB2  | 10                  | 0.18     | 0.02                | 0.18       |
| (1,2347) | 1:173:A:VAL:HB   | 1:173:A:VAL:HG21 | 10                  | 0.18     | 0.01                | 0.18       |
| (1,2347) | 1:173:A:VAL:HB   | 1:173:A:VAL:HG22 | 10                  | 0.18     | 0.01                | 0.18       |
| (1,2347) | 1:173:A:VAL:HB   | 1:173:A:VAL:HG23 | 10                  | 0.18     | 0.01                | 0.18       |
| (1,1892) | 1:134:A:TRP:HB3  | 1:135:A:VAL:H    | 10                  | 0.18     | 0.02                | 0.18       |
| (1,1383) | 1:87:A:THR:HB    | 1:87:A:THR:HG21  | 10                  | 0.18     | 0.01                | 0.17       |
| (1,1383) | 1:87:A:THR:HB    | 1:87:A:THR:HG22  | 10                  | 0.18     | 0.01                | 0.17       |
| (1,1383) | 1:87:A:THR:HB    | 1:87:A:THR:HG23  | 10                  | 0.18     | 0.01                | 0.17       |
| (1,553)  | 1:50:A:TRP:HB2   | 1:52:A:LYS:H     | 10                  | 0.18     | 0.03                | 0.18       |
| (1,568)  | 1:51:A:ILE:HA    | 1:51:A:ILE:HG21  | 10                  | 0.17     | 0.05                | 0.16       |
| (1,568)  | 1:51:A:ILE:HA    | 1:51:A:ILE:HG22  | 10                  | 0.17     | 0.05                | 0.16       |
| (1,568)  | 1:51:A:ILE:HA    | 1:51:A:ILE:HG23  | 10                  | 0.17     | 0.05                | 0.16       |
| (1,745)  | 1:63:A:THR:HB    | 1:63:A:THR:HG21  | 10                  | 0.17     | 0.01                | 0.17       |
| (1,745)  | 1:63:A:THR:HB    | 1:63:A:THR:HG22  | 10                  | 0.17     | 0.01                | 0.17       |
| (1,745)  | 1:63:A:THR:HB    | 1:63:A:THR:HG23  | 10                  | 0.17     | 0.01                | 0.17       |
| (1,92)   | 1:25:A:VAL:H     | 1:50:A:TRP:HE1   | 10                  | 0.17     | 0.03                | 0.18       |
| (1,1261) | 1:82:A:THR:HB    | 1:82:A:THR:HG21  | 10                  | 0.16     | 0.0                 | 0.16       |
| (1,1261) | 1:82:A:THR:HB    | 1:82:A:THR:HG22  | 10                  | 0.16     | 0.0                 | 0.16       |
| (1,1261) | 1:82:A:THR:HB    | 1:82:A:THR:HG23  | 10                  | 0.16     | 0.0                 | 0.16       |
| (1,632)  | 1:56:A:ASN:HD21  | 1:56:A:ASN:HD22  | 10                  | 0.16     | 0.0                 | 0.16       |
| (1,1006) | 1:74:A:PHE:HA    | 1:163:A:LYS:H    | 10                  | 0.15     | 0.03                | 0.15       |
| (1,1425) | 1:88:A:ASN:HD21  | 1:88:A:ASN:HD22  | 10                  | 0.15     | 0.0                 | 0.15       |
| (1,2207) | 1:159:A:PHE:HB2  | 1:159:A:PHE:H    | 10                  | 0.15     | 0.02                | 0.16       |
| (1,51)   | 1:24:A:ASP:HB2   | 1:25:A:VAL:H     | 10                  | 0.15     | 0.02                | 0.15       |
| (1,2139) | 1:155:A:ASN:H    | 1:156:A:PHE:HZ   | 10                  | 0.14     | 0.02                | 0.15       |
| (1,1207) | 1:81:A:ILE:HA    | 1:82:A:THR:H     | 10                  | 0.13     | 0.01                | 0.13       |
| (1,1250) | 1:81:A:ILE:H     | 1:156:A:PHE:HA   | 10                  | 0.13     | 0.02                | 0.12       |
| (1,291)  | 1:37:A:GLY:HA2   | 1:37:A:GLY:HA3   | 10                  | 0.12     | 0.0                 | 0.12       |
| (1,1826) | 1:132:A:SER:HA   | 1:133:A:ILE:HB   | 10                  | 0.12     | 0.01                | 0.12       |
| (1,2357) | 1:173:A:VAL:HG21 | 1:175:A:PHE:HE1  | 9                   | 0.73     | 0.01                | 0.73       |
| (1,2357) | 1:173:A:VAL:HG21 | 1:175:A:PHE:HE2  | 9                   | 0.73     | 0.01                | 0.73       |
| (1,2357) | 1:173:A:VAL:HG22 | 1:175:A:PHE:HE1  | 9                   | 0.73     | 0.01                | 0.73       |
| (1,2357) | 1:173:A:VAL:HG22 | 1:175:A:PHE:HE2  | 9                   | 0.73     | 0.01                | 0.73       |
| (1,2357) | 1:173:A:VAL:HG23 | 1:175:A:PHE:HE1  | 9                   | 0.73     | 0.01                | 0.73       |
| (1,2357) | 1:173:A:VAL:HG23 | 1:175:A:PHE:HE2  | 9                   | 0.73     | 0.01                | 0.73       |
| (1,145)  | 1:28:A:HIS:HE1   | 1:48:A:ILE:HD11  | 9                   | 0.7      | 0.02                | 0.7        |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,145)  | 1:28:A:HIS:HE1   | 1:48:A:ILE:HD12  | 9                   | 0.7      | 0.02                | 0.7        |
| (1,145)  | 1:28:A:HIS:HE1   | 1:48:A:ILE:HD13  | 9                   | 0.7      | 0.02                | 0.7        |
| (2,365)  | 1:66:A:ASN:HB3   | 1:173:A:VAL:HG21 | 9                   | 0.67     | 0.11                | 0.73       |
| (2,365)  | 1:66:A:ASN:HB3   | 1:173:A:VAL:HG22 | 9                   | 0.67     | 0.11                | 0.73       |
| (2,365)  | 1:66:A:ASN:HB3   | 1:173:A:VAL:HG23 | 9                   | 0.67     | 0.11                | 0.73       |
| (1,1243) | 1:81:A:ILE:HG21  | 1:156:A:PHE:HZ   | 9                   | 0.66     | 0.02                | 0.66       |
| (1,1243) | 1:81:A:ILE:HG22  | 1:156:A:PHE:HZ   | 9                   | 0.66     | 0.02                | 0.66       |
| (1,1243) | 1:81:A:ILE:HG23  | 1:156:A:PHE:HZ   | 9                   | 0.66     | 0.02                | 0.66       |
| (1,1548) | 1:102:A:ILE:HG21 | 1:109:A:ALA:HB1  | 9                   | 0.62     | 0.06                | 0.63       |
| (1,1548) | 1:102:A:ILE:HG21 | 1:109:A:ALA:HB2  | 9                   | 0.62     | 0.06                | 0.63       |
| (1,1548) | 1:102:A:ILE:HG21 | 1:109:A:ALA:HB3  | 9                   | 0.62     | 0.06                | 0.63       |
| (1,1548) | 1:102:A:ILE:HG22 | 1:109:A:ALA:HB1  | 9                   | 0.62     | 0.06                | 0.63       |
| (1,1548) | 1:102:A:ILE:HG22 | 1:109:A:ALA:HB2  | 9                   | 0.62     | 0.06                | 0.63       |
| (1,1548) | 1:102:A:ILE:HG22 | 1:109:A:ALA:HB3  | 9                   | 0.62     | 0.06                | 0.63       |
| (1,1548) | 1:102:A:ILE:HG23 | 1:109:A:ALA:HB1  | 9                   | 0.62     | 0.06                | 0.63       |
| (1,1548) | 1:102:A:ILE:HG23 | 1:109:A:ALA:HB2  | 9                   | 0.62     | 0.06                | 0.63       |
| (1,1548) | 1:102:A:ILE:HG23 | 1:109:A:ALA:HB3  | 9                   | 0.62     | 0.06                | 0.63       |
| (2,389)  | 1:70:A:LEU:HD21  | 1:172:A:PRO:HD2  | 9                   | 0.6      | 0.21                | 0.64       |
| (2,389)  | 1:70:A:LEU:HD22  | 1:172:A:PRO:HD2  | 9                   | 0.6      | 0.21                | 0.64       |
| (2,389)  | 1:70:A:LEU:HD23  | 1:172:A:PRO:HD2  | 9                   | 0.6      | 0.21                | 0.64       |
| (2,517)  | 1:84:A:GLY:HA2   | 1:85:A:TYR:HD1   | 9                   | 0.6      | 0.25                | 0.72       |
| (2,517)  | 1:84:A:GLY:HA2   | 1:85:A:TYR:HD2   | 9                   | 0.6      | 0.25                | 0.72       |
| (2,517)  | 1:84:A:GLY:HA3   | 1:85:A:TYR:HD1   | 9                   | 0.6      | 0.25                | 0.72       |
| (2,517)  | 1:84:A:GLY:HA3   | 1:85:A:TYR:HD2   | 9                   | 0.6      | 0.25                | 0.72       |
| (1,2245) | 1:162:A:ALA:HB1  | 1:168:A:PHE:HE1  | 9                   | 0.57     | 0.11                | 0.64       |
| (1,2245) | 1:162:A:ALA:HB1  | 1:168:A:PHE:HE2  | 9                   | 0.57     | 0.11                | 0.64       |
| (1,2245) | 1:162:A:ALA:HB2  | 1:168:A:PHE:HE1  | 9                   | 0.57     | 0.11                | 0.64       |
| (1,2245) | 1:162:A:ALA:HB2  | 1:168:A:PHE:HE2  | 9                   | 0.57     | 0.11                | 0.64       |
| (1,2245) | 1:162:A:ALA:HB3  | 1:168:A:PHE:HE1  | 9                   | 0.57     | 0.11                | 0.64       |
| (1,2245) | 1:162:A:ALA:HB3  | 1:168:A:PHE:HE2  | 9                   | 0.57     | 0.11                | 0.64       |
| (1,2324) | 1:171:A:LEU:HD21 | 1:171:A:LEU:H    | 9                   | 0.57     | 0.06                | 0.57       |
| (1,2324) | 1:171:A:LEU:HD22 | 1:171:A:LEU:H    | 9                   | 0.57     | 0.06                | 0.57       |
| (1,2324) | 1:171:A:LEU:HD23 | 1:171:A:LEU:H    | 9                   | 0.57     | 0.06                | 0.57       |
| (2,380)  | 1:69:A:GLN:HE22  | 1:73:A:TYR:HE1   | 9                   | 0.54     | 0.05                | 0.54       |
| (2,380)  | 1:69:A:GLN:HE22  | 1:73:A:TYR:HE2   | 9                   | 0.54     | 0.05                | 0.54       |
| (1,1777) | 1:121:A:LEU:HD21 | 1:121:A:LEU:H    | 9                   | 0.49     | 0.17                | 0.62       |
| (1,1777) | 1:121:A:LEU:HD22 | 1:121:A:LEU:H    | 9                   | 0.49     | 0.17                | 0.62       |
| (1,1777) | 1:121:A:LEU:HD23 | 1:121:A:LEU:H    | 9                   | 0.49     | 0.17                | 0.62       |
| (1,296)  | 1:38:A:ALA:HB1   | 1:39:A:GLN:H     | 9                   | 0.48     | 0.11                | 0.53       |
| (1,296)  | 1:38:A:ALA:HB2   | 1:39:A:GLN:H     | 9                   | 0.48     | 0.11                | 0.53       |
| (1,296)  | 1:38:A:ALA:HB3   | 1:39:A:GLN:H     | 9                   | 0.48     | 0.11                | 0.53       |
| (1,545)  | 1:50:A:TRP:HA    | 1:151:A:VAL:HG21 | 9                   | 0.48     | 0.1                 | 0.51       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,545)  | 1:50:A:TRP:HA    | 1:151:A:VAL:HG22 | 9                   | 0.48     | 0.1                 | 0.51       |
| (1,545)  | 1:50:A:TRP:HA    | 1:151:A:VAL:HG23 | 9                   | 0.48     | 0.1                 | 0.51       |
| (1,840)  | 1:66:A:ASN:HB2   | 1:174:A:ILE:HD11 | 9                   | 0.45     | 0.0                 | 0.45       |
| (1,840)  | 1:66:A:ASN:HB2   | 1:174:A:ILE:HD12 | 9                   | 0.45     | 0.0                 | 0.45       |
| (1,840)  | 1:66:A:ASN:HB2   | 1:174:A:ILE:HD13 | 9                   | 0.45     | 0.0                 | 0.45       |
| (2,523)  | 1:85:A:TYR:HD1   | 1:134:A:TRP:H    | 9                   | 0.45     | 0.09                | 0.49       |
| (2,523)  | 1:85:A:TYR:HD2   | 1:134:A:TRP:H    | 9                   | 0.45     | 0.09                | 0.49       |
| (1,1546) | 1:102:A:ILE:HG21 | 1:108:A:SER:HA   | 9                   | 0.4      | 0.1                 | 0.44       |
| (1,1546) | 1:102:A:ILE:HG22 | 1:108:A:SER:HA   | 9                   | 0.4      | 0.1                 | 0.44       |
| (1,1546) | 1:102:A:ILE:HG23 | 1:108:A:SER:HA   | 9                   | 0.4      | 0.1                 | 0.44       |
| (2,194)  | 1:38:A:ALA:HB1   | 1:39:A:GLN:HE21  | 9                   | 0.4      | 0.19                | 0.39       |
| (2,194)  | 1:38:A:ALA:HB2   | 1:39:A:GLN:HE21  | 9                   | 0.4      | 0.19                | 0.39       |
| (2,194)  | 1:38:A:ALA:HB3   | 1:39:A:GLN:HE21  | 9                   | 0.4      | 0.19                | 0.39       |
| (1,2110) | 1:154:A:LEU:HA   | 1:154:A:LEU:HD21 | 9                   | 0.4      | 0.03                | 0.41       |
| (1,2110) | 1:154:A:LEU:HA   | 1:154:A:LEU:HD22 | 9                   | 0.4      | 0.03                | 0.41       |
| (1,2110) | 1:154:A:LEU:HA   | 1:154:A:LEU:HD23 | 9                   | 0.4      | 0.03                | 0.41       |
| (1,1510) | 1:98:A:THR:HG21  | 1:100:A:ALA:H    | 9                   | 0.4      | 0.13                | 0.47       |
| (1,1510) | 1:98:A:THR:HG22  | 1:100:A:ALA:H    | 9                   | 0.4      | 0.13                | 0.47       |
| (1,1510) | 1:98:A:THR:HG23  | 1:100:A:ALA:H    | 9                   | 0.4      | 0.13                | 0.47       |
| (1,1954) | 1:136:A:PRO:HG2  | 1:155:A:ASN:HD21 | 9                   | 0.38     | 0.05                | 0.39       |
| (1,1954) | 1:136:A:PRO:HG2  | 1:155:A:ASN:HD22 | 9                   | 0.38     | 0.05                | 0.39       |
| (1,495)  | 1:48:A:ILE:HG21  | 1:50:A:TRP:HE1   | 9                   | 0.35     | 0.1                 | 0.32       |
| (1,495)  | 1:48:A:ILE:HG22  | 1:50:A:TRP:HE1   | 9                   | 0.35     | 0.1                 | 0.32       |
| (1,495)  | 1:48:A:ILE:HG23  | 1:50:A:TRP:HE1   | 9                   | 0.35     | 0.1                 | 0.32       |
| (1,286)  | 1:36:A:ALA:HA    | 1:37:A:GLY:H     | 9                   | 0.34     | 0.04                | 0.32       |
| (1,487)  | 1:48:A:ILE:HG12  | 1:48:A:ILE:HG21  | 9                   | 0.34     | 0.03                | 0.33       |
| (1,487)  | 1:48:A:ILE:HG12  | 1:48:A:ILE:HG22  | 9                   | 0.34     | 0.03                | 0.33       |
| (1,487)  | 1:48:A:ILE:HG12  | 1:48:A:ILE:HG23  | 9                   | 0.34     | 0.03                | 0.33       |
| (1,2246) | 1:162:A:ALA:HB1  | 1:168:A:PHE:HZ   | 9                   | 0.34     | 0.11                | 0.32       |
| (1,2246) | 1:162:A:ALA:HB2  | 1:168:A:PHE:HZ   | 9                   | 0.34     | 0.11                | 0.32       |
| (1,2246) | 1:162:A:ALA:HB3  | 1:168:A:PHE:HZ   | 9                   | 0.34     | 0.11                | 0.32       |
| (1,837)  | 1:66:A:ASN:HB2   | 1:66:A:ASN:HD22  | 9                   | 0.27     | 0.1                 | 0.24       |
| (1,1445) | 1:90:A:THR:HA    | 1:90:A:THR:HG21  | 9                   | 0.25     | 0.01                | 0.25       |
| (1,1445) | 1:90:A:THR:HA    | 1:90:A:THR:HG22  | 9                   | 0.25     | 0.01                | 0.25       |
| (1,1445) | 1:90:A:THR:HA    | 1:90:A:THR:HG23  | 9                   | 0.25     | 0.01                | 0.25       |
| (1,1399) | 1:87:A:THR:HG21  | 1:87:A:THR:H     | 9                   | 0.22     | 0.08                | 0.23       |
| (1,1399) | 1:87:A:THR:HG22  | 1:87:A:THR:H     | 9                   | 0.22     | 0.08                | 0.23       |
| (1,1399) | 1:87:A:THR:HG23  | 1:87:A:THR:H     | 9                   | 0.22     | 0.08                | 0.23       |
| (1,710)  | 1:62:A:VAL:HA    | 1:62:A:VAL:HG21  | 9                   | 0.17     | 0.03                | 0.17       |
| (1,710)  | 1:62:A:VAL:HA    | 1:62:A:VAL:HG22  | 9                   | 0.17     | 0.03                | 0.17       |
| (1,710)  | 1:62:A:VAL:HA    | 1:62:A:VAL:HG23  | 9                   | 0.17     | 0.03                | 0.17       |
| (1,2270) | 1:166:A:MET:HA   | 1:167:A:LEU:H    | 9                   | 0.15     | 0.02                | 0.15       |

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| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,230)  | 1:32:A:ILE:HG12  | 1:32:A:ILE:H    | 9                   | 0.14     | 0.01                | 0.13       |
| (1,1677) | 1:114:A:ASP:HA   | 1:118:A:ILE:H   | 9                   | 0.12     | 0.02                | 0.11       |
| (1,513)  | 1:49:A:VAL:HA    | 1:49:A:VAL:HG11 | 9                   | 0.12     | 0.02                | 0.12       |
| (1,513)  | 1:49:A:VAL:HA    | 1:49:A:VAL:HG12 | 9                   | 0.12     | 0.02                | 0.12       |
| (1,513)  | 1:49:A:VAL:HA    | 1:49:A:VAL:HG13 | 9                   | 0.12     | 0.02                | 0.12       |
| (2,733)  | 1:157:A:LYS:HE2  | 1:159:A:PHE:HD1 | 8                   | 0.58     | 0.2                 | 0.58       |
| (2,733)  | 1:157:A:LYS:HE2  | 1:159:A:PHE:HD2 | 8                   | 0.58     | 0.2                 | 0.58       |
| (2,733)  | 1:157:A:LYS:HE3  | 1:159:A:PHE:HD1 | 8                   | 0.58     | 0.2                 | 0.58       |
| (2,733)  | 1:157:A:LYS:HE3  | 1:159:A:PHE:HD2 | 8                   | 0.58     | 0.2                 | 0.58       |
| (2,518)  | 1:84:A:GLY:HA2   | 1:95:A:PHE:HE1  | 8                   | 0.57     | 0.29                | 0.64       |
| (2,518)  | 1:84:A:GLY:HA2   | 1:95:A:PHE:HE2  | 8                   | 0.57     | 0.29                | 0.64       |
| (2,518)  | 1:84:A:GLY:HA3   | 1:95:A:PHE:HE1  | 8                   | 0.57     | 0.29                | 0.64       |
| (2,518)  | 1:84:A:GLY:HA3   | 1:95:A:PHE:HE2  | 8                   | 0.57     | 0.29                | 0.64       |
| (1,679)  | 1:60:A:LEU:HD11  | 1:177:A:PHE:HD1 | 8                   | 0.53     | 0.19                | 0.48       |
| (1,679)  | 1:60:A:LEU:HD11  | 1:177:A:PHE:HD2 | 8                   | 0.53     | 0.19                | 0.48       |
| (1,679)  | 1:60:A:LEU:HD12  | 1:177:A:PHE:HD1 | 8                   | 0.53     | 0.19                | 0.48       |
| (1,679)  | 1:60:A:LEU:HD12  | 1:177:A:PHE:HD2 | 8                   | 0.53     | 0.19                | 0.48       |
| (1,679)  | 1:60:A:LEU:HD13  | 1:177:A:PHE:HD1 | 8                   | 0.53     | 0.19                | 0.48       |
| (1,679)  | 1:60:A:LEU:HD13  | 1:177:A:PHE:HD2 | 8                   | 0.53     | 0.19                | 0.48       |
| (2,614)  | 1:118:A:ILE:HG21 | 1:151:A:VAL:HA  | 8                   | 0.46     | 0.16                | 0.46       |
| (2,614)  | 1:118:A:ILE:HG22 | 1:151:A:VAL:HA  | 8                   | 0.46     | 0.16                | 0.46       |
| (2,614)  | 1:118:A:ILE:HG23 | 1:151:A:VAL:HA  | 8                   | 0.46     | 0.16                | 0.46       |
| (1,2083) | 1:151:A:VAL:HG21 | 1:152:A:ALA:H   | 8                   | 0.45     | 0.01                | 0.45       |
| (1,2083) | 1:151:A:VAL:HG22 | 1:152:A:ALA:H   | 8                   | 0.45     | 0.01                | 0.45       |
| (1,2083) | 1:151:A:VAL:HG23 | 1:152:A:ALA:H   | 8                   | 0.45     | 0.01                | 0.45       |
| (1,242)  | 1:32:A:ILE:HG21  | 1:160:A:TYR:HE1 | 8                   | 0.44     | 0.11                | 0.42       |
| (1,242)  | 1:32:A:ILE:HG21  | 1:160:A:TYR:HE2 | 8                   | 0.44     | 0.11                | 0.42       |
| (1,242)  | 1:32:A:ILE:HG22  | 1:160:A:TYR:HE1 | 8                   | 0.44     | 0.11                | 0.42       |
| (1,242)  | 1:32:A:ILE:HG22  | 1:160:A:TYR:HE2 | 8                   | 0.44     | 0.11                | 0.42       |
| (1,242)  | 1:32:A:ILE:HG23  | 1:160:A:TYR:HE1 | 8                   | 0.44     | 0.11                | 0.42       |
| (1,242)  | 1:32:A:ILE:HG23  | 1:160:A:TYR:HE2 | 8                   | 0.44     | 0.11                | 0.42       |
| (1,2354) | 1:173:A:VAL:HG11 | 1:175:A:PHE:HE1 | 8                   | 0.43     | 0.2                 | 0.44       |
| (1,2354) | 1:173:A:VAL:HG11 | 1:175:A:PHE:HE2 | 8                   | 0.43     | 0.2                 | 0.44       |
| (1,2354) | 1:173:A:VAL:HG12 | 1:175:A:PHE:HE1 | 8                   | 0.43     | 0.2                 | 0.44       |
| (1,2354) | 1:173:A:VAL:HG12 | 1:175:A:PHE:HE2 | 8                   | 0.43     | 0.2                 | 0.44       |
| (1,2354) | 1:173:A:VAL:HG13 | 1:175:A:PHE:HE1 | 8                   | 0.43     | 0.2                 | 0.44       |
| (1,2354) | 1:173:A:VAL:HG13 | 1:175:A:PHE:HE2 | 8                   | 0.43     | 0.2                 | 0.44       |
| (2,592)  | 1:114:A:ASP:HB3  | 1:116:A:GLU:HG2 | 8                   | 0.34     | 0.15                | 0.38       |
| (2,592)  | 1:114:A:ASP:HB3  | 1:116:A:GLU:HG3 | 8                   | 0.34     | 0.15                | 0.38       |
| (2,607)  | 1:115:A:LYS:H    | 1:116:A:GLU:HG2 | 8                   | 0.31     | 0.12                | 0.34       |
| (2,607)  | 1:115:A:LYS:H    | 1:116:A:GLU:HG3 | 8                   | 0.31     | 0.12                | 0.34       |
| (1,2286) | 1:168:A:PHE:HD1  | 1:168:A:PHE:H   | 8                   | 0.31     | 0.04                | 0.32       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2286) | 1:168:A:PHE:HD2  | 1:168:A:PHE:H    | 8                   | 0.31     | 0.04                | 0.32       |
| (1,170)  | 1:29:A:LEU:HD21  | 1:175:A:PHE:HD1  | 8                   | 0.29     | 0.15                | 0.26       |
| (1,170)  | 1:29:A:LEU:HD21  | 1:175:A:PHE:HD2  | 8                   | 0.29     | 0.15                | 0.26       |
| (1,170)  | 1:29:A:LEU:HD22  | 1:175:A:PHE:HD1  | 8                   | 0.29     | 0.15                | 0.26       |
| (1,170)  | 1:29:A:LEU:HD22  | 1:175:A:PHE:HD2  | 8                   | 0.29     | 0.15                | 0.26       |
| (1,170)  | 1:29:A:LEU:HD23  | 1:175:A:PHE:HD1  | 8                   | 0.29     | 0.15                | 0.26       |
| (1,170)  | 1:29:A:LEU:HD23  | 1:175:A:PHE:HD2  | 8                   | 0.29     | 0.15                | 0.26       |
| (1,2106) | 1:153:A:ILE:HG21 | 1:155:A:ASN:HD21 | 8                   | 0.29     | 0.12                | 0.3        |
| (1,2106) | 1:153:A:ILE:HG21 | 1:155:A:ASN:HD22 | 8                   | 0.29     | 0.12                | 0.3        |
| (1,2106) | 1:153:A:ILE:HG22 | 1:155:A:ASN:HD21 | 8                   | 0.29     | 0.12                | 0.3        |
| (1,2106) | 1:153:A:ILE:HG22 | 1:155:A:ASN:HD22 | 8                   | 0.29     | 0.12                | 0.3        |
| (1,2106) | 1:153:A:ILE:HG23 | 1:155:A:ASN:HD21 | 8                   | 0.29     | 0.12                | 0.3        |
| (1,2106) | 1:153:A:ILE:HG23 | 1:155:A:ASN:HD22 | 8                   | 0.29     | 0.12                | 0.3        |
| (1,467)  | 1:47:A:ALA:H     | 1:156:A:PHE:HE1  | 8                   | 0.25     | 0.06                | 0.26       |
| (1,467)  | 1:47:A:ALA:H     | 1:156:A:PHE:HE2  | 8                   | 0.25     | 0.06                | 0.26       |
| (1,556)  | 1:50:A:TRP:HD1   | 1:151:A:VAL:HG21 | 8                   | 0.25     | 0.03                | 0.26       |
| (1,556)  | 1:50:A:TRP:HD1   | 1:151:A:VAL:HG22 | 8                   | 0.25     | 0.03                | 0.26       |
| (1,556)  | 1:50:A:TRP:HD1   | 1:151:A:VAL:HG23 | 8                   | 0.25     | 0.03                | 0.26       |
| (1,543)  | 1:50:A:TRP:HA    | 1:151:A:VAL:HA   | 8                   | 0.21     | 0.02                | 0.2        |
| (1,2370) | 1:174:A:ILE:HG21 | 1:175:A:PHE:HA   | 8                   | 0.2      | 0.04                | 0.2        |
| (1,2370) | 1:174:A:ILE:HG22 | 1:175:A:PHE:HA   | 8                   | 0.2      | 0.04                | 0.2        |
| (1,2370) | 1:174:A:ILE:HG23 | 1:175:A:PHE:HA   | 8                   | 0.2      | 0.04                | 0.2        |
| (1,268)  | 1:34:A:PRO:HD3   | 1:35:A:ALA:H     | 8                   | 0.2      | 0.06                | 0.18       |
| (1,2349) | 1:173:A:VAL:HB   | 1:174:A:ILE:H    | 8                   | 0.2      | 0.03                | 0.2        |
| (1,2079) | 1:151:A:VAL:HG11 | 1:151:A:VAL:H    | 8                   | 0.16     | 0.03                | 0.16       |
| (1,2079) | 1:151:A:VAL:HG12 | 1:151:A:VAL:H    | 8                   | 0.16     | 0.03                | 0.16       |
| (1,2079) | 1:151:A:VAL:HG13 | 1:151:A:VAL:H    | 8                   | 0.16     | 0.03                | 0.16       |
| (1,1075) | 1:76:A:TYR:H     | 1:162:A:ALA:HA   | 8                   | 0.14     | 0.03                | 0.14       |
| (1,2089) | 1:152:A:ALA:HB1  | 1:152:A:ALA:H    | 8                   | 0.14     | 0.06                | 0.11       |
| (1,2089) | 1:152:A:ALA:HB2  | 1:152:A:ALA:H    | 8                   | 0.14     | 0.06                | 0.11       |
| (1,2089) | 1:152:A:ALA:HB3  | 1:152:A:ALA:H    | 8                   | 0.14     | 0.06                | 0.11       |
| (1,1894) | 1:134:A:TRP:HB3  | 1:142:A:ILE:HA   | 8                   | 0.13     | 0.02                | 0.13       |
| (1,975)  | 1:73:A:TYR:HA    | 1:73:A:TYR:HB3   | 8                   | 0.12     | 0.01                | 0.12       |
| (1,1532) | 1:102:A:ILE:HB   | 1:102:A:ILE:H    | 8                   | 0.12     | 0.02                | 0.12       |
| (1,82)   | 1:25:A:VAL:HG21  | 1:25:A:VAL:HG11  | 8                   | 0.11     | 0.0                 | 0.11       |
| (1,82)   | 1:25:A:VAL:HG21  | 1:25:A:VAL:HG12  | 8                   | 0.11     | 0.0                 | 0.11       |
| (1,82)   | 1:25:A:VAL:HG21  | 1:25:A:VAL:HG13  | 8                   | 0.11     | 0.0                 | 0.11       |
| (1,82)   | 1:25:A:VAL:HG22  | 1:25:A:VAL:HG11  | 8                   | 0.11     | 0.0                 | 0.11       |
| (1,82)   | 1:25:A:VAL:HG22  | 1:25:A:VAL:HG12  | 8                   | 0.11     | 0.0                 | 0.11       |
| (1,82)   | 1:25:A:VAL:HG22  | 1:25:A:VAL:HG13  | 8                   | 0.11     | 0.0                 | 0.11       |
| (1,82)   | 1:25:A:VAL:HG23  | 1:25:A:VAL:HG11  | 8                   | 0.11     | 0.0                 | 0.11       |
| (1,82)   | 1:25:A:VAL:HG23  | 1:25:A:VAL:HG12  | 8                   | 0.11     | 0.0                 | 0.11       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,82)   | 1:25:A:VAL:HG23  | 1:25:A:VAL:HG13  | 8                   | 0.11     | 0.0                 | 0.11       |
| (1,2183) | 1:158:A:ALA:HA   | 1:159:A:PHE:HB3  | 8                   | 0.11     | 0.01                | 0.11       |
| (1,1103) | 1:77:A:LEU:H     | 1:104:A:LEU:HD11 | 7                   | 0.53     | 0.01                | 0.53       |
| (1,1103) | 1:77:A:LEU:H     | 1:104:A:LEU:HD12 | 7                   | 0.53     | 0.01                | 0.53       |
| (1,1103) | 1:77:A:LEU:H     | 1:104:A:LEU:HD13 | 7                   | 0.53     | 0.01                | 0.53       |
| (1,599)  | 1:53:A:ASP:H     | 1:55:A:VAL:HG11  | 7                   | 0.5      | 0.1                 | 0.53       |
| (1,599)  | 1:53:A:ASP:H     | 1:55:A:VAL:HG12  | 7                   | 0.5      | 0.1                 | 0.53       |
| (1,599)  | 1:53:A:ASP:H     | 1:55:A:VAL:HG13  | 7                   | 0.5      | 0.1                 | 0.53       |
| (1,2131) | 1:155:A:ASN:HD21 | 1:155:A:ASN:HA   | 7                   | 0.49     | 0.01                | 0.49       |
| (1,2131) | 1:155:A:ASN:HD22 | 1:155:A:ASN:HA   | 7                   | 0.49     | 0.01                | 0.49       |
| (1,1088) | 1:77:A:LEU:HD11  | 1:78:A:GLN:H     | 7                   | 0.49     | 0.07                | 0.51       |
| (1,1088) | 1:77:A:LEU:HD12  | 1:78:A:GLN:H     | 7                   | 0.49     | 0.07                | 0.51       |
| (1,1088) | 1:77:A:LEU:HD13  | 1:78:A:GLN:H     | 7                   | 0.49     | 0.07                | 0.51       |
| (1,1088) | 1:77:A:LEU:HD21  | 1:78:A:GLN:H     | 7                   | 0.49     | 0.07                | 0.51       |
| (1,1088) | 1:77:A:LEU:HD22  | 1:78:A:GLN:H     | 7                   | 0.49     | 0.07                | 0.51       |
| (1,1088) | 1:77:A:LEU:HD23  | 1:78:A:GLN:H     | 7                   | 0.49     | 0.07                | 0.51       |
| (1,2449) | 1:179:A:VAL:HG21 | 1:179:A:VAL:H    | 7                   | 0.46     | 0.03                | 0.45       |
| (1,2449) | 1:179:A:VAL:HG22 | 1:179:A:VAL:H    | 7                   | 0.46     | 0.03                | 0.45       |
| (1,2449) | 1:179:A:VAL:HG23 | 1:179:A:VAL:H    | 7                   | 0.46     | 0.03                | 0.45       |
| (1,1475) | 1:95:A:PHE:HB2   | 1:96:A:SER:H     | 7                   | 0.4      | 0.03                | 0.4        |
| (1,1475) | 1:95:A:PHE:HB3   | 1:96:A:SER:H     | 7                   | 0.4      | 0.03                | 0.4        |
| (1,852)  | 1:66:A:ASN:HD22  | 1:70:A:LEU:HD21  | 7                   | 0.4      | 0.08                | 0.45       |
| (1,852)  | 1:66:A:ASN:HD22  | 1:70:A:LEU:HD22  | 7                   | 0.4      | 0.08                | 0.45       |
| (1,852)  | 1:66:A:ASN:HD22  | 1:70:A:LEU:HD23  | 7                   | 0.4      | 0.08                | 0.45       |
| (1,1556) | 1:103:A:SER:HA   | 1:104:A:LEU:HB3  | 7                   | 0.33     | 0.02                | 0.33       |
| (1,1189) | 1:80:A:GLN:HG2   | 1:98:A:THR:HG21  | 7                   | 0.32     | 0.05                | 0.31       |
| (1,1189) | 1:80:A:GLN:HG2   | 1:98:A:THR:HG22  | 7                   | 0.32     | 0.05                | 0.31       |
| (1,1189) | 1:80:A:GLN:HG2   | 1:98:A:THR:HG23  | 7                   | 0.32     | 0.05                | 0.31       |
| (1,1189) | 1:80:A:GLN:HG3   | 1:98:A:THR:HG21  | 7                   | 0.32     | 0.05                | 0.31       |
| (1,1189) | 1:80:A:GLN:HG3   | 1:98:A:THR:HG22  | 7                   | 0.32     | 0.05                | 0.31       |
| (1,1189) | 1:80:A:GLN:HG3   | 1:98:A:THR:HG23  | 7                   | 0.32     | 0.05                | 0.31       |
| (1,2327) | 1:171:A:LEU:HG   | 1:171:A:LEU:H    | 7                   | 0.31     | 0.05                | 0.32       |
| (1,1818) | 1:131:A:THR:HG21 | 1:131:A:THR:H    | 7                   | 0.31     | 0.18                | 0.23       |
| (1,1818) | 1:131:A:THR:HG22 | 1:131:A:THR:H    | 7                   | 0.31     | 0.18                | 0.23       |
| (1,1818) | 1:131:A:THR:HG23 | 1:131:A:THR:H    | 7                   | 0.31     | 0.18                | 0.23       |
| (2,425)  | 1:74:A:PHE:HZ    | 1:160:A:TYR:HE1  | 7                   | 0.31     | 0.14                | 0.31       |
| (2,425)  | 1:74:A:PHE:HZ    | 1:160:A:TYR:HE2  | 7                   | 0.31     | 0.14                | 0.31       |
| (2,632)  | 1:122:A:TYR:HD1  | 1:125:A:LYS:H    | 7                   | 0.3      | 0.17                | 0.24       |
| (2,632)  | 1:122:A:TYR:HD2  | 1:125:A:LYS:H    | 7                   | 0.3      | 0.17                | 0.24       |
| (1,1338) | 1:85:A:TYR:HD1   | 1:86:A:GLU:H     | 7                   | 0.3      | 0.09                | 0.3        |
| (1,1338) | 1:85:A:TYR:HD2   | 1:86:A:GLU:H     | 7                   | 0.3      | 0.09                | 0.3        |
| (1,1706) | 1:115:A:LYS:HG2  | 1:115:A:LYS:H    | 7                   | 0.28     | 0.06                | 0.28       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1706) | 1:115:A:LYS:HG3  | 1:115:A:LYS:H    | 7                   | 0.28     | 0.06                | 0.28       |
| (1,1767) | 1:120:A:VAL:HG11 | 1:121:A:LEU:H    | 7                   | 0.27     | 0.03                | 0.27       |
| (1,1767) | 1:120:A:VAL:HG12 | 1:121:A:LEU:H    | 7                   | 0.27     | 0.03                | 0.27       |
| (1,1767) | 1:120:A:VAL:HG13 | 1:121:A:LEU:H    | 7                   | 0.27     | 0.03                | 0.27       |
| (2,732)  | 1:155:A:ASN:H    | 1:156:A:PHE:HE1  | 7                   | 0.24     | 0.1                 | 0.22       |
| (2,732)  | 1:155:A:ASN:H    | 1:156:A:PHE:HE2  | 7                   | 0.24     | 0.1                 | 0.22       |
| (1,2021) | 1:143:A:ILE:HA   | 1:143:A:ILE:HD11 | 7                   | 0.24     | 0.02                | 0.24       |
| (1,2021) | 1:143:A:ILE:HA   | 1:143:A:ILE:HD12 | 7                   | 0.24     | 0.02                | 0.24       |
| (1,2021) | 1:143:A:ILE:HA   | 1:143:A:ILE:HD13 | 7                   | 0.24     | 0.02                | 0.24       |
| (1,2030) | 1:143:A:ILE:HG21 | 1:143:A:ILE:HD11 | 7                   | 0.24     | 0.02                | 0.23       |
| (1,2030) | 1:143:A:ILE:HG21 | 1:143:A:ILE:HD12 | 7                   | 0.24     | 0.02                | 0.23       |
| (1,2030) | 1:143:A:ILE:HG21 | 1:143:A:ILE:HD13 | 7                   | 0.24     | 0.02                | 0.23       |
| (1,2030) | 1:143:A:ILE:HG22 | 1:143:A:ILE:HD11 | 7                   | 0.24     | 0.02                | 0.23       |
| (1,2030) | 1:143:A:ILE:HG22 | 1:143:A:ILE:HD12 | 7                   | 0.24     | 0.02                | 0.23       |
| (1,2030) | 1:143:A:ILE:HG22 | 1:143:A:ILE:HD13 | 7                   | 0.24     | 0.02                | 0.23       |
| (1,2030) | 1:143:A:ILE:HG23 | 1:143:A:ILE:HD11 | 7                   | 0.24     | 0.02                | 0.23       |
| (1,2030) | 1:143:A:ILE:HG23 | 1:143:A:ILE:HD12 | 7                   | 0.24     | 0.02                | 0.23       |
| (1,2030) | 1:143:A:ILE:HG23 | 1:143:A:ILE:HD13 | 7                   | 0.24     | 0.02                | 0.23       |
| (1,1653) | 1:113:A:LEU:HA   | 1:113:A:LEU:HD21 | 7                   | 0.23     | 0.06                | 0.23       |
| (1,1653) | 1:113:A:LEU:HA   | 1:113:A:LEU:HD22 | 7                   | 0.23     | 0.06                | 0.23       |
| (1,1653) | 1:113:A:LEU:HA   | 1:113:A:LEU:HD23 | 7                   | 0.23     | 0.06                | 0.23       |
| (2,178)  | 1:36:A:ALA:H     | 1:37:A:GLY:H     | 7                   | 0.21     | 0.08                | 0.21       |
| (1,1505) | 1:98:A:THR:HA    | 1:100:A:ALA:H    | 7                   | 0.16     | 0.03                | 0.16       |
| (1,914)  | 1:69:A:GLN:HG3   | 1:69:A:GLN:H     | 7                   | 0.16     | 0.04                | 0.16       |
| (1,857)  | 1:66:A:ASN:HD22  | 1:174:A:ILE:H    | 7                   | 0.15     | 0.03                | 0.16       |
| (1,1371) | 1:86:A:GLU:H     | 1:134:A:TRP:HE1  | 7                   | 0.14     | 0.03                | 0.13       |
| (1,1923) | 1:134:A:TRP:HE1  | 1:139:A:PRO:HD2  | 7                   | 0.13     | 0.05                | 0.11       |
| (1,548)  | 1:50:A:TRP:HB3   | 1:50:A:TRP:H     | 7                   | 0.12     | 0.01                | 0.12       |
| (1,1127) | 1:78:A:GLN:H     | 1:104:A:LEU:H    | 7                   | 0.12     | 0.02                | 0.13       |
| (1,1618) | 1:108:A:SER:H    | 1:109:A:ALA:H    | 7                   | 0.1      | 0.0                 | 0.1        |
| (1,206)  | 1:32:A:ILE:HA    | 1:32:A:ILE:HD11  | 6                   | 0.75     | 0.03                | 0.75       |
| (1,206)  | 1:32:A:ILE:HA    | 1:32:A:ILE:HD12  | 6                   | 0.75     | 0.03                | 0.75       |
| (1,206)  | 1:32:A:ILE:HA    | 1:32:A:ILE:HD13  | 6                   | 0.75     | 0.03                | 0.75       |
| (1,2462) | 1:182:A:VAL:HG11 | 1:183:A:GLY:H    | 6                   | 0.49     | 0.01                | 0.49       |
| (1,2462) | 1:182:A:VAL:HG12 | 1:183:A:GLY:H    | 6                   | 0.49     | 0.01                | 0.49       |
| (1,2462) | 1:182:A:VAL:HG13 | 1:183:A:GLY:H    | 6                   | 0.49     | 0.01                | 0.49       |
| (2,635)  | 1:122:A:TYR:HD1  | 1:126:A:THR:H    | 6                   | 0.47     | 0.1                 | 0.51       |
| (2,635)  | 1:122:A:TYR:HD2  | 1:126:A:THR:H    | 6                   | 0.47     | 0.1                 | 0.51       |
| (1,1647) | 1:112:A:VAL:HG11 | 1:112:A:VAL:H    | 6                   | 0.46     | 0.01                | 0.46       |
| (1,1647) | 1:112:A:VAL:HG12 | 1:112:A:VAL:H    | 6                   | 0.46     | 0.01                | 0.46       |
| (1,1647) | 1:112:A:VAL:HG13 | 1:112:A:VAL:H    | 6                   | 0.46     | 0.01                | 0.46       |
| (1,205)  | 1:32:A:ILE:HA    | 1:32:A:ILE:HD11  | 6                   | 0.46     | 0.03                | 0.45       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,205)  | 1:32:A:ILE:HA    | 1:32:A:ILE:HD12  | 6                   | 0.46     | 0.03                | 0.45       |
| (1,205)  | 1:32:A:ILE:HA    | 1:32:A:ILE:HD13  | 6                   | 0.46     | 0.03                | 0.45       |
| (1,582)  | 1:51:A:ILE:HG21  | 1:55:A:VAL:H     | 6                   | 0.4      | 0.09                | 0.42       |
| (1,582)  | 1:51:A:ILE:HG22  | 1:55:A:VAL:H     | 6                   | 0.4      | 0.09                | 0.42       |
| (1,582)  | 1:51:A:ILE:HG23  | 1:55:A:VAL:H     | 6                   | 0.4      | 0.09                | 0.42       |
| (1,1342) | 1:85:A:TYR:HE1   | 1:143:A:ILE:HG21 | 6                   | 0.4      | 0.16                | 0.36       |
| (1,1342) | 1:85:A:TYR:HE1   | 1:143:A:ILE:HG22 | 6                   | 0.4      | 0.16                | 0.36       |
| (1,1342) | 1:85:A:TYR:HE1   | 1:143:A:ILE:HG23 | 6                   | 0.4      | 0.16                | 0.36       |
| (1,1342) | 1:85:A:TYR:HE2   | 1:143:A:ILE:HG21 | 6                   | 0.4      | 0.16                | 0.36       |
| (1,1342) | 1:85:A:TYR:HE2   | 1:143:A:ILE:HG22 | 6                   | 0.4      | 0.16                | 0.36       |
| (1,1342) | 1:85:A:TYR:HE2   | 1:143:A:ILE:HG23 | 6                   | 0.4      | 0.16                | 0.36       |
| (1,1953) | 1:136:A:PRO:HG3  | 1:155:A:ASN:HD21 | 6                   | 0.35     | 0.1                 | 0.38       |
| (1,1953) | 1:136:A:PRO:HG3  | 1:155:A:ASN:HD22 | 6                   | 0.35     | 0.1                 | 0.38       |
| (2,383)  | 1:70:A:LEU:HA    | 1:74:A:PHE:HD1   | 6                   | 0.3      | 0.12                | 0.28       |
| (2,383)  | 1:70:A:LEU:HA    | 1:74:A:PHE:HD2   | 6                   | 0.3      | 0.12                | 0.28       |
| (1,2028) | 1:143:A:ILE:HD11 | 1:143:A:ILE:H    | 6                   | 0.3      | 0.18                | 0.24       |
| (1,2028) | 1:143:A:ILE:HD12 | 1:143:A:ILE:H    | 6                   | 0.3      | 0.18                | 0.24       |
| (1,2028) | 1:143:A:ILE:HD13 | 1:143:A:ILE:H    | 6                   | 0.3      | 0.18                | 0.24       |
| (1,731)  | 1:62:A:VAL:HG21  | 1:177:A:PHE:HD1  | 6                   | 0.3      | 0.1                 | 0.34       |
| (1,731)  | 1:62:A:VAL:HG21  | 1:177:A:PHE:HD2  | 6                   | 0.3      | 0.1                 | 0.34       |
| (1,731)  | 1:62:A:VAL:HG22  | 1:177:A:PHE:HD1  | 6                   | 0.3      | 0.1                 | 0.34       |
| (1,731)  | 1:62:A:VAL:HG22  | 1:177:A:PHE:HD2  | 6                   | 0.3      | 0.1                 | 0.34       |
| (1,731)  | 1:62:A:VAL:HG23  | 1:177:A:PHE:HD1  | 6                   | 0.3      | 0.1                 | 0.34       |
| (1,731)  | 1:62:A:VAL:HG23  | 1:177:A:PHE:HD2  | 6                   | 0.3      | 0.1                 | 0.34       |
| (1,436)  | 1:46:A:TYR:HB2   | 1:153:A:ILE:HG21 | 6                   | 0.29     | 0.13                | 0.27       |
| (1,436)  | 1:46:A:TYR:HB2   | 1:153:A:ILE:HG22 | 6                   | 0.29     | 0.13                | 0.27       |
| (1,436)  | 1:46:A:TYR:HB2   | 1:153:A:ILE:HG23 | 6                   | 0.29     | 0.13                | 0.27       |
| (1,873)  | 1:67:A:ALA:HB1   | 1:68:A:GLU:H     | 6                   | 0.25     | 0.03                | 0.25       |
| (1,873)  | 1:67:A:ALA:HB2   | 1:68:A:GLU:H     | 6                   | 0.25     | 0.03                | 0.25       |
| (1,873)  | 1:67:A:ALA:HB3   | 1:68:A:GLU:H     | 6                   | 0.25     | 0.03                | 0.25       |
| (2,714)  | 1:141:A:LYS:HD2  | 1:142:A:ILE:H    | 6                   | 0.24     | 0.06                | 0.22       |
| (2,714)  | 1:141:A:LYS:HD3  | 1:142:A:ILE:H    | 6                   | 0.24     | 0.06                | 0.22       |
| (1,2371) | 1:174:A:ILE:HG21 | 1:175:A:PHE:H    | 6                   | 0.23     | 0.07                | 0.22       |
| (1,2371) | 1:174:A:ILE:HG22 | 1:175:A:PHE:H    | 6                   | 0.23     | 0.07                | 0.22       |
| (1,2371) | 1:174:A:ILE:HG23 | 1:175:A:PHE:H    | 6                   | 0.23     | 0.07                | 0.22       |
| (1,1769) | 1:120:A:VAL:HG21 | 1:120:A:VAL:H    | 6                   | 0.23     | 0.01                | 0.23       |
| (1,1769) | 1:120:A:VAL:HG22 | 1:120:A:VAL:H    | 6                   | 0.23     | 0.01                | 0.23       |
| (1,1769) | 1:120:A:VAL:HG23 | 1:120:A:VAL:H    | 6                   | 0.23     | 0.01                | 0.23       |
| (1,1298) | 1:83:A:SER:HA    | 1:154:A:LEU:HD21 | 6                   | 0.23     | 0.04                | 0.24       |
| (1,1298) | 1:83:A:SER:HA    | 1:154:A:LEU:HD22 | 6                   | 0.23     | 0.04                | 0.24       |
| (1,1298) | 1:83:A:SER:HA    | 1:154:A:LEU:HD23 | 6                   | 0.23     | 0.04                | 0.24       |
| (1,427)  | 1:46:A:TYR:HA    | 1:156:A:PHE:HE1  | 6                   | 0.22     | 0.08                | 0.22       |

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| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,427)  | 1:46:A:TYR:HA    | 1:156:A:PHE:HE2 | 6                   | 0.22     | 0.08                | 0.22       |
| (1,1216) | 1:81:A:ILE:HD11  | 1:100:A:ALA:H   | 6                   | 0.21     | 0.07                | 0.19       |
| (1,1216) | 1:81:A:ILE:HD12  | 1:100:A:ALA:H   | 6                   | 0.21     | 0.07                | 0.19       |
| (1,1216) | 1:81:A:ILE:HD13  | 1:100:A:ALA:H   | 6                   | 0.21     | 0.07                | 0.19       |
| (1,1169) | 1:79:A:ILE:HG21  | 1:79:A:ILE:HD11 | 6                   | 0.2      | 0.11                | 0.16       |
| (1,1169) | 1:79:A:ILE:HG21  | 1:79:A:ILE:HD12 | 6                   | 0.2      | 0.11                | 0.16       |
| (1,1169) | 1:79:A:ILE:HG21  | 1:79:A:ILE:HD13 | 6                   | 0.2      | 0.11                | 0.16       |
| (1,1169) | 1:79:A:ILE:HG22  | 1:79:A:ILE:HD11 | 6                   | 0.2      | 0.11                | 0.16       |
| (1,1169) | 1:79:A:ILE:HG22  | 1:79:A:ILE:HD12 | 6                   | 0.2      | 0.11                | 0.16       |
| (1,1169) | 1:79:A:ILE:HG22  | 1:79:A:ILE:HD13 | 6                   | 0.2      | 0.11                | 0.16       |
| (1,1169) | 1:79:A:ILE:HG23  | 1:79:A:ILE:HD11 | 6                   | 0.2      | 0.11                | 0.16       |
| (1,1169) | 1:79:A:ILE:HG23  | 1:79:A:ILE:HD12 | 6                   | 0.2      | 0.11                | 0.16       |
| (1,1169) | 1:79:A:ILE:HG23  | 1:79:A:ILE:HD13 | 6                   | 0.2      | 0.11                | 0.16       |
| (1,1089) | 1:77:A:LEU:HD11  | 1:79:A:ILE:HD11 | 6                   | 0.2      | 0.02                | 0.2        |
| (1,1089) | 1:77:A:LEU:HD11  | 1:79:A:ILE:HD12 | 6                   | 0.2      | 0.02                | 0.2        |
| (1,1089) | 1:77:A:LEU:HD11  | 1:79:A:ILE:HD13 | 6                   | 0.2      | 0.02                | 0.2        |
| (1,1089) | 1:77:A:LEU:HD12  | 1:79:A:ILE:HD11 | 6                   | 0.2      | 0.02                | 0.2        |
| (1,1089) | 1:77:A:LEU:HD12  | 1:79:A:ILE:HD12 | 6                   | 0.2      | 0.02                | 0.2        |
| (1,1089) | 1:77:A:LEU:HD12  | 1:79:A:ILE:HD13 | 6                   | 0.2      | 0.02                | 0.2        |
| (1,1089) | 1:77:A:LEU:HD13  | 1:79:A:ILE:HD11 | 6                   | 0.2      | 0.02                | 0.2        |
| (1,1089) | 1:77:A:LEU:HD13  | 1:79:A:ILE:HD12 | 6                   | 0.2      | 0.02                | 0.2        |
| (1,1089) | 1:77:A:LEU:HD13  | 1:79:A:ILE:HD13 | 6                   | 0.2      | 0.02                | 0.2        |
| (1,1089) | 1:77:A:LEU:HD21  | 1:79:A:ILE:HD11 | 6                   | 0.2      | 0.02                | 0.2        |
| (1,1089) | 1:77:A:LEU:HD21  | 1:79:A:ILE:HD12 | 6                   | 0.2      | 0.02                | 0.2        |
| (1,1089) | 1:77:A:LEU:HD21  | 1:79:A:ILE:HD13 | 6                   | 0.2      | 0.02                | 0.2        |
| (1,1089) | 1:77:A:LEU:HD22  | 1:79:A:ILE:HD11 | 6                   | 0.2      | 0.02                | 0.2        |
| (1,1089) | 1:77:A:LEU:HD22  | 1:79:A:ILE:HD12 | 6                   | 0.2      | 0.02                | 0.2        |
| (1,1089) | 1:77:A:LEU:HD22  | 1:79:A:ILE:HD13 | 6                   | 0.2      | 0.02                | 0.2        |
| (1,1089) | 1:77:A:LEU:HD23  | 1:79:A:ILE:HD11 | 6                   | 0.2      | 0.02                | 0.2        |
| (1,1089) | 1:77:A:LEU:HD23  | 1:79:A:ILE:HD12 | 6                   | 0.2      | 0.02                | 0.2        |
| (1,1089) | 1:77:A:LEU:HD23  | 1:79:A:ILE:HD13 | 6                   | 0.2      | 0.02                | 0.2        |
| (1,1640) | 1:111:A:ILE:HG21 | 1:112:A:VAL:H   | 6                   | 0.18     | 0.07                | 0.17       |
| (1,1640) | 1:111:A:ILE:HG22 | 1:112:A:VAL:H   | 6                   | 0.18     | 0.07                | 0.17       |
| (1,1640) | 1:111:A:ILE:HG23 | 1:112:A:VAL:H   | 6                   | 0.18     | 0.07                | 0.17       |
| (1,1774) | 1:121:A:LEU:HB3  | 1:121:A:LEU:H   | 6                   | 0.18     | 0.02                | 0.18       |
| (1,235)  | 1:32:A:ILE:HG21  | 1:33:A:THR:H    | 6                   | 0.18     | 0.02                | 0.18       |
| (1,235)  | 1:32:A:ILE:HG22  | 1:33:A:THR:H    | 6                   | 0.18     | 0.02                | 0.18       |
| (1,235)  | 1:32:A:ILE:HG23  | 1:33:A:THR:H    | 6                   | 0.18     | 0.02                | 0.18       |
| (1,845)  | 1:66:A:ASN:HD21  | 1:173:A:VAL:HA  | 6                   | 0.16     | 0.02                | 0.17       |
| (1,1723) | 1:116:A:GLU:HG2  | 1:116:A:GLU:H   | 6                   | 0.16     | 0.05                | 0.12       |
| (1,1723) | 1:116:A:GLU:HG3  | 1:116:A:GLU:H   | 6                   | 0.16     | 0.05                | 0.12       |
| (1,1128) | 1:78:A:GLN:H     | 1:158:A:ALA:HA  | 6                   | 0.16     | 0.02                | 0.16       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,554)  | 1:50:A:TRP:HD1   | 1:50:A:TRP:H     | 6                   | 0.15     | 0.02                | 0.15       |
| (1,2260) | 1:163:A:LYS:H    | 1:168:A:PHE:HZ   | 6                   | 0.14     | 0.03                | 0.14       |
| (1,227)  | 1:32:A:ILE:HG13  | 1:33:A:THR:H     | 6                   | 0.14     | 0.01                | 0.14       |
| (1,426)  | 1:46:A:TYR:HA    | 1:156:A:PHE:HA   | 6                   | 0.13     | 0.02                | 0.13       |
| (1,761)  | 1:63:A:THR:H     | 1:175:A:PHE:HA   | 6                   | 0.12     | 0.02                | 0.12       |
| (1,795)  | 1:64:A:LEU:HG    | 1:67:A:ALA:HA    | 6                   | 0.11     | 0.01                | 0.12       |
| (1,1787) | 1:123:A:PRO:HD2  | 1:124:A:ASP:H    | 6                   | 0.11     | 0.02                | 0.1        |
| (1,2459) | 1:182:A:VAL:HB   | 1:183:A:GLY:H    | 6                   | 0.1      | 0.0                 | 0.11       |
| (1,282)  | 1:35:A:ALA:HB1   | 1:36:A:ALA:H     | 5                   | 0.6      | 0.06                | 0.57       |
| (1,282)  | 1:35:A:ALA:HB2   | 1:36:A:ALA:H     | 5                   | 0.6      | 0.06                | 0.57       |
| (1,282)  | 1:35:A:ALA:HB3   | 1:36:A:ALA:H     | 5                   | 0.6      | 0.06                | 0.57       |
| (1,579)  | 1:51:A:ILE:HG21  | 1:53:A:ASP:HB2   | 5                   | 0.58     | 0.36                | 0.79       |
| (1,579)  | 1:51:A:ILE:HG21  | 1:53:A:ASP:HB3   | 5                   | 0.58     | 0.36                | 0.79       |
| (1,579)  | 1:51:A:ILE:HG22  | 1:53:A:ASP:HB2   | 5                   | 0.58     | 0.36                | 0.79       |
| (1,579)  | 1:51:A:ILE:HG22  | 1:53:A:ASP:HB3   | 5                   | 0.58     | 0.36                | 0.79       |
| (1,579)  | 1:51:A:ILE:HG23  | 1:53:A:ASP:HB2   | 5                   | 0.58     | 0.36                | 0.79       |
| (1,579)  | 1:51:A:ILE:HG23  | 1:53:A:ASP:HB3   | 5                   | 0.58     | 0.36                | 0.79       |
| (1,2304) | 1:170:A:SER:HA   | 1:171:A:LEU:HD21 | 5                   | 0.55     | 0.2                 | 0.65       |
| (1,2304) | 1:170:A:SER:HA   | 1:171:A:LEU:HD22 | 5                   | 0.55     | 0.2                 | 0.65       |
| (1,2304) | 1:170:A:SER:HA   | 1:171:A:LEU:HD23 | 5                   | 0.55     | 0.2                 | 0.65       |
| (2,765)  | 1:169:A:ASP:H    | 1:171:A:LEU:HD11 | 5                   | 0.55     | 0.3                 | 0.52       |
| (2,765)  | 1:169:A:ASP:H    | 1:171:A:LEU:HD12 | 5                   | 0.55     | 0.3                 | 0.52       |
| (2,765)  | 1:169:A:ASP:H    | 1:171:A:LEU:HD13 | 5                   | 0.55     | 0.3                 | 0.52       |
| (2,631)  | 1:122:A:TYR:HD1  | 1:124:A:ASP:H    | 5                   | 0.5      | 0.01                | 0.5        |
| (2,631)  | 1:122:A:TYR:HD2  | 1:124:A:ASP:H    | 5                   | 0.5      | 0.01                | 0.5        |
| (1,1097) | 1:77:A:LEU:HD11  | 1:160:A:TYR:HB3  | 5                   | 0.43     | 0.16                | 0.47       |
| (1,1097) | 1:77:A:LEU:HD12  | 1:160:A:TYR:HB3  | 5                   | 0.43     | 0.16                | 0.47       |
| (1,1097) | 1:77:A:LEU:HD13  | 1:160:A:TYR:HB3  | 5                   | 0.43     | 0.16                | 0.47       |
| (1,1097) | 1:77:A:LEU:HD21  | 1:160:A:TYR:HB3  | 5                   | 0.43     | 0.16                | 0.47       |
| (1,1097) | 1:77:A:LEU:HD22  | 1:160:A:TYR:HB3  | 5                   | 0.43     | 0.16                | 0.47       |
| (1,1097) | 1:77:A:LEU:HD23  | 1:160:A:TYR:HB3  | 5                   | 0.43     | 0.16                | 0.47       |
| (1,1537) | 1:102:A:ILE:HD11 | 1:107:A:PRO:HA   | 5                   | 0.43     | 0.11                | 0.51       |
| (1,1537) | 1:102:A:ILE:HD12 | 1:107:A:PRO:HA   | 5                   | 0.43     | 0.11                | 0.51       |
| (1,1537) | 1:102:A:ILE:HD13 | 1:107:A:PRO:HA   | 5                   | 0.43     | 0.11                | 0.51       |
| (1,23)   | 1:23:A:ILE:HA    | 1:23:A:ILE:HD11  | 5                   | 0.41     | 0.01                | 0.41       |
| (1,23)   | 1:23:A:ILE:HA    | 1:23:A:ILE:HD12  | 5                   | 0.41     | 0.01                | 0.41       |
| (1,23)   | 1:23:A:ILE:HA    | 1:23:A:ILE:HD13  | 5                   | 0.41     | 0.01                | 0.41       |
| (1,2448) | 1:179:A:VAL:HG11 | 1:179:A:VAL:H    | 5                   | 0.39     | 0.1                 | 0.47       |
| (1,2448) | 1:179:A:VAL:HG12 | 1:179:A:VAL:H    | 5                   | 0.39     | 0.1                 | 0.47       |
| (1,2448) | 1:179:A:VAL:HG13 | 1:179:A:VAL:H    | 5                   | 0.39     | 0.1                 | 0.47       |
| (1,11)   | 1:20:A:SER:HB2   | 1:21:A:GLU:H     | 5                   | 0.34     | 0.09                | 0.39       |
| (1,11)   | 1:20:A:SER:HB3   | 1:21:A:GLU:H     | 5                   | 0.34     | 0.09                | 0.39       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (2,735)  | 1:158:A:ALA:H    | 1:160:A:TYR:HE1  | 5                   | 0.33     | 0.09                | 0.29       |
| (2,735)  | 1:158:A:ALA:H    | 1:160:A:TYR:HE2  | 5                   | 0.33     | 0.09                | 0.29       |
| (1,166)  | 1:29:A:LEU:HD11  | 1:175:A:PHE:H    | 5                   | 0.31     | 0.16                | 0.29       |
| (1,166)  | 1:29:A:LEU:HD12  | 1:175:A:PHE:H    | 5                   | 0.31     | 0.16                | 0.29       |
| (1,166)  | 1:29:A:LEU:HD13  | 1:175:A:PHE:H    | 5                   | 0.31     | 0.16                | 0.29       |
| (1,2054) | 1:145:A:TYR:HD1  | 1:146:A:ASN:H    | 5                   | 0.3      | 0.09                | 0.34       |
| (1,2054) | 1:145:A:TYR:HD2  | 1:146:A:ASN:H    | 5                   | 0.3      | 0.09                | 0.34       |
| (1,2303) | 1:170:A:SER:HA   | 1:171:A:LEU:HD11 | 5                   | 0.28     | 0.2                 | 0.19       |
| (1,2303) | 1:170:A:SER:HA   | 1:171:A:LEU:HD12 | 5                   | 0.28     | 0.2                 | 0.19       |
| (1,2303) | 1:170:A:SER:HA   | 1:171:A:LEU:HD13 | 5                   | 0.28     | 0.2                 | 0.19       |
| (2,534)  | 1:85:A:TYR:HE1   | 1:151:A:VAL:H    | 5                   | 0.28     | 0.15                | 0.19       |
| (2,534)  | 1:85:A:TYR:HE2   | 1:151:A:VAL:H    | 5                   | 0.28     | 0.15                | 0.19       |
| (1,1859) | 1:133:A:ILE:HD11 | 1:144:A:VAL:HB   | 5                   | 0.27     | 0.11                | 0.27       |
| (1,1859) | 1:133:A:ILE:HD12 | 1:144:A:VAL:HB   | 5                   | 0.27     | 0.11                | 0.27       |
| (1,1859) | 1:133:A:ILE:HD13 | 1:144:A:VAL:HB   | 5                   | 0.27     | 0.11                | 0.27       |
| (1,1241) | 1:81:A:ILE:HG21  | 1:156:A:PHE:HD1  | 5                   | 0.27     | 0.27                | 0.13       |
| (1,1241) | 1:81:A:ILE:HG21  | 1:156:A:PHE:HD2  | 5                   | 0.27     | 0.27                | 0.13       |
| (1,1241) | 1:81:A:ILE:HG22  | 1:156:A:PHE:HD1  | 5                   | 0.27     | 0.27                | 0.13       |
| (1,1241) | 1:81:A:ILE:HG22  | 1:156:A:PHE:HD2  | 5                   | 0.27     | 0.27                | 0.13       |
| (1,1241) | 1:81:A:ILE:HG23  | 1:156:A:PHE:HD1  | 5                   | 0.27     | 0.27                | 0.13       |
| (1,1241) | 1:81:A:ILE:HG23  | 1:156:A:PHE:HD2  | 5                   | 0.27     | 0.27                | 0.13       |
| (1,915)  | 1:69:A:GLN:HG3   | 1:70:A:LEU:H     | 5                   | 0.24     | 0.04                | 0.23       |
| (2,731)  | 1:155:A:ASN:H    | 1:156:A:PHE:HD1  | 5                   | 0.24     | 0.07                | 0.23       |
| (2,731)  | 1:155:A:ASN:H    | 1:156:A:PHE:HD2  | 5                   | 0.24     | 0.07                | 0.23       |
| (1,909)  | 1:69:A:GLN:HB2   | 1:70:A:LEU:H     | 5                   | 0.21     | 0.06                | 0.2        |
| (1,922)  | 1:70:A:LEU:HD11  | 1:70:A:LEU:H     | 5                   | 0.19     | 0.08                | 0.16       |
| (1,922)  | 1:70:A:LEU:HD12  | 1:70:A:LEU:H     | 5                   | 0.19     | 0.08                | 0.16       |
| (1,922)  | 1:70:A:LEU:HD13  | 1:70:A:LEU:H     | 5                   | 0.19     | 0.08                | 0.16       |
| (1,455)  | 1:47:A:ALA:HB1   | 1:48:A:ILE:H     | 5                   | 0.19     | 0.07                | 0.16       |
| (1,455)  | 1:47:A:ALA:HB2   | 1:48:A:ILE:H     | 5                   | 0.19     | 0.07                | 0.16       |
| (1,455)  | 1:47:A:ALA:HB3   | 1:48:A:ILE:H     | 5                   | 0.19     | 0.07                | 0.16       |
| (1,2013) | 1:142:A:ILE:HG21 | 1:143:A:ILE:H    | 5                   | 0.18     | 0.06                | 0.15       |
| (1,2013) | 1:142:A:ILE:HG22 | 1:143:A:ILE:H    | 5                   | 0.18     | 0.06                | 0.15       |
| (1,2013) | 1:142:A:ILE:HG23 | 1:143:A:ILE:H    | 5                   | 0.18     | 0.06                | 0.15       |
| (1,849)  | 1:66:A:ASN:HD22  | 1:66:A:ASN:H     | 5                   | 0.18     | 0.01                | 0.18       |
| (1,25)   | 1:23:A:ILE:HA    | 1:23:A:ILE:HG21  | 5                   | 0.18     | 0.05                | 0.17       |
| (1,25)   | 1:23:A:ILE:HA    | 1:23:A:ILE:HG22  | 5                   | 0.18     | 0.05                | 0.17       |
| (1,25)   | 1:23:A:ILE:HA    | 1:23:A:ILE:HG23  | 5                   | 0.18     | 0.05                | 0.17       |
| (1,292)  | 1:37:A:GLY:HA2   | 1:37:A:GLY:H     | 5                   | 0.17     | 0.05                | 0.15       |
| (1,894)  | 1:68:A:GLU:H     | 1:69:A:GLN:H     | 5                   | 0.15     | 0.03                | 0.15       |
| (1,541)  | 1:50:A:TRP:HA    | 1:51:A:ILE:HB    | 5                   | 0.15     | 0.03                | 0.17       |
| (2,205)  | 1:39:A:GLN:HB3   | 1:39:A:GLN:HE21  | 5                   | 0.14     | 0.0                 | 0.14       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1363) | 1:86:A:GLU:HG3   | 1:86:A:GLU:H     | 5                   | 0.13     | 0.01                | 0.13       |
| (1,2258) | 1:163:A:LYS:HG2  | 1:163:A:LYS:H    | 5                   | 0.13     | 0.01                | 0.14       |
| (1,683)  | 1:60:A:LEU:HG    | 1:60:A:LEU:H     | 5                   | 0.13     | 0.01                | 0.12       |
| (1,1778) | 1:121:A:LEU:HG   | 1:121:A:LEU:H    | 5                   | 0.12     | 0.01                | 0.12       |
| (1,1379) | 1:87:A:THR:HA    | 1:134:A:TRP:HE3  | 5                   | 0.12     | 0.01                | 0.12       |
| (1,643)  | 1:57:A:ASP:HB2   | 1:115:A:LYS:H    | 5                   | 0.12     | 0.01                | 0.12       |
| (1,1974) | 1:138:A:GLU:H    | 1:139:A:PRO:HD2  | 5                   | 0.11     | 0.0                 | 0.11       |
| (1,2275) | 1:167:A:LEU:HA   | 1:168:A:PHE:H    | 5                   | 0.1      | 0.0                 | 0.1        |
| (2,7)    | 1:16:A:ALA:HB1   | 1:18:A:ALA:H     | 4                   | 0.65     | 0.09                | 0.64       |
| (2,7)    | 1:16:A:ALA:HB2   | 1:18:A:ALA:H     | 4                   | 0.65     | 0.09                | 0.64       |
| (2,7)    | 1:16:A:ALA:HB3   | 1:18:A:ALA:H     | 4                   | 0.65     | 0.09                | 0.64       |
| (1,923)  | 1:70:A:LEU:HD11  | 1:71:A:LYS:H     | 4                   | 0.6      | 0.03                | 0.6        |
| (1,923)  | 1:70:A:LEU:HD12  | 1:71:A:LYS:H     | 4                   | 0.6      | 0.03                | 0.6        |
| (1,923)  | 1:70:A:LEU:HD13  | 1:71:A:LYS:H     | 4                   | 0.6      | 0.03                | 0.6        |
| (1,991)  | 1:73:A:TYR:HE1   | 1:171:A:LEU:HD11 | 4                   | 0.59     | 0.03                | 0.6        |
| (1,991)  | 1:73:A:TYR:HE1   | 1:171:A:LEU:HD12 | 4                   | 0.59     | 0.03                | 0.6        |
| (1,991)  | 1:73:A:TYR:HE1   | 1:171:A:LEU:HD13 | 4                   | 0.59     | 0.03                | 0.6        |
| (1,991)  | 1:73:A:TYR:HE2   | 1:171:A:LEU:HD11 | 4                   | 0.59     | 0.03                | 0.6        |
| (1,991)  | 1:73:A:TYR:HE2   | 1:171:A:LEU:HD12 | 4                   | 0.59     | 0.03                | 0.6        |
| (1,991)  | 1:73:A:TYR:HE2   | 1:171:A:LEU:HD13 | 4                   | 0.59     | 0.03                | 0.6        |
| (1,223)  | 1:32:A:ILE:HD11  | 1:160:A:TYR:HE1  | 4                   | 0.52     | 0.22                | 0.54       |
| (1,223)  | 1:32:A:ILE:HD11  | 1:160:A:TYR:HE2  | 4                   | 0.52     | 0.22                | 0.54       |
| (1,223)  | 1:32:A:ILE:HD12  | 1:160:A:TYR:HE1  | 4                   | 0.52     | 0.22                | 0.54       |
| (1,223)  | 1:32:A:ILE:HD12  | 1:160:A:TYR:HE2  | 4                   | 0.52     | 0.22                | 0.54       |
| (1,223)  | 1:32:A:ILE:HD13  | 1:160:A:TYR:HE1  | 4                   | 0.52     | 0.22                | 0.54       |
| (1,223)  | 1:32:A:ILE:HD13  | 1:160:A:TYR:HE2  | 4                   | 0.52     | 0.22                | 0.54       |
| (1,2010) | 1:142:A:ILE:HD11 | 1:145:A:TYR:HD1  | 4                   | 0.5      | 0.2                 | 0.5        |
| (1,2010) | 1:142:A:ILE:HD11 | 1:145:A:TYR:HD2  | 4                   | 0.5      | 0.2                 | 0.5        |
| (1,2010) | 1:142:A:ILE:HD12 | 1:145:A:TYR:HD1  | 4                   | 0.5      | 0.2                 | 0.5        |
| (1,2010) | 1:142:A:ILE:HD12 | 1:145:A:TYR:HD2  | 4                   | 0.5      | 0.2                 | 0.5        |
| (1,2010) | 1:142:A:ILE:HD13 | 1:145:A:TYR:HD1  | 4                   | 0.5      | 0.2                 | 0.5        |
| (1,2010) | 1:142:A:ILE:HD13 | 1:145:A:TYR:HD2  | 4                   | 0.5      | 0.2                 | 0.5        |
| (2,94)   | 1:23:A:ILE:HD11  | 1:53:A:ASP:H     | 4                   | 0.48     | 0.23                | 0.53       |
| (2,94)   | 1:23:A:ILE:HD12  | 1:53:A:ASP:H     | 4                   | 0.48     | 0.23                | 0.53       |
| (2,94)   | 1:23:A:ILE:HD13  | 1:53:A:ASP:H     | 4                   | 0.48     | 0.23                | 0.53       |
| (1,353)  | 1:42:A:ASP:HB2   | 1:158:A:ALA:HB1  | 4                   | 0.48     | 0.18                | 0.44       |
| (1,353)  | 1:42:A:ASP:HB2   | 1:158:A:ALA:HB2  | 4                   | 0.48     | 0.18                | 0.44       |
| (1,353)  | 1:42:A:ASP:HB2   | 1:158:A:ALA:HB3  | 4                   | 0.48     | 0.18                | 0.44       |
| (1,353)  | 1:42:A:ASP:HB3   | 1:158:A:ALA:HB1  | 4                   | 0.48     | 0.18                | 0.44       |
| (1,353)  | 1:42:A:ASP:HB3   | 1:158:A:ALA:HB2  | 4                   | 0.48     | 0.18                | 0.44       |
| (1,353)  | 1:42:A:ASP:HB3   | 1:158:A:ALA:HB3  | 4                   | 0.48     | 0.18                | 0.44       |
| (2,702)  | 1:132:A:SER:HB2  | 1:145:A:TYR:HE1  | 4                   | 0.46     | 0.09                | 0.5        |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (2,702)  | 1:132:A:SER:HB2  | 1:145:A:TYR:HE2  | 4                   | 0.46     | 0.09                | 0.5        |
| (1,1840) | 1:132:A:SER:HB3  | 1:142:A:ILE:HG21 | 4                   | 0.46     | 0.02                | 0.45       |
| (1,1840) | 1:132:A:SER:HB3  | 1:142:A:ILE:HG22 | 4                   | 0.46     | 0.02                | 0.45       |
| (1,1840) | 1:132:A:SER:HB3  | 1:142:A:ILE:HG23 | 4                   | 0.46     | 0.02                | 0.45       |
| (1,1090) | 1:77:A:LEU:HD11  | 1:79:A:ILE:H     | 4                   | 0.42     | 0.07                | 0.42       |
| (1,1090) | 1:77:A:LEU:HD12  | 1:79:A:ILE:H     | 4                   | 0.42     | 0.07                | 0.42       |
| (1,1090) | 1:77:A:LEU:HD13  | 1:79:A:ILE:H     | 4                   | 0.42     | 0.07                | 0.42       |
| (1,1090) | 1:77:A:LEU:HD21  | 1:79:A:ILE:H     | 4                   | 0.42     | 0.07                | 0.42       |
| (1,1090) | 1:77:A:LEU:HD22  | 1:79:A:ILE:H     | 4                   | 0.42     | 0.07                | 0.42       |
| (1,1090) | 1:77:A:LEU:HD23  | 1:79:A:ILE:H     | 4                   | 0.42     | 0.07                | 0.42       |
| (1,1747) | 1:118:A:ILE:HD11 | 1:118:A:ILE:H    | 4                   | 0.4      | 0.17                | 0.45       |
| (1,1747) | 1:118:A:ILE:HD12 | 1:118:A:ILE:H    | 4                   | 0.4      | 0.17                | 0.45       |
| (1,1747) | 1:118:A:ILE:HD13 | 1:118:A:ILE:H    | 4                   | 0.4      | 0.17                | 0.45       |
| (2,593)  | 1:114:A:ASP:HB2  | 1:116:A:GLU:HG2  | 4                   | 0.39     | 0.12                | 0.42       |
| (2,593)  | 1:114:A:ASP:HB2  | 1:116:A:GLU:HG3  | 4                   | 0.39     | 0.12                | 0.42       |
| (1,289)  | 1:37:A:GLY:HA3   | 1:37:A:GLY:H     | 4                   | 0.37     | 0.09                | 0.39       |
| (1,1707) | 1:115:A:LYS:HG2  | 1:116:A:GLU:H    | 4                   | 0.36     | 0.01                | 0.36       |
| (1,1707) | 1:115:A:LYS:HG3  | 1:116:A:GLU:H    | 4                   | 0.36     | 0.01                | 0.36       |
| (1,1522) | 1:100:A:ALA:H    | 1:111:A:ILE:HD11 | 4                   | 0.35     | 0.15                | 0.32       |
| (1,1522) | 1:100:A:ALA:H    | 1:111:A:ILE:HD12 | 4                   | 0.35     | 0.15                | 0.32       |
| (1,1522) | 1:100:A:ALA:H    | 1:111:A:ILE:HD13 | 4                   | 0.35     | 0.15                | 0.32       |
| (1,270)  | 1:34:A:PRO:HD3   | 1:168:A:PHE:HE1  | 4                   | 0.34     | 0.03                | 0.34       |
| (1,270)  | 1:34:A:PRO:HD3   | 1:168:A:PHE:HE2  | 4                   | 0.34     | 0.03                | 0.34       |
| (2,397)  | 1:73:A:TYR:HD1   | 1:74:A:PHE:HA    | 4                   | 0.31     | 0.15                | 0.3        |
| (2,397)  | 1:73:A:TYR:HD2   | 1:74:A:PHE:HA    | 4                   | 0.31     | 0.15                | 0.3        |
| (1,212)  | 1:32:A:ILE:HB    | 1:32:A:ILE:HD11  | 4                   | 0.3      | 0.04                | 0.29       |
| (1,212)  | 1:32:A:ILE:HB    | 1:32:A:ILE:HD12  | 4                   | 0.3      | 0.04                | 0.29       |
| (1,212)  | 1:32:A:ILE:HB    | 1:32:A:ILE:HD13  | 4                   | 0.3      | 0.04                | 0.29       |
| (1,1483) | 1:95:A:PHE:HE1   | 1:116:A:GLU:HB3  | 4                   | 0.27     | 0.05                | 0.29       |
| (1,1483) | 1:95:A:PHE:HE2   | 1:116:A:GLU:HB3  | 4                   | 0.27     | 0.05                | 0.29       |
| (2,481)  | 1:80:A:GLN:HE22  | 1:98:A:THR:HG21  | 4                   | 0.24     | 0.04                | 0.26       |
| (2,481)  | 1:80:A:GLN:HE22  | 1:98:A:THR:HG22  | 4                   | 0.24     | 0.04                | 0.26       |
| (2,481)  | 1:80:A:GLN:HE22  | 1:98:A:THR:HG23  | 4                   | 0.24     | 0.04                | 0.26       |
| (1,597)  | 1:53:A:ASP:HB2   | 1:54:A:GLN:H     | 4                   | 0.22     | 0.1                 | 0.21       |
| (1,597)  | 1:53:A:ASP:HB3   | 1:54:A:GLN:H     | 4                   | 0.22     | 0.1                 | 0.21       |
| (1,2154) | 1:156:A:PHE:HD1  | 1:156:A:PHE:H    | 4                   | 0.22     | 0.01                | 0.22       |
| (1,2154) | 1:156:A:PHE:HD2  | 1:156:A:PHE:H    | 4                   | 0.22     | 0.01                | 0.22       |
| (1,908)  | 1:69:A:GLN:HB3   | 1:70:A:LEU:H     | 4                   | 0.2      | 0.05                | 0.18       |
| (1,911)  | 1:69:A:GLN:HE22  | 1:70:A:LEU:H     | 4                   | 0.2      | 0.03                | 0.2        |
| (1,2343) | 1:173:A:VAL:HA   | 1:173:A:VAL:HG21 | 4                   | 0.2      | 0.01                | 0.2        |
| (1,2343) | 1:173:A:VAL:HA   | 1:173:A:VAL:HG22 | 4                   | 0.2      | 0.01                | 0.2        |
| (1,2343) | 1:173:A:VAL:HA   | 1:173:A:VAL:HG23 | 4                   | 0.2      | 0.01                | 0.2        |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,755)  | 1:63:A:THR:HG21  | 1:108:A:SER:HA   | 4                   | 0.19     | 0.08                | 0.19       |
| (1,755)  | 1:63:A:THR:HG22  | 1:108:A:SER:HA   | 4                   | 0.19     | 0.08                | 0.19       |
| (1,755)  | 1:63:A:THR:HG23  | 1:108:A:SER:HA   | 4                   | 0.19     | 0.08                | 0.19       |
| (1,2455) | 1:182:A:VAL:HA   | 1:182:A:VAL:HB   | 4                   | 0.17     | 0.0                 | 0.17       |
| (1,470)  | 1:48:A:ILE:HA    | 1:48:A:ILE:HG21  | 4                   | 0.16     | 0.01                | 0.16       |
| (1,470)  | 1:48:A:ILE:HA    | 1:48:A:ILE:HG22  | 4                   | 0.16     | 0.01                | 0.16       |
| (1,470)  | 1:48:A:ILE:HA    | 1:48:A:ILE:HG23  | 4                   | 0.16     | 0.01                | 0.16       |
| (1,1790) | 1:126:A:THR:HA   | 1:126:A:THR:HG21 | 4                   | 0.16     | 0.02                | 0.15       |
| (1,1790) | 1:126:A:THR:HA   | 1:126:A:THR:HG22 | 4                   | 0.16     | 0.02                | 0.15       |
| (1,1790) | 1:126:A:THR:HA   | 1:126:A:THR:HG23 | 4                   | 0.16     | 0.02                | 0.15       |
| (1,48)   | 1:24:A:ASP:HB3   | 1:50:A:TRP:HD1   | 4                   | 0.15     | 0.03                | 0.15       |
| (1,1369) | 1:86:A:GLU:H     | 1:133:A:ILE:HG21 | 4                   | 0.14     | 0.03                | 0.15       |
| (1,1369) | 1:86:A:GLU:H     | 1:133:A:ILE:HG22 | 4                   | 0.14     | 0.03                | 0.15       |
| (1,1369) | 1:86:A:GLU:H     | 1:133:A:ILE:HG23 | 4                   | 0.14     | 0.03                | 0.15       |
| (1,831)  | 1:66:A:ASN:HA    | 1:174:A:ILE:HB   | 4                   | 0.14     | 0.01                | 0.14       |
| (1,854)  | 1:66:A:ASN:HD22  | 1:172:A:PRO:HD3  | 4                   | 0.14     | 0.03                | 0.13       |
| (1,77)   | 1:25:A:VAL:HG11  | 1:25:A:VAL:H     | 4                   | 0.14     | 0.03                | 0.12       |
| (1,77)   | 1:25:A:VAL:HG12  | 1:25:A:VAL:H     | 4                   | 0.14     | 0.03                | 0.12       |
| (1,77)   | 1:25:A:VAL:HG13  | 1:25:A:VAL:H     | 4                   | 0.14     | 0.03                | 0.12       |
| (2,761)  | 1:168:A:PHE:H    | 1:169:A:ASP:H    | 4                   | 0.13     | 0.02                | 0.12       |
| (2,206)  | 1:39:A:GLN:HB2   | 1:39:A:GLN:HE21  | 4                   | 0.13     | 0.02                | 0.14       |
| (1,834)  | 1:66:A:ASN:HB3   | 1:66:A:ASN:H     | 4                   | 0.12     | 0.01                | 0.13       |
| (1,2299) | 1:169:A:ASP:H    | 1:170:A:SER:H    | 4                   | 0.12     | 0.02                | 0.12       |
| (1,1380) | 1:87:A:THR:HA    | 1:134:A:TRP:HH2  | 4                   | 0.12     | 0.02                | 0.12       |
| (1,1520) | 1:100:A:ALA:HB1  | 1:111:A:ILE:HG21 | 3                   | 0.71     | 0.15                | 0.81       |
| (1,1520) | 1:100:A:ALA:HB1  | 1:111:A:ILE:HG22 | 3                   | 0.71     | 0.15                | 0.81       |
| (1,1520) | 1:100:A:ALA:HB1  | 1:111:A:ILE:HG23 | 3                   | 0.71     | 0.15                | 0.81       |
| (1,1520) | 1:100:A:ALA:HB2  | 1:111:A:ILE:HG21 | 3                   | 0.71     | 0.15                | 0.81       |
| (1,1520) | 1:100:A:ALA:HB2  | 1:111:A:ILE:HG22 | 3                   | 0.71     | 0.15                | 0.81       |
| (1,1520) | 1:100:A:ALA:HB2  | 1:111:A:ILE:HG23 | 3                   | 0.71     | 0.15                | 0.81       |
| (1,1520) | 1:100:A:ALA:HB3  | 1:111:A:ILE:HG21 | 3                   | 0.71     | 0.15                | 0.81       |
| (1,1520) | 1:100:A:ALA:HB3  | 1:111:A:ILE:HG22 | 3                   | 0.71     | 0.15                | 0.81       |
| (1,1520) | 1:100:A:ALA:HB3  | 1:111:A:ILE:HG23 | 3                   | 0.71     | 0.15                | 0.81       |
| (2,718)  | 1:142:A:ILE:HD11 | 1:145:A:TYR:HE1  | 3                   | 0.65     | 0.43                | 0.65       |
| (2,718)  | 1:142:A:ILE:HD11 | 1:145:A:TYR:HE2  | 3                   | 0.65     | 0.43                | 0.65       |
| (2,718)  | 1:142:A:ILE:HD12 | 1:145:A:TYR:HE1  | 3                   | 0.65     | 0.43                | 0.65       |
| (2,718)  | 1:142:A:ILE:HD12 | 1:145:A:TYR:HE2  | 3                   | 0.65     | 0.43                | 0.65       |
| (2,718)  | 1:142:A:ILE:HD13 | 1:145:A:TYR:HE1  | 3                   | 0.65     | 0.43                | 0.65       |
| (2,718)  | 1:142:A:ILE:HD13 | 1:145:A:TYR:HE2  | 3                   | 0.65     | 0.43                | 0.65       |
| (1,1884) | 1:134:A:TRP:HA   | 1:143:A:ILE:HD11 | 3                   | 0.61     | 0.02                | 0.61       |
| (1,1884) | 1:134:A:TRP:HA   | 1:143:A:ILE:HD12 | 3                   | 0.61     | 0.02                | 0.61       |
| (1,1884) | 1:134:A:TRP:HA   | 1:143:A:ILE:HD13 | 3                   | 0.61     | 0.02                | 0.61       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,508)  | 1:48:A:ILE:HG21  | 1:153:A:ILE:HG13 | 3                   | 0.58     | 0.01                | 0.58       |
| (1,508)  | 1:48:A:ILE:HG22  | 1:153:A:ILE:HG13 | 3                   | 0.58     | 0.01                | 0.58       |
| (1,508)  | 1:48:A:ILE:HG23  | 1:153:A:ILE:HG13 | 3                   | 0.58     | 0.01                | 0.58       |
| (1,650)  | 1:58:A:VAL:HG11  | 1:58:A:VAL:H     | 3                   | 0.58     | 0.03                | 0.6        |
| (1,650)  | 1:58:A:VAL:HG12  | 1:58:A:VAL:H     | 3                   | 0.58     | 0.03                | 0.6        |
| (1,650)  | 1:58:A:VAL:HG13  | 1:58:A:VAL:H     | 3                   | 0.58     | 0.03                | 0.6        |
| (1,650)  | 1:58:A:VAL:HG21  | 1:58:A:VAL:H     | 3                   | 0.58     | 0.03                | 0.6        |
| (1,650)  | 1:58:A:VAL:HG22  | 1:58:A:VAL:H     | 3                   | 0.58     | 0.03                | 0.6        |
| (1,650)  | 1:58:A:VAL:HG23  | 1:58:A:VAL:H     | 3                   | 0.58     | 0.03                | 0.6        |
| (1,1274) | 1:82:A:THR:HG21  | 1:96:A:SER:HB3   | 3                   | 0.58     | 0.02                | 0.58       |
| (1,1274) | 1:82:A:THR:HG22  | 1:96:A:SER:HB3   | 3                   | 0.58     | 0.02                | 0.58       |
| (1,1274) | 1:82:A:THR:HG23  | 1:96:A:SER:HB3   | 3                   | 0.58     | 0.02                | 0.58       |
| (1,1275) | 1:82:A:THR:HG21  | 1:96:A:SER:HB2   | 3                   | 0.53     | 0.08                | 0.59       |
| (1,1275) | 1:82:A:THR:HG22  | 1:96:A:SER:HB2   | 3                   | 0.53     | 0.08                | 0.59       |
| (1,1275) | 1:82:A:THR:HG23  | 1:96:A:SER:HB2   | 3                   | 0.53     | 0.08                | 0.59       |
| (1,1104) | 1:77:A:LEU:H     | 1:104:A:LEU:HD21 | 3                   | 0.53     | 0.01                | 0.53       |
| (1,1104) | 1:77:A:LEU:H     | 1:104:A:LEU:HD22 | 3                   | 0.53     | 0.01                | 0.53       |
| (1,1104) | 1:77:A:LEU:H     | 1:104:A:LEU:HD23 | 3                   | 0.53     | 0.01                | 0.53       |
| (1,1766) | 1:120:A:VAL:HG11 | 1:120:A:VAL:H    | 3                   | 0.44     | 0.0                 | 0.44       |
| (1,1766) | 1:120:A:VAL:HG12 | 1:120:A:VAL:H    | 3                   | 0.44     | 0.0                 | 0.44       |
| (1,1766) | 1:120:A:VAL:HG13 | 1:120:A:VAL:H    | 3                   | 0.44     | 0.0                 | 0.44       |
| (2,295)  | 1:52:A:LYS:HE2   | 1:54:A:GLN:HE22  | 3                   | 0.38     | 0.05                | 0.4        |
| (2,295)  | 1:52:A:LYS:HE3   | 1:54:A:GLN:HE22  | 3                   | 0.38     | 0.05                | 0.4        |
| (2,689)  | 1:131:A:THR:HA   | 1:145:A:TYR:HD1  | 3                   | 0.37     | 0.09                | 0.44       |
| (2,689)  | 1:131:A:THR:HA   | 1:145:A:TYR:HD2  | 3                   | 0.37     | 0.09                | 0.44       |
| (1,844)  | 1:66:A:ASN:HD21  | 1:70:A:LEU:HD21  | 3                   | 0.34     | 0.05                | 0.34       |
| (1,844)  | 1:66:A:ASN:HD21  | 1:70:A:LEU:HD22  | 3                   | 0.34     | 0.05                | 0.34       |
| (1,844)  | 1:66:A:ASN:HD21  | 1:70:A:LEU:HD23  | 3                   | 0.34     | 0.05                | 0.34       |
| (2,673)  | 1:127:A:GLY:H    | 1:128:A:TYR:HD1  | 3                   | 0.33     | 0.12                | 0.25       |
| (2,673)  | 1:127:A:GLY:H    | 1:128:A:TYR:HD2  | 3                   | 0.33     | 0.12                | 0.25       |
| (1,1557) | 1:103:A:SER:HA   | 1:104:A:LEU:HB2  | 3                   | 0.32     | 0.01                | 0.32       |
| (2,618)  | 1:119:A:ALA:HB1  | 1:149:A:LYS:H    | 3                   | 0.31     | 0.18                | 0.21       |
| (2,618)  | 1:119:A:ALA:HB2  | 1:149:A:LYS:H    | 3                   | 0.31     | 0.18                | 0.21       |
| (2,618)  | 1:119:A:ALA:HB3  | 1:149:A:LYS:H    | 3                   | 0.31     | 0.18                | 0.21       |
| (1,1485) | 1:95:A:PHE:HE1   | 1:117:A:ASP:HA   | 3                   | 0.3      | 0.01                | 0.29       |
| (1,1485) | 1:95:A:PHE:HE2   | 1:117:A:ASP:HA   | 3                   | 0.3      | 0.01                | 0.29       |
| (1,2191) | 1:158:A:ALA:HB1  | 1:160:A:TYR:HE1  | 3                   | 0.29     | 0.11                | 0.33       |
| (1,2191) | 1:158:A:ALA:HB1  | 1:160:A:TYR:HE2  | 3                   | 0.29     | 0.11                | 0.33       |
| (1,2191) | 1:158:A:ALA:HB2  | 1:160:A:TYR:HE1  | 3                   | 0.29     | 0.11                | 0.33       |
| (1,2191) | 1:158:A:ALA:HB2  | 1:160:A:TYR:HE2  | 3                   | 0.29     | 0.11                | 0.33       |
| (1,2191) | 1:158:A:ALA:HB3  | 1:160:A:TYR:HE1  | 3                   | 0.29     | 0.11                | 0.33       |
| (1,2191) | 1:158:A:ALA:HB3  | 1:160:A:TYR:HE2  | 3                   | 0.29     | 0.11                | 0.33       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1845) | 1:132:A:SER:HB2  | 1:145:A:TYR:HD1  | 3                   | 0.28     | 0.04                | 0.3        |
| (1,1845) | 1:132:A:SER:HB2  | 1:145:A:TYR:HD2  | 3                   | 0.28     | 0.04                | 0.3        |
| (1,2262) | 1:164:A:GLU:HA   | 1:164:A:GLU:HG2  | 3                   | 0.28     | 0.01                | 0.27       |
| (1,2262) | 1:164:A:GLU:HA   | 1:164:A:GLU:HG3  | 3                   | 0.28     | 0.01                | 0.27       |
| (2,729)  | 1:151:A:VAL:H    | 1:153:A:ILE:HD11 | 3                   | 0.27     | 0.08                | 0.23       |
| (2,729)  | 1:151:A:VAL:H    | 1:153:A:ILE:HD12 | 3                   | 0.27     | 0.08                | 0.23       |
| (2,729)  | 1:151:A:VAL:H    | 1:153:A:ILE:HD13 | 3                   | 0.27     | 0.08                | 0.23       |
| (1,1789) | 1:125:A:LYS:HG2  | 1:125:A:LYS:HE2  | 3                   | 0.26     | 0.0                 | 0.26       |
| (1,1789) | 1:125:A:LYS:HG2  | 1:125:A:LYS:HE3  | 3                   | 0.26     | 0.0                 | 0.26       |
| (1,1789) | 1:125:A:LYS:HG3  | 1:125:A:LYS:HE2  | 3                   | 0.26     | 0.0                 | 0.26       |
| (1,1789) | 1:125:A:LYS:HG3  | 1:125:A:LYS:HE3  | 3                   | 0.26     | 0.0                 | 0.26       |
| (1,1770) | 1:120:A:VAL:HG21 | 1:121:A:LEU:H    | 3                   | 0.26     | 0.04                | 0.25       |
| (1,1770) | 1:120:A:VAL:HG22 | 1:121:A:LEU:H    | 3                   | 0.26     | 0.04                | 0.25       |
| (1,1770) | 1:120:A:VAL:HG23 | 1:121:A:LEU:H    | 3                   | 0.26     | 0.04                | 0.25       |
| (1,1803) | 1:129:A:THR:HA   | 1:129:A:THR:HG21 | 3                   | 0.24     | 0.0                 | 0.24       |
| (1,1803) | 1:129:A:THR:HA   | 1:129:A:THR:HG22 | 3                   | 0.24     | 0.0                 | 0.24       |
| (1,1803) | 1:129:A:THR:HA   | 1:129:A:THR:HG23 | 3                   | 0.24     | 0.0                 | 0.24       |
| (2,468)  | 1:79:A:ILE:HG21  | 1:156:A:PHE:HE1  | 3                   | 0.24     | 0.02                | 0.25       |
| (2,468)  | 1:79:A:ILE:HG21  | 1:156:A:PHE:HE2  | 3                   | 0.24     | 0.02                | 0.25       |
| (2,468)  | 1:79:A:ILE:HG22  | 1:156:A:PHE:HE1  | 3                   | 0.24     | 0.02                | 0.25       |
| (2,468)  | 1:79:A:ILE:HG22  | 1:156:A:PHE:HE2  | 3                   | 0.24     | 0.02                | 0.25       |
| (2,468)  | 1:79:A:ILE:HG23  | 1:156:A:PHE:HE1  | 3                   | 0.24     | 0.02                | 0.25       |
| (2,468)  | 1:79:A:ILE:HG23  | 1:156:A:PHE:HE2  | 3                   | 0.24     | 0.02                | 0.25       |
| (1,1233) | 1:81:A:ILE:HG21  | 1:100:A:ALA:HB1  | 3                   | 0.22     | 0.07                | 0.19       |
| (1,1233) | 1:81:A:ILE:HG21  | 1:100:A:ALA:HB2  | 3                   | 0.22     | 0.07                | 0.19       |
| (1,1233) | 1:81:A:ILE:HG21  | 1:100:A:ALA:HB3  | 3                   | 0.22     | 0.07                | 0.19       |
| (1,1233) | 1:81:A:ILE:HG22  | 1:100:A:ALA:HB1  | 3                   | 0.22     | 0.07                | 0.19       |
| (1,1233) | 1:81:A:ILE:HG22  | 1:100:A:ALA:HB2  | 3                   | 0.22     | 0.07                | 0.19       |
| (1,1233) | 1:81:A:ILE:HG22  | 1:100:A:ALA:HB3  | 3                   | 0.22     | 0.07                | 0.19       |
| (1,1233) | 1:81:A:ILE:HG23  | 1:100:A:ALA:HB1  | 3                   | 0.22     | 0.07                | 0.19       |
| (1,1233) | 1:81:A:ILE:HG23  | 1:100:A:ALA:HB2  | 3                   | 0.22     | 0.07                | 0.19       |
| (1,1233) | 1:81:A:ILE:HG23  | 1:100:A:ALA:HB3  | 3                   | 0.22     | 0.07                | 0.19       |
| (1,1474) | 1:95:A:PHE:HB2   | 1:95:A:PHE:H     | 3                   | 0.22     | 0.06                | 0.25       |
| (1,1474) | 1:95:A:PHE:HB3   | 1:95:A:PHE:H     | 3                   | 0.22     | 0.06                | 0.25       |
| (1,1635) | 1:111:A:ILE:HB   | 1:111:A:ILE:H    | 3                   | 0.21     | 0.02                | 0.21       |
| (1,1020) | 1:74:A:PHE:HD1   | 1:162:A:ALA:HA   | 3                   | 0.2      | 0.08                | 0.22       |
| (1,1020) | 1:74:A:PHE:HD2   | 1:162:A:ALA:HA   | 3                   | 0.2      | 0.08                | 0.22       |
| (1,647)  | 1:58:A:VAL:HB    | 1:58:A:VAL:H     | 3                   | 0.2      | 0.0                 | 0.2        |
| (1,2425) | 1:177:A:PHE:HD1  | 1:177:A:PHE:H    | 3                   | 0.19     | 0.06                | 0.22       |
| (1,2425) | 1:177:A:PHE:HD2  | 1:177:A:PHE:H    | 3                   | 0.19     | 0.06                | 0.22       |
| (1,1232) | 1:81:A:ILE:HG21  | 1:99:A:LYS:H     | 3                   | 0.19     | 0.08                | 0.16       |
| (1,1232) | 1:81:A:ILE:HG22  | 1:99:A:LYS:H     | 3                   | 0.19     | 0.08                | 0.16       |

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| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1232) | 1:81:A:ILE:HG23  | 1:99:A:LYS:H    | 3                   | 0.19     | 0.08                | 0.16       |
| (1,356)  | 1:42:A:ASP:HB2   | 1:160:A:TYR:HE1 | 3                   | 0.19     | 0.12                | 0.11       |
| (1,356)  | 1:42:A:ASP:HB2   | 1:160:A:TYR:HE2 | 3                   | 0.19     | 0.12                | 0.11       |
| (1,356)  | 1:42:A:ASP:HB3   | 1:160:A:TYR:HE1 | 3                   | 0.19     | 0.12                | 0.11       |
| (1,356)  | 1:42:A:ASP:HB3   | 1:160:A:TYR:HE2 | 3                   | 0.19     | 0.12                | 0.11       |
| (1,1882) | 1:134:A:TRP:HA   | 1:143:A:ILE:HA  | 3                   | 0.18     | 0.01                | 0.19       |
| (1,1775) | 1:121:A:LEU:HB2  | 1:121:A:LEU:H   | 3                   | 0.18     | 0.03                | 0.19       |
| (1,1572) | 1:104:A:LEU:HD11 | 1:104:A:LEU:H   | 3                   | 0.17     | 0.02                | 0.17       |
| (1,1572) | 1:104:A:LEU:HD12 | 1:104:A:LEU:H   | 3                   | 0.17     | 0.02                | 0.17       |
| (1,1572) | 1:104:A:LEU:HD13 | 1:104:A:LEU:H   | 3                   | 0.17     | 0.02                | 0.17       |
| (1,886)  | 1:68:A:GLU:HA    | 1:71:A:LYS:HD2  | 3                   | 0.16     | 0.06                | 0.14       |
| (1,886)  | 1:68:A:GLU:HA    | 1:71:A:LYS:HD3  | 3                   | 0.16     | 0.06                | 0.14       |
| (1,240)  | 1:32:A:ILE:HG21  | 1:74:A:PHE:HE1  | 3                   | 0.16     | 0.06                | 0.13       |
| (1,240)  | 1:32:A:ILE:HG21  | 1:74:A:PHE:HE2  | 3                   | 0.16     | 0.06                | 0.13       |
| (1,240)  | 1:32:A:ILE:HG22  | 1:74:A:PHE:HE1  | 3                   | 0.16     | 0.06                | 0.13       |
| (1,240)  | 1:32:A:ILE:HG22  | 1:74:A:PHE:HE2  | 3                   | 0.16     | 0.06                | 0.13       |
| (1,240)  | 1:32:A:ILE:HG23  | 1:74:A:PHE:HE1  | 3                   | 0.16     | 0.06                | 0.13       |
| (1,240)  | 1:32:A:ILE:HG23  | 1:74:A:PHE:HE2  | 3                   | 0.16     | 0.06                | 0.13       |
| (2,298)  | 1:54:A:GLN:HB3   | 1:54:A:GLN:HE21 | 3                   | 0.16     | 0.03                | 0.14       |
| (3,2)    | 1:33:A:THR:HA    | 1:34:A:PRO:HD3  | 3                   | 0.16     | 0.03                | 0.15       |
| (1,190)  | 1:31:A:SER:HA    | 1:32:A:ILE:HD11 | 3                   | 0.15     | 0.03                | 0.17       |
| (1,190)  | 1:31:A:SER:HA    | 1:32:A:ILE:HD12 | 3                   | 0.15     | 0.03                | 0.17       |
| (1,190)  | 1:31:A:SER:HA    | 1:32:A:ILE:HD13 | 3                   | 0.15     | 0.03                | 0.17       |
| (1,2316) | 1:171:A:LEU:HA   | 1:172:A:PRO:HD3 | 3                   | 0.15     | 0.03                | 0.16       |
| (1,256)  | 1:33:A:THR:HA    | 1:168:A:PHE:HZ  | 3                   | 0.14     | 0.03                | 0.14       |
| (1,12)   | 1:21:A:GLU:HA    | 1:21:A:GLU:HG2  | 3                   | 0.13     | 0.0                 | 0.13       |
| (1,12)   | 1:21:A:GLU:HA    | 1:21:A:GLU:HG3  | 3                   | 0.13     | 0.0                 | 0.13       |
| (1,424)  | 1:46:A:TYR:HA    | 1:155:A:ASN:HB2 | 3                   | 0.12     | 0.01                | 0.12       |
| (1,272)  | 1:34:A:PRO:HD2   | 1:35:A:ALA:H    | 3                   | 0.11     | 0.01                | 0.12       |
| (1,432)  | 1:46:A:TYR:HB3   | 1:154:A:LEU:H   | 3                   | 0.11     | 0.01                | 0.11       |
| (1,1422) | 1:88:A:ASN:HB2   | 1:88:A:ASN:HD21 | 3                   | 0.11     | 0.01                | 0.12       |
| (1,1629) | 1:110:A:VAL:HG11 | 1:111:A:ILE:H   | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,1629) | 1:110:A:VAL:HG12 | 1:111:A:ILE:H   | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,1629) | 1:110:A:VAL:HG13 | 1:111:A:ILE:H   | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,2086) | 1:152:A:ALA:HA   | 1:152:A:ALA:HB1 | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,2086) | 1:152:A:ALA:HA   | 1:152:A:ALA:HB2 | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,2086) | 1:152:A:ALA:HA   | 1:152:A:ALA:HB3 | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,678)  | 1:60:A:LEU:HA    | 1:111:A:ILE:H   | 3                   | 0.1      | 0.0                 | 0.1        |
| (1,1457) | 1:92:A:LEU:HD11  | 1:93:A:GLY:H    | 2                   | 0.72     | 0.03                | 0.72       |
| (1,1457) | 1:92:A:LEU:HD12  | 1:93:A:GLY:H    | 2                   | 0.72     | 0.03                | 0.72       |
| (1,1457) | 1:92:A:LEU:HD13  | 1:93:A:GLY:H    | 2                   | 0.72     | 0.03                | 0.72       |
| (2,5)    | 1:16:A:ALA:HB1   | 1:17:A:GLN:HE21 | 2                   | 0.65     | 0.1                 | 0.65       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (2,5)    | 1:16:A:ALA:HB2   | 1:17:A:GLN:HE21  | 2                   | 0.65     | 0.1                 | 0.65       |
| (2,5)    | 1:16:A:ALA:HB3   | 1:17:A:GLN:HE21  | 2                   | 0.65     | 0.1                 | 0.65       |
| (2,184)  | 1:37:A:GLY:H     | 1:38:A:ALA:HB1   | 2                   | 0.65     | 0.03                | 0.65       |
| (2,184)  | 1:37:A:GLY:H     | 1:38:A:ALA:HB2   | 2                   | 0.65     | 0.03                | 0.65       |
| (2,184)  | 1:37:A:GLY:H     | 1:38:A:ALA:HB3   | 2                   | 0.65     | 0.03                | 0.65       |
| (1,1091) | 1:77:A:LEU:HD11  | 1:103:A:SER:HA   | 2                   | 0.53     | 0.14                | 0.53       |
| (1,1091) | 1:77:A:LEU:HD12  | 1:103:A:SER:HA   | 2                   | 0.53     | 0.14                | 0.53       |
| (1,1091) | 1:77:A:LEU:HD13  | 1:103:A:SER:HA   | 2                   | 0.53     | 0.14                | 0.53       |
| (1,1091) | 1:77:A:LEU:HD21  | 1:103:A:SER:HA   | 2                   | 0.53     | 0.14                | 0.53       |
| (1,1091) | 1:77:A:LEU:HD22  | 1:103:A:SER:HA   | 2                   | 0.53     | 0.14                | 0.53       |
| (1,1091) | 1:77:A:LEU:HD23  | 1:103:A:SER:HA   | 2                   | 0.53     | 0.14                | 0.53       |
| (1,1242) | 1:81:A:ILE:HG21  | 1:156:A:PHE:HE1  | 2                   | 0.52     | 0.26                | 0.52       |
| (1,1242) | 1:81:A:ILE:HG21  | 1:156:A:PHE:HE2  | 2                   | 0.52     | 0.26                | 0.52       |
| (1,1242) | 1:81:A:ILE:HG22  | 1:156:A:PHE:HE1  | 2                   | 0.52     | 0.26                | 0.52       |
| (1,1242) | 1:81:A:ILE:HG22  | 1:156:A:PHE:HE2  | 2                   | 0.52     | 0.26                | 0.52       |
| (1,1242) | 1:81:A:ILE:HG23  | 1:156:A:PHE:HE1  | 2                   | 0.52     | 0.26                | 0.52       |
| (1,1242) | 1:81:A:ILE:HG23  | 1:156:A:PHE:HE2  | 2                   | 0.52     | 0.26                | 0.52       |
| (2,700)  | 1:132:A:SER:HB3  | 1:145:A:TYR:HE1  | 2                   | 0.51     | 0.0                 | 0.51       |
| (2,700)  | 1:132:A:SER:HB3  | 1:145:A:TYR:HE2  | 2                   | 0.51     | 0.0                 | 0.51       |
| (2,716)  | 1:142:A:ILE:HB   | 1:145:A:TYR:HE1  | 2                   | 0.51     | 0.0                 | 0.51       |
| (2,716)  | 1:142:A:ILE:HB   | 1:145:A:TYR:HE2  | 2                   | 0.51     | 0.0                 | 0.51       |
| (1,2284) | 1:168:A:PHE:HB2  | 1:171:A:LEU:HD11 | 2                   | 0.49     | 0.09                | 0.49       |
| (1,2284) | 1:168:A:PHE:HB2  | 1:171:A:LEU:HD12 | 2                   | 0.49     | 0.09                | 0.49       |
| (1,2284) | 1:168:A:PHE:HB2  | 1:171:A:LEU:HD13 | 2                   | 0.49     | 0.09                | 0.49       |
| (1,1662) | 1:113:A:LEU:HD11 | 1:113:A:LEU:H    | 2                   | 0.48     | 0.0                 | 0.48       |
| (1,1662) | 1:113:A:LEU:HD12 | 1:113:A:LEU:H    | 2                   | 0.48     | 0.0                 | 0.48       |
| (1,1662) | 1:113:A:LEU:HD13 | 1:113:A:LEU:H    | 2                   | 0.48     | 0.0                 | 0.48       |
| (2,661)  | 1:125:A:LYS:HG2  | 1:126:A:THR:H    | 2                   | 0.46     | 0.06                | 0.46       |
| (2,661)  | 1:125:A:LYS:HG3  | 1:126:A:THR:H    | 2                   | 0.46     | 0.06                | 0.46       |
| (1,992)  | 1:73:A:TYR:HE1   | 1:171:A:LEU:HD21 | 2                   | 0.44     | 0.25                | 0.44       |
| (1,992)  | 1:73:A:TYR:HE1   | 1:171:A:LEU:HD22 | 2                   | 0.44     | 0.25                | 0.44       |
| (1,992)  | 1:73:A:TYR:HE1   | 1:171:A:LEU:HD23 | 2                   | 0.44     | 0.25                | 0.44       |
| (1,992)  | 1:73:A:TYR:HE2   | 1:171:A:LEU:HD21 | 2                   | 0.44     | 0.25                | 0.44       |
| (1,992)  | 1:73:A:TYR:HE2   | 1:171:A:LEU:HD22 | 2                   | 0.44     | 0.25                | 0.44       |
| (1,992)  | 1:73:A:TYR:HE2   | 1:171:A:LEU:HD23 | 2                   | 0.44     | 0.25                | 0.44       |
| (1,2081) | 1:151:A:VAL:HG11 | 1:153:A:ILE:H    | 2                   | 0.44     | 0.03                | 0.44       |
| (1,2081) | 1:151:A:VAL:HG12 | 1:153:A:ILE:H    | 2                   | 0.44     | 0.03                | 0.44       |
| (1,2081) | 1:151:A:VAL:HG13 | 1:153:A:ILE:H    | 2                   | 0.44     | 0.03                | 0.44       |
| (2,240)  | 1:46:A:TYR:HB2   | 1:155:A:ASN:HD21 | 2                   | 0.44     | 0.03                | 0.44       |
| (2,240)  | 1:46:A:TYR:HB2   | 1:155:A:ASN:HD22 | 2                   | 0.44     | 0.03                | 0.44       |
| (1,2080) | 1:151:A:VAL:HG11 | 1:152:A:ALA:H    | 2                   | 0.42     | 0.01                | 0.42       |
| (1,2080) | 1:151:A:VAL:HG12 | 1:152:A:ALA:H    | 2                   | 0.42     | 0.01                | 0.42       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2080) | 1:151:A:VAL:HG13 | 1:152:A:ALA:H    | 2                   | 0.42     | 0.01                | 0.42       |
| (2,355)  | 1:64:A:LEU:H     | 1:175:A:PHE:HE1  | 2                   | 0.4      | 0.1                 | 0.4        |
| (2,355)  | 1:64:A:LEU:H     | 1:175:A:PHE:HE2  | 2                   | 0.4      | 0.1                 | 0.4        |
| (1,1844) | 1:132:A:SER:HB2  | 1:142:A:ILE:HG21 | 2                   | 0.4      | 0.05                | 0.4        |
| (1,1844) | 1:132:A:SER:HB2  | 1:142:A:ILE:HG22 | 2                   | 0.4      | 0.05                | 0.4        |
| (1,1844) | 1:132:A:SER:HB2  | 1:142:A:ILE:HG23 | 2                   | 0.4      | 0.05                | 0.4        |
| (1,2287) | 1:168:A:PHE:HD1  | 1:169:A:ASP:H    | 2                   | 0.38     | 0.21                | 0.38       |
| (1,2287) | 1:168:A:PHE:HD2  | 1:169:A:ASP:H    | 2                   | 0.38     | 0.21                | 0.38       |
| (2,721)  | 1:144:A:VAL:HA   | 1:145:A:TYR:HD1  | 2                   | 0.37     | 0.2                 | 0.37       |
| (2,721)  | 1:144:A:VAL:HA   | 1:145:A:TYR:HD2  | 2                   | 0.37     | 0.2                 | 0.37       |
| (1,126)  | 1:27:A:SER:HB2   | 1:177:A:PHE:HE1  | 2                   | 0.36     | 0.12                | 0.36       |
| (1,126)  | 1:27:A:SER:HB2   | 1:177:A:PHE:HE2  | 2                   | 0.36     | 0.12                | 0.36       |
| (1,126)  | 1:27:A:SER:HB3   | 1:177:A:PHE:HE1  | 2                   | 0.36     | 0.12                | 0.36       |
| (1,126)  | 1:27:A:SER:HB3   | 1:177:A:PHE:HE2  | 2                   | 0.36     | 0.12                | 0.36       |
| (2,601)  | 1:115:A:LYS:HE2  | 1:116:A:GLU:H    | 2                   | 0.36     | 0.04                | 0.36       |
| (2,601)  | 1:115:A:LYS:HE3  | 1:116:A:GLU:H    | 2                   | 0.36     | 0.04                | 0.36       |
| (2,725)  | 1:145:A:TYR:HD1  | 1:147:A:GLU:H    | 2                   | 0.36     | 0.01                | 0.36       |
| (2,725)  | 1:145:A:TYR:HD2  | 1:147:A:GLU:H    | 2                   | 0.36     | 0.01                | 0.36       |
| (2,590)  | 1:110:A:VAL:H    | 1:111:A:ILE:HD11 | 2                   | 0.36     | 0.14                | 0.36       |
| (2,590)  | 1:110:A:VAL:H    | 1:111:A:ILE:HD12 | 2                   | 0.36     | 0.14                | 0.36       |
| (2,590)  | 1:110:A:VAL:H    | 1:111:A:ILE:HD13 | 2                   | 0.36     | 0.14                | 0.36       |
| (1,86)   | 1:25:A:VAL:HG21  | 1:49:A:VAL:HG21  | 2                   | 0.34     | 0.1                 | 0.34       |
| (1,86)   | 1:25:A:VAL:HG21  | 1:49:A:VAL:HG22  | 2                   | 0.34     | 0.1                 | 0.34       |
| (1,86)   | 1:25:A:VAL:HG21  | 1:49:A:VAL:HG23  | 2                   | 0.34     | 0.1                 | 0.34       |
| (1,86)   | 1:25:A:VAL:HG22  | 1:49:A:VAL:HG21  | 2                   | 0.34     | 0.1                 | 0.34       |
| (1,86)   | 1:25:A:VAL:HG22  | 1:49:A:VAL:HG22  | 2                   | 0.34     | 0.1                 | 0.34       |
| (1,86)   | 1:25:A:VAL:HG22  | 1:49:A:VAL:HG23  | 2                   | 0.34     | 0.1                 | 0.34       |
| (1,86)   | 1:25:A:VAL:HG23  | 1:49:A:VAL:HG21  | 2                   | 0.34     | 0.1                 | 0.34       |
| (1,86)   | 1:25:A:VAL:HG23  | 1:49:A:VAL:HG22  | 2                   | 0.34     | 0.1                 | 0.34       |
| (1,86)   | 1:25:A:VAL:HG23  | 1:49:A:VAL:HG23  | 2                   | 0.34     | 0.1                 | 0.34       |
| (1,2069) | 1:148:A:THR:HG21 | 1:148:A:THR:H    | 2                   | 0.34     | 0.2                 | 0.34       |
| (1,2069) | 1:148:A:THR:HG22 | 1:148:A:THR:H    | 2                   | 0.34     | 0.2                 | 0.34       |
| (1,2069) | 1:148:A:THR:HG23 | 1:148:A:THR:H    | 2                   | 0.34     | 0.2                 | 0.34       |
| (2,724)  | 1:145:A:TYR:HD1  | 1:147:A:GLU:HG2  | 2                   | 0.34     | 0.04                | 0.34       |
| (2,724)  | 1:145:A:TYR:HD1  | 1:147:A:GLU:HG3  | 2                   | 0.34     | 0.04                | 0.34       |
| (2,724)  | 1:145:A:TYR:HD2  | 1:147:A:GLU:HG2  | 2                   | 0.34     | 0.04                | 0.34       |
| (2,724)  | 1:145:A:TYR:HD2  | 1:147:A:GLU:HG3  | 2                   | 0.34     | 0.04                | 0.34       |
| (1,238)  | 1:32:A:ILE:HG21  | 1:42:A:ASP:HB2   | 2                   | 0.32     | 0.01                | 0.32       |
| (1,238)  | 1:32:A:ILE:HG21  | 1:42:A:ASP:HB3   | 2                   | 0.32     | 0.01                | 0.32       |
| (1,238)  | 1:32:A:ILE:HG22  | 1:42:A:ASP:HB2   | 2                   | 0.32     | 0.01                | 0.32       |
| (1,238)  | 1:32:A:ILE:HG22  | 1:42:A:ASP:HB3   | 2                   | 0.32     | 0.01                | 0.32       |
| (1,238)  | 1:32:A:ILE:HG23  | 1:42:A:ASP:HB2   | 2                   | 0.32     | 0.01                | 0.32       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,238)  | 1:32:A:ILE:HG23  | 1:42:A:ASP:HB3   | 2                   | 0.32     | 0.01                | 0.32       |
| (2,443)  | 1:76:A:TYR:HE1   | 1:78:A:GLN:HE22  | 2                   | 0.32     | 0.2                 | 0.32       |
| (2,443)  | 1:76:A:TYR:HE2   | 1:78:A:GLN:HE22  | 2                   | 0.32     | 0.2                 | 0.32       |
| (1,2176) | 1:157:A:LYS:HE2  | 1:159:A:PHE:HE1  | 2                   | 0.32     | 0.15                | 0.32       |
| (1,2176) | 1:157:A:LYS:HE2  | 1:159:A:PHE:HE2  | 2                   | 0.32     | 0.15                | 0.32       |
| (1,2176) | 1:157:A:LYS:HE3  | 1:159:A:PHE:HE1  | 2                   | 0.32     | 0.15                | 0.32       |
| (1,2176) | 1:157:A:LYS:HE3  | 1:159:A:PHE:HE2  | 2                   | 0.32     | 0.15                | 0.32       |
| (1,2446) | 1:179:A:VAL:HB   | 1:179:A:VAL:H    | 2                   | 0.32     | 0.01                | 0.32       |
| (2,227)  | 1:43:A:ASP:HB3   | 1:46:A:TYR:HE1   | 2                   | 0.32     | 0.08                | 0.32       |
| (2,227)  | 1:43:A:ASP:HB3   | 1:46:A:TYR:HE2   | 2                   | 0.32     | 0.08                | 0.32       |
| (1,1460) | 1:92:A:LEU:HG    | 1:93:A:GLY:H     | 2                   | 0.31     | 0.16                | 0.31       |
| (1,1841) | 1:132:A:SER:HB3  | 1:145:A:TYR:HD1  | 2                   | 0.3      | 0.01                | 0.3        |
| (1,1841) | 1:132:A:SER:HB3  | 1:145:A:TYR:HD2  | 2                   | 0.3      | 0.01                | 0.3        |
| (1,260)  | 1:33:A:THR:HG21  | 1:34:A:PRO:HD3   | 2                   | 0.29     | 0.1                 | 0.29       |
| (1,260)  | 1:33:A:THR:HG22  | 1:34:A:PRO:HD3   | 2                   | 0.29     | 0.1                 | 0.29       |
| (1,260)  | 1:33:A:THR:HG23  | 1:34:A:PRO:HD3   | 2                   | 0.29     | 0.1                 | 0.29       |
| (1,2321) | 1:171:A:LEU:HD11 | 1:171:A:LEU:H    | 2                   | 0.29     | 0.06                | 0.29       |
| (1,2321) | 1:171:A:LEU:HD12 | 1:171:A:LEU:H    | 2                   | 0.29     | 0.06                | 0.29       |
| (1,2321) | 1:171:A:LEU:HD13 | 1:171:A:LEU:H    | 2                   | 0.29     | 0.06                | 0.29       |
| (1,1032) | 1:74:A:PHE:HE1   | 1:168:A:PHE:HZ   | 2                   | 0.28     | 0.03                | 0.28       |
| (1,1032) | 1:74:A:PHE:HE2   | 1:168:A:PHE:HZ   | 2                   | 0.28     | 0.03                | 0.28       |
| (1,655)  | 1:58:A:VAL:H     | 1:113:A:LEU:HD11 | 2                   | 0.27     | 0.1                 | 0.27       |
| (1,655)  | 1:58:A:VAL:H     | 1:113:A:LEU:HD12 | 2                   | 0.27     | 0.1                 | 0.27       |
| (1,655)  | 1:58:A:VAL:H     | 1:113:A:LEU:HD13 | 2                   | 0.27     | 0.1                 | 0.27       |
| (1,724)  | 1:62:A:VAL:HG11  | 1:63:A:THR:H     | 2                   | 0.27     | 0.01                | 0.27       |
| (1,724)  | 1:62:A:VAL:HG12  | 1:63:A:THR:H     | 2                   | 0.27     | 0.01                | 0.27       |
| (1,724)  | 1:62:A:VAL:HG13  | 1:63:A:THR:H     | 2                   | 0.27     | 0.01                | 0.27       |
| (1,1400) | 1:87:A:THR:HG21  | 1:88:A:ASN:HA    | 2                   | 0.27     | 0.05                | 0.27       |
| (1,1400) | 1:87:A:THR:HG22  | 1:88:A:ASN:HA    | 2                   | 0.27     | 0.05                | 0.27       |
| (1,1400) | 1:87:A:THR:HG23  | 1:88:A:ASN:HA    | 2                   | 0.27     | 0.05                | 0.27       |
| (2,522)  | 1:85:A:TYR:HD1   | 1:134:A:TRP:HA   | 2                   | 0.27     | 0.01                | 0.27       |
| (2,522)  | 1:85:A:TYR:HD2   | 1:134:A:TRP:HA   | 2                   | 0.27     | 0.01                | 0.27       |
| (1,651)  | 1:58:A:VAL:HG11  | 1:59:A:LYS:H     | 2                   | 0.26     | 0.11                | 0.26       |
| (1,651)  | 1:58:A:VAL:HG12  | 1:59:A:LYS:H     | 2                   | 0.26     | 0.11                | 0.26       |
| (1,651)  | 1:58:A:VAL:HG13  | 1:59:A:LYS:H     | 2                   | 0.26     | 0.11                | 0.26       |
| (1,651)  | 1:58:A:VAL:HG21  | 1:59:A:LYS:H     | 2                   | 0.26     | 0.11                | 0.26       |
| (1,651)  | 1:58:A:VAL:HG22  | 1:59:A:LYS:H     | 2                   | 0.26     | 0.11                | 0.26       |
| (1,651)  | 1:58:A:VAL:HG23  | 1:59:A:LYS:H     | 2                   | 0.26     | 0.11                | 0.26       |
| (1,727)  | 1:62:A:VAL:HG11  | 1:177:A:PHE:HE1  | 2                   | 0.26     | 0.02                | 0.26       |
| (1,727)  | 1:62:A:VAL:HG11  | 1:177:A:PHE:HE2  | 2                   | 0.26     | 0.02                | 0.26       |
| (1,727)  | 1:62:A:VAL:HG12  | 1:177:A:PHE:HE1  | 2                   | 0.26     | 0.02                | 0.26       |
| (1,727)  | 1:62:A:VAL:HG12  | 1:177:A:PHE:HE2  | 2                   | 0.26     | 0.02                | 0.26       |

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| Key      | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,727)  | 1:62:A:VAL:HG13 | 1:177:A:PHE:HE1  | 2                   | 0.26     | 0.02                | 0.26       |
| (1,727)  | 1:62:A:VAL:HG13 | 1:177:A:PHE:HE2  | 2                   | 0.26     | 0.02                | 0.26       |
| (2,547)  | 1:87:A:THR:HG21 | 1:91:A:ALA:H     | 2                   | 0.26     | 0.03                | 0.26       |
| (2,547)  | 1:87:A:THR:HG22 | 1:91:A:ALA:H     | 2                   | 0.26     | 0.03                | 0.26       |
| (2,547)  | 1:87:A:THR:HG23 | 1:91:A:ALA:H     | 2                   | 0.26     | 0.03                | 0.26       |
| (1,445)  | 1:46:A:TYR:HE1  | 1:141:A:LYS:HE3  | 2                   | 0.25     | 0.06                | 0.25       |
| (1,445)  | 1:46:A:TYR:HE2  | 1:141:A:LYS:HE3  | 2                   | 0.25     | 0.06                | 0.25       |
| (1,728)  | 1:62:A:VAL:HG21 | 1:62:A:VAL:H     | 2                   | 0.23     | 0.01                | 0.23       |
| (1,728)  | 1:62:A:VAL:HG22 | 1:62:A:VAL:H     | 2                   | 0.23     | 0.01                | 0.23       |
| (1,728)  | 1:62:A:VAL:HG23 | 1:62:A:VAL:H     | 2                   | 0.23     | 0.01                | 0.23       |
| (2,552)  | 1:87:A:THR:H    | 1:92:A:LEU:HB2   | 2                   | 0.23     | 0.02                | 0.23       |
| (1,392)  | 1:44:A:ILE:HG21 | 1:158:A:ALA:H    | 2                   | 0.22     | 0.02                | 0.22       |
| (1,392)  | 1:44:A:ILE:HG22 | 1:158:A:ALA:H    | 2                   | 0.22     | 0.02                | 0.22       |
| (1,392)  | 1:44:A:ILE:HG23 | 1:158:A:ALA:H    | 2                   | 0.22     | 0.02                | 0.22       |
| (1,941)  | 1:71:A:LYS:HA   | 1:74:A:PHE:HD1   | 2                   | 0.22     | 0.02                | 0.22       |
| (1,941)  | 1:71:A:LYS:HA   | 1:74:A:PHE:HD2   | 2                   | 0.22     | 0.02                | 0.22       |
| (1,498)  | 1:48:A:ILE:HG21 | 1:50:A:TRP:HZ2   | 2                   | 0.2      | 0.03                | 0.2        |
| (1,498)  | 1:48:A:ILE:HG22 | 1:50:A:TRP:HZ2   | 2                   | 0.2      | 0.03                | 0.2        |
| (1,498)  | 1:48:A:ILE:HG23 | 1:50:A:TRP:HZ2   | 2                   | 0.2      | 0.03                | 0.2        |
| (2,625)  | 1:121:A:LEU:H   | 1:122:A:TYR:HD1  | 2                   | 0.2      | 0.08                | 0.2        |
| (2,625)  | 1:121:A:LEU:H   | 1:122:A:TYR:HD2  | 2                   | 0.2      | 0.08                | 0.2        |
| (1,1793) | 1:128:A:TYR:HA  | 1:128:A:TYR:HB3  | 2                   | 0.2      | 0.05                | 0.2        |
| (1,461)  | 1:47:A:ALA:H    | 1:153:A:ILE:HG21 | 2                   | 0.18     | 0.04                | 0.18       |
| (1,461)  | 1:47:A:ALA:H    | 1:153:A:ILE:HG22 | 2                   | 0.18     | 0.04                | 0.18       |
| (1,461)  | 1:47:A:ALA:H    | 1:153:A:ILE:HG23 | 2                   | 0.18     | 0.04                | 0.18       |
| (1,912)  | 1:69:A:GLN:HG3  | 1:69:A:GLN:HE21  | 2                   | 0.18     | 0.03                | 0.18       |
| (1,46)   | 1:24:A:ASP:HB3  | 1:50:A:TRP:HB3   | 2                   | 0.18     | 0.0                 | 0.18       |
| (1,1446) | 1:90:A:THR:HA   | 1:93:A:GLY:H     | 2                   | 0.18     | 0.04                | 0.18       |
| (1,2272) | 1:166:A:MET:HB2 | 1:167:A:LEU:H    | 2                   | 0.18     | 0.0                 | 0.18       |
| (1,530)  | 1:49:A:VAL:H    | 1:152:A:ALA:HA   | 2                   | 0.17     | 0.0                 | 0.17       |
| (1,989)  | 1:73:A:TYR:HD1  | 1:74:A:PHE:HE1   | 2                   | 0.17     | 0.02                | 0.17       |
| (1,989)  | 1:73:A:TYR:HD1  | 1:74:A:PHE:HE2   | 2                   | 0.17     | 0.02                | 0.17       |
| (1,989)  | 1:73:A:TYR:HD2  | 1:74:A:PHE:HE1   | 2                   | 0.17     | 0.02                | 0.17       |
| (1,989)  | 1:73:A:TYR:HD2  | 1:74:A:PHE:HE2   | 2                   | 0.17     | 0.02                | 0.17       |
| (1,2313) | 1:171:A:LEU:HA  | 1:171:A:LEU:HD11 | 2                   | 0.16     | 0.02                | 0.16       |
| (1,2313) | 1:171:A:LEU:HA  | 1:171:A:LEU:HD12 | 2                   | 0.16     | 0.02                | 0.16       |
| (1,2313) | 1:171:A:LEU:HA  | 1:171:A:LEU:HD13 | 2                   | 0.16     | 0.02                | 0.16       |
| (2,760)  | 1:168:A:PHE:HE1 | 1:171:A:LEU:HG   | 2                   | 0.16     | 0.02                | 0.16       |
| (2,760)  | 1:168:A:PHE:HE2 | 1:171:A:LEU:HG   | 2                   | 0.16     | 0.02                | 0.16       |
| (1,337)  | 1:41:A:SER:HB2  | 1:42:A:ASP:HA    | 2                   | 0.14     | 0.0                 | 0.14       |
| (1,1272) | 1:82:A:THR:HG21 | 1:96:A:SER:HA    | 2                   | 0.14     | 0.0                 | 0.14       |
| (1,1272) | 1:82:A:THR:HG22 | 1:96:A:SER:HA    | 2                   | 0.14     | 0.0                 | 0.14       |

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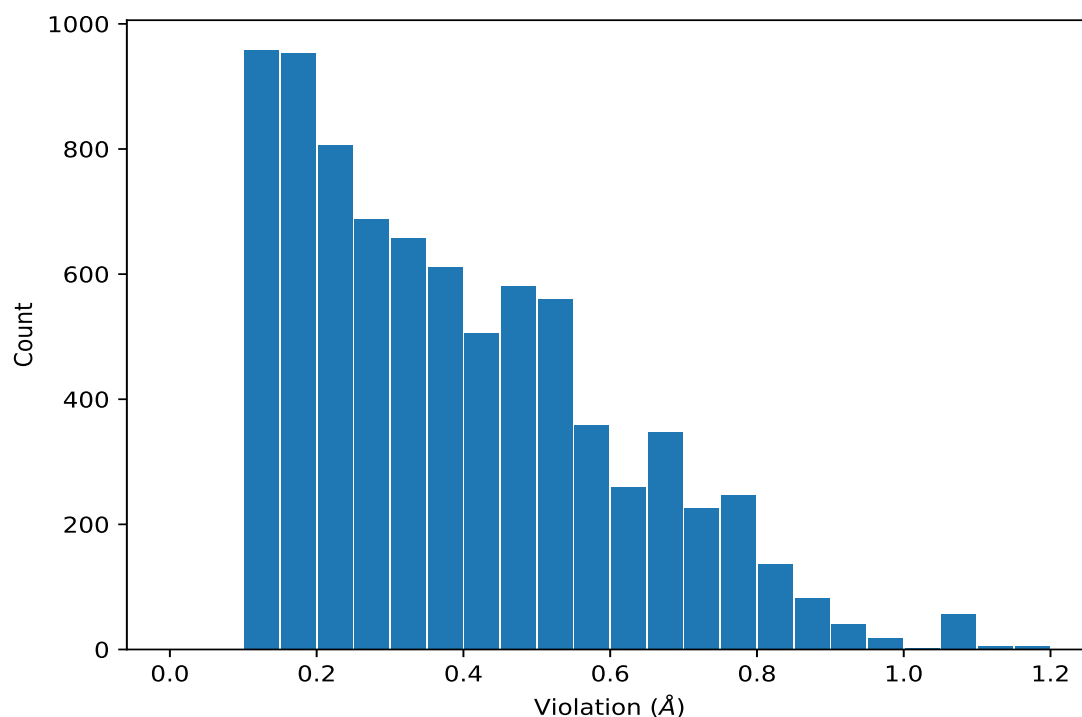
| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1272) | 1:82:A:THR:HG23 | 1:96:A:SER:HA   | 2                   | 0.14     | 0.0                 | 0.14       |
| (1,1273) | 1:82:A:THR:HG21 | 1:96:A:SER:HA   | 2                   | 0.14     | 0.0                 | 0.14       |
| (1,1273) | 1:82:A:THR:HG22 | 1:96:A:SER:HA   | 2                   | 0.14     | 0.0                 | 0.14       |
| (1,1273) | 1:82:A:THR:HG23 | 1:96:A:SER:HA   | 2                   | 0.14     | 0.0                 | 0.14       |
| (1,1335) | 1:85:A:TYR:HB2  | 1:86:A:GLU:H    | 2                   | 0.14     | 0.0                 | 0.14       |
| (1,2276) | 1:167:A:LEU:H   | 1:168:A:PHE:H   | 2                   | 0.14     | 0.03                | 0.14       |
| (2,12)   | 1:17:A:GLN:HB2  | 1:17:A:GLN:HE21 | 2                   | 0.14     | 0.0                 | 0.14       |
| (1,259)  | 1:33:A:THR:HB   | 1:35:A:ALA:H    | 2                   | 0.13     | 0.0                 | 0.13       |
| (1,863)  | 1:66:A:ASN:H    | 1:175:A:PHE:HA  | 2                   | 0.13     | 0.01                | 0.13       |
| (1,1100) | 1:77:A:LEU:HG   | 1:78:A:GLN:H    | 2                   | 0.13     | 0.02                | 0.13       |
| (1,54)   | 1:24:A:ASP:HB2  | 1:50:A:TRP:HB2  | 2                   | 0.12     | 0.02                | 0.12       |
| (1,447)  | 1:46:A:TYR:HE1  | 1:141:A:LYS:HG3 | 2                   | 0.12     | 0.02                | 0.12       |
| (1,447)  | 1:46:A:TYR:HE2  | 1:141:A:LYS:HG3 | 2                   | 0.12     | 0.02                | 0.12       |
| (1,529)  | 1:49:A:VAL:H    | 1:151:A:VAL:HA  | 2                   | 0.12     | 0.02                | 0.12       |
| (1,1333) | 1:85:A:TYR:HA   | 1:86:A:GLU:H    | 2                   | 0.12     | 0.01                | 0.12       |
| (1,254)  | 1:33:A:THR:HA   | 1:33:A:THR:HG21 | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,254)  | 1:33:A:THR:HA   | 1:33:A:THR:HG22 | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,254)  | 1:33:A:THR:HA   | 1:33:A:THR:HG23 | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,1086) | 1:77:A:LEU:HB2  | 1:78:A:GLN:H    | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,1282) | 1:82:A:THR:H    | 1:155:A:ASN:HB3 | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,1690) | 1:115:A:LYS:HA  | 1:115:A:LYS:HG2 | 2                   | 0.12     | 0.01                | 0.12       |
| (1,1690) | 1:115:A:LYS:HA  | 1:115:A:LYS:HG3 | 2                   | 0.12     | 0.01                | 0.12       |
| (1,1817) | 1:131:A:THR:HB  | 1:132:A:SER:H   | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,2271) | 1:166:A:MET:HB3 | 1:167:A:LEU:H   | 2                   | 0.12     | 0.01                | 0.12       |
| (2,26)   | 1:19:A:VAL:H    | 1:20:A:SER:HB2  | 2                   | 0.12     | 0.0                 | 0.12       |
| (2,26)   | 1:19:A:VAL:H    | 1:20:A:SER:HB3  | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,1439) | 1:88:A:ASN:H    | 1:134:A:TRP:HZ3 | 2                   | 0.12     | 0.02                | 0.12       |
| (1,1271) | 1:82:A:THR:HG21 | 1:83:A:SER:H    | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,1271) | 1:82:A:THR:HG22 | 1:83:A:SER:H    | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,1271) | 1:82:A:THR:HG23 | 1:83:A:SER:H    | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,188)  | 1:30:A:GLY:H    | 1:46:A:TYR:H    | 2                   | 0.11     | 0.0                 | 0.11       |
| (2,27)   | 1:19:A:VAL:H    | 1:20:A:SER:H    | 2                   | 0.11     | 0.01                | 0.11       |
| (2,123)  | 1:28:A:HIS:HD2  | 1:46:A:TYR:HE1  | 2                   | 0.11     | 0.0                 | 0.11       |
| (2,123)  | 1:28:A:HIS:HD2  | 1:46:A:TYR:HE2  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,141)  | 1:28:A:HIS:HD2  | 1:48:A:ILE:HA   | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,290)  | 1:37:A:GLY:HA3  | 1:38:A:ALA:H    | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,639)  | 1:57:A:ASP:HB3  | 1:58:A:VAL:H    | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,828)  | 1:66:A:ASN:HA   | 1:69:A:GLN:HG3  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1761) | 1:119:A:ALA:H   | 1:151:A:VAL:H   | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,2295) | 1:169:A:ASP:HB3 | 1:170:A:SER:H   | 2                   | 0.11     | 0.0                 | 0.11       |

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

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

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

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



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

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

| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (2,718) | 1:142:A:ILE:HD11 | 1:145:A:TYR:HE1 | 6        | 1.18          |
| (2,718) | 1:142:A:ILE:HD11 | 1:145:A:TYR:HE2 | 6        | 1.18          |
| (2,718) | 1:142:A:ILE:HD12 | 1:145:A:TYR:HE1 | 6        | 1.18          |
| (2,718) | 1:142:A:ILE:HD12 | 1:145:A:TYR:HE2 | 6        | 1.18          |
| (2,718) | 1:142:A:ILE:HD13 | 1:145:A:TYR:HE1 | 6        | 1.18          |
| (2,718) | 1:142:A:ILE:HD13 | 1:145:A:TYR:HE2 | 6        | 1.18          |
| (1,10)  | 1:19:A:VAL:HG11  | 1:19:A:VAL:H    | 5        | 1.11          |
| (1,10)  | 1:19:A:VAL:HG12  | 1:19:A:VAL:H    | 5        | 1.11          |
| (1,10)  | 1:19:A:VAL:HG13  | 1:19:A:VAL:H    | 5        | 1.11          |
| (1,10)  | 1:19:A:VAL:HG21  | 1:19:A:VAL:H    | 5        | 1.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,10)   | 1:19:A:VAL:HG22 | 1:19:A:VAL:H    | 5        | 1.11          |
| (1,10)   | 1:19:A:VAL:HG23 | 1:19:A:VAL:H    | 5        | 1.11          |
| (1,1030) | 1:74:A:PHE:HE1  | 1:162:A:ALA:HB1 | 4        | 1.08          |
| (1,1030) | 1:74:A:PHE:HE1  | 1:162:A:ALA:HB2 | 4        | 1.08          |
| (1,1030) | 1:74:A:PHE:HE1  | 1:162:A:ALA:HB3 | 4        | 1.08          |
| (1,1030) | 1:74:A:PHE:HE2  | 1:162:A:ALA:HB1 | 4        | 1.08          |
| (1,1030) | 1:74:A:PHE:HE2  | 1:162:A:ALA:HB2 | 4        | 1.08          |
| (1,1030) | 1:74:A:PHE:HE2  | 1:162:A:ALA:HB3 | 4        | 1.08          |
| (1,1030) | 1:74:A:PHE:HE1  | 1:162:A:ALA:HB1 | 9        | 1.08          |
| (1,1030) | 1:74:A:PHE:HE1  | 1:162:A:ALA:HB2 | 9        | 1.08          |
| (1,1030) | 1:74:A:PHE:HE1  | 1:162:A:ALA:HB3 | 9        | 1.08          |
| (1,1030) | 1:74:A:PHE:HE2  | 1:162:A:ALA:HB1 | 9        | 1.08          |
| (1,1030) | 1:74:A:PHE:HE2  | 1:162:A:ALA:HB2 | 9        | 1.08          |
| (1,1030) | 1:74:A:PHE:HE2  | 1:162:A:ALA:HB3 | 9        | 1.08          |
| (1,1030) | 1:74:A:PHE:HE1  | 1:162:A:ALA:HB1 | 1        | 1.07          |
| (1,1030) | 1:74:A:PHE:HE1  | 1:162:A:ALA:HB2 | 1        | 1.07          |
| (1,1030) | 1:74:A:PHE:HE1  | 1:162:A:ALA:HB3 | 1        | 1.07          |
| (1,1030) | 1:74:A:PHE:HE2  | 1:162:A:ALA:HB1 | 1        | 1.07          |
| (1,1030) | 1:74:A:PHE:HE2  | 1:162:A:ALA:HB2 | 1        | 1.07          |
| (1,1030) | 1:74:A:PHE:HE2  | 1:162:A:ALA:HB3 | 1        | 1.07          |
| (1,1030) | 1:74:A:PHE:HE1  | 1:162:A:ALA:HB1 | 7        | 1.07          |
| (1,1030) | 1:74:A:PHE:HE1  | 1:162:A:ALA:HB2 | 7        | 1.07          |
| (1,1030) | 1:74:A:PHE:HE1  | 1:162:A:ALA:HB3 | 7        | 1.07          |
| (1,1030) | 1:74:A:PHE:HE2  | 1:162:A:ALA:HB1 | 7        | 1.07          |
| (1,1030) | 1:74:A:PHE:HE2  | 1:162:A:ALA:HB2 | 7        | 1.07          |
| (1,1030) | 1:74:A:PHE:HE2  | 1:162:A:ALA:HB3 | 7        | 1.07          |
| (1,288)  | 1:36:A:ALA:HB1  | 1:37:A:GLY:H    | 7        | 1.07          |
| (1,288)  | 1:36:A:ALA:HB2  | 1:37:A:GLY:H    | 7        | 1.07          |
| (1,288)  | 1:36:A:ALA:HB3  | 1:37:A:GLY:H    | 7        | 1.07          |
| (1,10)   | 1:19:A:VAL:HG11 | 1:19:A:VAL:H    | 4        | 1.07          |
| (1,10)   | 1:19:A:VAL:HG12 | 1:19:A:VAL:H    | 4        | 1.07          |
| (1,10)   | 1:19:A:VAL:HG13 | 1:19:A:VAL:H    | 4        | 1.07          |
| (1,10)   | 1:19:A:VAL:HG21 | 1:19:A:VAL:H    | 4        | 1.07          |
| (1,10)   | 1:19:A:VAL:HG22 | 1:19:A:VAL:H    | 4        | 1.07          |
| (1,10)   | 1:19:A:VAL:HG23 | 1:19:A:VAL:H    | 4        | 1.07          |
| (1,1030) | 1:74:A:PHE:HE1  | 1:162:A:ALA:HB1 | 5        | 1.06          |
| (1,1030) | 1:74:A:PHE:HE1  | 1:162:A:ALA:HB2 | 5        | 1.06          |
| (1,1030) | 1:74:A:PHE:HE1  | 1:162:A:ALA:HB3 | 5        | 1.06          |
| (1,1030) | 1:74:A:PHE:HE2  | 1:162:A:ALA:HB1 | 5        | 1.06          |
| (1,1030) | 1:74:A:PHE:HE2  | 1:162:A:ALA:HB2 | 5        | 1.06          |
| (1,1030) | 1:74:A:PHE:HE2  | 1:162:A:ALA:HB3 | 5        | 1.06          |
| (1,10)   | 1:19:A:VAL:HG11 | 1:19:A:VAL:H    | 8        | 1.06          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,10)   | 1:19:A:VAL:HG12  | 1:19:A:VAL:H     | 8        | 1.06          |
| (1,10)   | 1:19:A:VAL:HG13  | 1:19:A:VAL:H     | 8        | 1.06          |
| (1,10)   | 1:19:A:VAL:HG21  | 1:19:A:VAL:H     | 8        | 1.06          |
| (1,10)   | 1:19:A:VAL:HG22  | 1:19:A:VAL:H     | 8        | 1.06          |
| (1,10)   | 1:19:A:VAL:HG23  | 1:19:A:VAL:H     | 8        | 1.06          |
| (1,10)   | 1:19:A:VAL:HG11  | 1:19:A:VAL:H     | 9        | 1.06          |
| (1,10)   | 1:19:A:VAL:HG12  | 1:19:A:VAL:H     | 9        | 1.06          |
| (1,10)   | 1:19:A:VAL:HG13  | 1:19:A:VAL:H     | 9        | 1.06          |
| (1,10)   | 1:19:A:VAL:HG21  | 1:19:A:VAL:H     | 9        | 1.06          |
| (1,10)   | 1:19:A:VAL:HG22  | 1:19:A:VAL:H     | 9        | 1.06          |
| (1,10)   | 1:19:A:VAL:HG23  | 1:19:A:VAL:H     | 9        | 1.06          |
| (1,10)   | 1:19:A:VAL:HG11  | 1:19:A:VAL:H     | 7        | 1.05          |
| (1,10)   | 1:19:A:VAL:HG12  | 1:19:A:VAL:H     | 7        | 1.05          |
| (1,10)   | 1:19:A:VAL:HG13  | 1:19:A:VAL:H     | 7        | 1.05          |
| (1,10)   | 1:19:A:VAL:HG21  | 1:19:A:VAL:H     | 7        | 1.05          |
| (1,10)   | 1:19:A:VAL:HG22  | 1:19:A:VAL:H     | 7        | 1.05          |
| (1,10)   | 1:19:A:VAL:HG23  | 1:19:A:VAL:H     | 7        | 1.05          |
| (2,765)  | 1:169:A:ASP:H    | 1:171:A:LEU:HD11 | 2        | 1.01          |
| (2,765)  | 1:169:A:ASP:H    | 1:171:A:LEU:HD12 | 2        | 1.01          |
| (2,765)  | 1:169:A:ASP:H    | 1:171:A:LEU:HD13 | 2        | 1.01          |
| (1,1030) | 1:74:A:PHE:HE1   | 1:162:A:ALA:HB1  | 3        | 0.98          |
| (1,1030) | 1:74:A:PHE:HE1   | 1:162:A:ALA:HB2  | 3        | 0.98          |
| (1,1030) | 1:74:A:PHE:HE1   | 1:162:A:ALA:HB3  | 3        | 0.98          |
| (1,1030) | 1:74:A:PHE:HE2   | 1:162:A:ALA:HB1  | 3        | 0.98          |
| (1,1030) | 1:74:A:PHE:HE2   | 1:162:A:ALA:HB2  | 3        | 0.98          |
| (1,1030) | 1:74:A:PHE:HE2   | 1:162:A:ALA:HB3  | 3        | 0.98          |
| (1,579)  | 1:51:A:ILE:HG21  | 1:53:A:ASP:HB2   | 7        | 0.97          |
| (1,579)  | 1:51:A:ILE:HG21  | 1:53:A:ASP:HB3   | 7        | 0.97          |
| (1,579)  | 1:51:A:ILE:HG22  | 1:53:A:ASP:HB2   | 7        | 0.97          |
| (1,579)  | 1:51:A:ILE:HG22  | 1:53:A:ASP:HB3   | 7        | 0.97          |
| (1,579)  | 1:51:A:ILE:HG23  | 1:53:A:ASP:HB2   | 7        | 0.97          |
| (1,579)  | 1:51:A:ILE:HG23  | 1:53:A:ASP:HB3   | 7        | 0.97          |
| (1,2017) | 1:142:A:ILE:HG21 | 1:145:A:TYR:HE1  | 6        | 0.96          |
| (1,2017) | 1:142:A:ILE:HG21 | 1:145:A:TYR:HE2  | 6        | 0.96          |
| (1,2017) | 1:142:A:ILE:HG22 | 1:145:A:TYR:HE1  | 6        | 0.96          |
| (1,2017) | 1:142:A:ILE:HG22 | 1:145:A:TYR:HE2  | 6        | 0.96          |
| (1,2017) | 1:142:A:ILE:HG23 | 1:145:A:TYR:HE1  | 6        | 0.96          |
| (1,2017) | 1:142:A:ILE:HG23 | 1:145:A:TYR:HE2  | 6        | 0.96          |
| (2,518)  | 1:84:A:GLY:HA2   | 1:95:A:PHE:HE1   | 4        | 0.94          |
| (2,518)  | 1:84:A:GLY:HA2   | 1:95:A:PHE:HE2   | 4        | 0.94          |
| (2,518)  | 1:84:A:GLY:HA3   | 1:95:A:PHE:HE1   | 4        | 0.94          |
| (2,518)  | 1:84:A:GLY:HA3   | 1:95:A:PHE:HE2   | 4        | 0.94          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,520)  | 1:84:A:GLY:HA2   | 1:155:A:ASN:HD21 | 3        | 0.93          |
| (2,520)  | 1:84:A:GLY:HA2   | 1:155:A:ASN:HD22 | 3        | 0.93          |
| (2,520)  | 1:84:A:GLY:HA3   | 1:155:A:ASN:HD21 | 3        | 0.93          |
| (2,520)  | 1:84:A:GLY:HA3   | 1:155:A:ASN:HD22 | 3        | 0.93          |
| (2,517)  | 1:84:A:GLY:HA2   | 1:85:A:TYR:HD1   | 9        | 0.93          |
| (2,517)  | 1:84:A:GLY:HA2   | 1:85:A:TYR:HD2   | 9        | 0.93          |
| (2,517)  | 1:84:A:GLY:HA3   | 1:85:A:TYR:HD1   | 9        | 0.93          |
| (2,517)  | 1:84:A:GLY:HA3   | 1:85:A:TYR:HD2   | 9        | 0.93          |
| (2,437)  | 1:76:A:TYR:HD1   | 1:104:A:LEU:HD11 | 10       | 0.93          |
| (2,437)  | 1:76:A:TYR:HD1   | 1:104:A:LEU:HD12 | 10       | 0.93          |
| (2,437)  | 1:76:A:TYR:HD1   | 1:104:A:LEU:HD13 | 10       | 0.93          |
| (2,437)  | 1:76:A:TYR:HD2   | 1:104:A:LEU:HD11 | 10       | 0.93          |
| (2,437)  | 1:76:A:TYR:HD2   | 1:104:A:LEU:HD12 | 10       | 0.93          |
| (2,437)  | 1:76:A:TYR:HD2   | 1:104:A:LEU:HD13 | 10       | 0.93          |
| (1,1940) | 1:135:A:VAL:HG11 | 1:155:A:ASN:HD21 | 6        | 0.93          |
| (1,1940) | 1:135:A:VAL:HG11 | 1:155:A:ASN:HD22 | 6        | 0.93          |
| (1,1940) | 1:135:A:VAL:HG12 | 1:155:A:ASN:HD21 | 6        | 0.93          |
| (1,1940) | 1:135:A:VAL:HG12 | 1:155:A:ASN:HD22 | 6        | 0.93          |
| (1,1940) | 1:135:A:VAL:HG13 | 1:155:A:ASN:HD21 | 6        | 0.93          |
| (1,1940) | 1:135:A:VAL:HG13 | 1:155:A:ASN:HD22 | 6        | 0.93          |
| (1,21)   | 1:22:A:PRO:HD2   | 1:23:A:ILE:H     | 3        | 0.93          |
| (2,469)  | 1:79:A:ILE:HG21  | 1:157:A:LYS:H    | 6        | 0.92          |
| (2,469)  | 1:79:A:ILE:HG22  | 1:157:A:LYS:H    | 6        | 0.92          |
| (2,469)  | 1:79:A:ILE:HG23  | 1:157:A:LYS:H    | 6        | 0.92          |
| (1,1940) | 1:135:A:VAL:HG11 | 1:155:A:ASN:HD21 | 10       | 0.91          |
| (1,1940) | 1:135:A:VAL:HG11 | 1:155:A:ASN:HD22 | 10       | 0.91          |
| (1,1940) | 1:135:A:VAL:HG12 | 1:155:A:ASN:HD21 | 10       | 0.91          |
| (1,1940) | 1:135:A:VAL:HG12 | 1:155:A:ASN:HD22 | 10       | 0.91          |
| (1,1940) | 1:135:A:VAL:HG13 | 1:155:A:ASN:HD21 | 10       | 0.91          |
| (1,1940) | 1:135:A:VAL:HG13 | 1:155:A:ASN:HD22 | 10       | 0.91          |
| (1,1940) | 1:135:A:VAL:HG11 | 1:155:A:ASN:HD21 | 5        | 0.9           |
| (1,1940) | 1:135:A:VAL:HG11 | 1:155:A:ASN:HD22 | 5        | 0.9           |
| (1,1940) | 1:135:A:VAL:HG12 | 1:155:A:ASN:HD21 | 5        | 0.9           |
| (1,1940) | 1:135:A:VAL:HG12 | 1:155:A:ASN:HD22 | 5        | 0.9           |
| (1,1940) | 1:135:A:VAL:HG13 | 1:155:A:ASN:HD21 | 5        | 0.9           |
| (1,1940) | 1:135:A:VAL:HG13 | 1:155:A:ASN:HD22 | 5        | 0.9           |
| (2,733)  | 1:157:A:LYS:HE2  | 1:159:A:PHE:HD1  | 10       | 0.89          |
| (2,733)  | 1:157:A:LYS:HE2  | 1:159:A:PHE:HD2  | 10       | 0.89          |
| (2,733)  | 1:157:A:LYS:HE3  | 1:159:A:PHE:HD1  | 10       | 0.89          |
| (2,733)  | 1:157:A:LYS:HE3  | 1:159:A:PHE:HD2  | 10       | 0.89          |
| (2,469)  | 1:79:A:ILE:HG21  | 1:157:A:LYS:H    | 1        | 0.89          |
| (2,469)  | 1:79:A:ILE:HG22  | 1:157:A:LYS:H    | 1        | 0.89          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,469)  | 1:79:A:ILE:HG23  | 1:157:A:LYS:H    | 1        | 0.89          |
| (2,469)  | 1:79:A:ILE:HG21  | 1:157:A:LYS:H    | 9        | 0.89          |
| (2,469)  | 1:79:A:ILE:HG22  | 1:157:A:LYS:H    | 9        | 0.89          |
| (2,469)  | 1:79:A:ILE:HG23  | 1:157:A:LYS:H    | 9        | 0.89          |
| (1,1940) | 1:135:A:VAL:HG11 | 1:155:A:ASN:HD21 | 1        | 0.89          |
| (1,1940) | 1:135:A:VAL:HG11 | 1:155:A:ASN:HD22 | 1        | 0.89          |
| (1,1940) | 1:135:A:VAL:HG12 | 1:155:A:ASN:HD21 | 1        | 0.89          |
| (1,1940) | 1:135:A:VAL:HG12 | 1:155:A:ASN:HD22 | 1        | 0.89          |
| (1,1940) | 1:135:A:VAL:HG13 | 1:155:A:ASN:HD21 | 1        | 0.89          |
| (1,1940) | 1:135:A:VAL:HG13 | 1:155:A:ASN:HD22 | 1        | 0.89          |
| (2,469)  | 1:79:A:ILE:HG21  | 1:157:A:LYS:H    | 2        | 0.88          |
| (2,469)  | 1:79:A:ILE:HG22  | 1:157:A:LYS:H    | 2        | 0.88          |
| (2,469)  | 1:79:A:ILE:HG23  | 1:157:A:LYS:H    | 2        | 0.88          |
| (2,469)  | 1:79:A:ILE:HG21  | 1:157:A:LYS:H    | 4        | 0.88          |
| (2,469)  | 1:79:A:ILE:HG22  | 1:157:A:LYS:H    | 4        | 0.88          |
| (2,469)  | 1:79:A:ILE:HG23  | 1:157:A:LYS:H    | 4        | 0.88          |
| (2,469)  | 1:79:A:ILE:HG21  | 1:157:A:LYS:H    | 5        | 0.88          |
| (2,469)  | 1:79:A:ILE:HG22  | 1:157:A:LYS:H    | 5        | 0.88          |
| (2,469)  | 1:79:A:ILE:HG23  | 1:157:A:LYS:H    | 5        | 0.88          |
| (1,1940) | 1:135:A:VAL:HG11 | 1:155:A:ASN:HD21 | 8        | 0.88          |
| (1,1940) | 1:135:A:VAL:HG11 | 1:155:A:ASN:HD22 | 8        | 0.88          |
| (1,1940) | 1:135:A:VAL:HG12 | 1:155:A:ASN:HD21 | 8        | 0.88          |
| (1,1940) | 1:135:A:VAL:HG12 | 1:155:A:ASN:HD22 | 8        | 0.88          |
| (1,1940) | 1:135:A:VAL:HG13 | 1:155:A:ASN:HD21 | 8        | 0.88          |
| (1,1940) | 1:135:A:VAL:HG13 | 1:155:A:ASN:HD22 | 8        | 0.88          |
| (1,1030) | 1:74:A:PHE:HE1   | 1:162:A:ALA:HB1  | 8        | 0.88          |
| (1,1030) | 1:74:A:PHE:HE1   | 1:162:A:ALA:HB2  | 8        | 0.88          |
| (1,1030) | 1:74:A:PHE:HE1   | 1:162:A:ALA:HB3  | 8        | 0.88          |
| (1,1030) | 1:74:A:PHE:HE2   | 1:162:A:ALA:HB1  | 8        | 0.88          |
| (1,1030) | 1:74:A:PHE:HE2   | 1:162:A:ALA:HB2  | 8        | 0.88          |
| (1,1030) | 1:74:A:PHE:HE2   | 1:162:A:ALA:HB3  | 8        | 0.88          |
| (2,469)  | 1:79:A:ILE:HG21  | 1:157:A:LYS:H    | 7        | 0.87          |
| (2,469)  | 1:79:A:ILE:HG22  | 1:157:A:LYS:H    | 7        | 0.87          |
| (2,469)  | 1:79:A:ILE:HG23  | 1:157:A:LYS:H    | 7        | 0.87          |
| (2,466)  | 1:79:A:ILE:HG21  | 1:102:A:ILE:H    | 4        | 0.87          |
| (2,466)  | 1:79:A:ILE:HG22  | 1:102:A:ILE:H    | 4        | 0.87          |
| (2,466)  | 1:79:A:ILE:HG23  | 1:102:A:ILE:H    | 4        | 0.87          |
| (2,466)  | 1:79:A:ILE:HG21  | 1:102:A:ILE:H    | 9        | 0.87          |
| (2,466)  | 1:79:A:ILE:HG22  | 1:102:A:ILE:H    | 9        | 0.87          |
| (2,466)  | 1:79:A:ILE:HG23  | 1:102:A:ILE:H    | 9        | 0.87          |
| (1,1940) | 1:135:A:VAL:HG11 | 1:155:A:ASN:HD21 | 3        | 0.87          |
| (1,1940) | 1:135:A:VAL:HG11 | 1:155:A:ASN:HD22 | 3        | 0.87          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1940) | 1:135:A:VAL:HG12 | 1:155:A:ASN:HD21 | 3        | 0.87          |
| (1,1940) | 1:135:A:VAL:HG12 | 1:155:A:ASN:HD22 | 3        | 0.87          |
| (1,1940) | 1:135:A:VAL:HG13 | 1:155:A:ASN:HD21 | 3        | 0.87          |
| (1,1940) | 1:135:A:VAL:HG13 | 1:155:A:ASN:HD22 | 3        | 0.87          |
| (1,1940) | 1:135:A:VAL:HG11 | 1:155:A:ASN:HD21 | 4        | 0.87          |
| (1,1940) | 1:135:A:VAL:HG11 | 1:155:A:ASN:HD22 | 4        | 0.87          |
| (1,1940) | 1:135:A:VAL:HG12 | 1:155:A:ASN:HD21 | 4        | 0.87          |
| (1,1940) | 1:135:A:VAL:HG12 | 1:155:A:ASN:HD22 | 4        | 0.87          |
| (1,1940) | 1:135:A:VAL:HG13 | 1:155:A:ASN:HD21 | 4        | 0.87          |
| (1,1940) | 1:135:A:VAL:HG13 | 1:155:A:ASN:HD22 | 4        | 0.87          |
| (1,579)  | 1:51:A:ILE:HG21  | 1:53:A:ASP:HB2   | 4        | 0.87          |
| (1,579)  | 1:51:A:ILE:HG21  | 1:53:A:ASP:HB3   | 4        | 0.87          |
| (1,579)  | 1:51:A:ILE:HG22  | 1:53:A:ASP:HB2   | 4        | 0.87          |
| (1,579)  | 1:51:A:ILE:HG22  | 1:53:A:ASP:HB3   | 4        | 0.87          |
| (1,579)  | 1:51:A:ILE:HG23  | 1:53:A:ASP:HB2   | 4        | 0.87          |
| (1,579)  | 1:51:A:ILE:HG23  | 1:53:A:ASP:HB3   | 4        | 0.87          |
| (2,469)  | 1:79:A:ILE:HG21  | 1:157:A:LYS:H    | 3        | 0.86          |
| (2,469)  | 1:79:A:ILE:HG22  | 1:157:A:LYS:H    | 3        | 0.86          |
| (2,469)  | 1:79:A:ILE:HG23  | 1:157:A:LYS:H    | 3        | 0.86          |
| (1,1940) | 1:135:A:VAL:HG11 | 1:155:A:ASN:HD21 | 7        | 0.86          |
| (1,1940) | 1:135:A:VAL:HG11 | 1:155:A:ASN:HD22 | 7        | 0.86          |
| (1,1940) | 1:135:A:VAL:HG12 | 1:155:A:ASN:HD21 | 7        | 0.86          |
| (1,1940) | 1:135:A:VAL:HG12 | 1:155:A:ASN:HD22 | 7        | 0.86          |
| (1,1940) | 1:135:A:VAL:HG13 | 1:155:A:ASN:HD21 | 7        | 0.86          |
| (1,1940) | 1:135:A:VAL:HG13 | 1:155:A:ASN:HD22 | 7        | 0.86          |
| (2,469)  | 1:79:A:ILE:HG21  | 1:157:A:LYS:H    | 8        | 0.85          |
| (2,469)  | 1:79:A:ILE:HG22  | 1:157:A:LYS:H    | 8        | 0.85          |
| (2,469)  | 1:79:A:ILE:HG23  | 1:157:A:LYS:H    | 8        | 0.85          |
| (2,469)  | 1:79:A:ILE:HG21  | 1:157:A:LYS:H    | 10       | 0.85          |
| (2,469)  | 1:79:A:ILE:HG22  | 1:157:A:LYS:H    | 10       | 0.85          |
| (2,469)  | 1:79:A:ILE:HG23  | 1:157:A:LYS:H    | 10       | 0.85          |
| (1,288)  | 1:36:A:ALA:HB1   | 1:37:A:GLY:H     | 10       | 0.85          |
| (1,288)  | 1:36:A:ALA:HB2   | 1:37:A:GLY:H     | 10       | 0.85          |
| (1,288)  | 1:36:A:ALA:HB3   | 1:37:A:GLY:H     | 10       | 0.85          |
| (2,517)  | 1:84:A:GLY:HA2   | 1:85:A:TYR:HD1   | 8        | 0.84          |
| (2,517)  | 1:84:A:GLY:HA2   | 1:85:A:TYR:HD2   | 8        | 0.84          |
| (2,517)  | 1:84:A:GLY:HA3   | 1:85:A:TYR:HD1   | 8        | 0.84          |
| (2,517)  | 1:84:A:GLY:HA3   | 1:85:A:TYR:HD2   | 8        | 0.84          |
| (2,466)  | 1:79:A:ILE:HG21  | 1:102:A:ILE:H    | 1        | 0.84          |
| (2,466)  | 1:79:A:ILE:HG22  | 1:102:A:ILE:H    | 1        | 0.84          |
| (2,466)  | 1:79:A:ILE:HG23  | 1:102:A:ILE:H    | 1        | 0.84          |
| (2,466)  | 1:79:A:ILE:HG21  | 1:102:A:ILE:H    | 7        | 0.84          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,466)  | 1:79:A:ILE:HG22  | 1:102:A:ILE:H    | 7        | 0.84          |
| (2,466)  | 1:79:A:ILE:HG23  | 1:102:A:ILE:H    | 7        | 0.84          |
| (1,288)  | 1:36:A:ALA:HB1   | 1:37:A:GLY:H     | 3        | 0.84          |
| (1,288)  | 1:36:A:ALA:HB2   | 1:37:A:GLY:H     | 3        | 0.84          |
| (1,288)  | 1:36:A:ALA:HB3   | 1:37:A:GLY:H     | 3        | 0.84          |
| (1,288)  | 1:36:A:ALA:HB1   | 1:37:A:GLY:H     | 9        | 0.84          |
| (1,288)  | 1:36:A:ALA:HB2   | 1:37:A:GLY:H     | 9        | 0.84          |
| (1,288)  | 1:36:A:ALA:HB3   | 1:37:A:GLY:H     | 9        | 0.84          |
| (1,1030) | 1:74:A:PHE:HE1   | 1:162:A:ALA:HB1  | 10       | 0.83          |
| (1,1030) | 1:74:A:PHE:HE1   | 1:162:A:ALA:HB2  | 10       | 0.83          |
| (1,1030) | 1:74:A:PHE:HE1   | 1:162:A:ALA:HB3  | 10       | 0.83          |
| (1,1030) | 1:74:A:PHE:HE2   | 1:162:A:ALA:HB1  | 10       | 0.83          |
| (1,1030) | 1:74:A:PHE:HE2   | 1:162:A:ALA:HB2  | 10       | 0.83          |
| (1,1030) | 1:74:A:PHE:HE2   | 1:162:A:ALA:HB3  | 10       | 0.83          |
| (2,719)  | 1:142:A:ILE:HG21 | 1:145:A:TYR:HA   | 4        | 0.82          |
| (2,719)  | 1:142:A:ILE:HG22 | 1:145:A:TYR:HA   | 4        | 0.82          |
| (2,719)  | 1:142:A:ILE:HG23 | 1:145:A:TYR:HA   | 4        | 0.82          |
| (2,466)  | 1:79:A:ILE:HG21  | 1:102:A:ILE:H    | 8        | 0.82          |
| (2,466)  | 1:79:A:ILE:HG22  | 1:102:A:ILE:H    | 8        | 0.82          |
| (2,466)  | 1:79:A:ILE:HG23  | 1:102:A:ILE:H    | 8        | 0.82          |
| (1,1520) | 1:100:A:ALA:HB1  | 1:111:A:ILE:HG21 | 7        | 0.82          |
| (1,1520) | 1:100:A:ALA:HB1  | 1:111:A:ILE:HG22 | 7        | 0.82          |
| (1,1520) | 1:100:A:ALA:HB1  | 1:111:A:ILE:HG23 | 7        | 0.82          |
| (1,1520) | 1:100:A:ALA:HB2  | 1:111:A:ILE:HG21 | 7        | 0.82          |
| (1,1520) | 1:100:A:ALA:HB2  | 1:111:A:ILE:HG22 | 7        | 0.82          |
| (1,1520) | 1:100:A:ALA:HB2  | 1:111:A:ILE:HG23 | 7        | 0.82          |
| (1,1520) | 1:100:A:ALA:HB3  | 1:111:A:ILE:HG21 | 7        | 0.82          |
| (1,1520) | 1:100:A:ALA:HB3  | 1:111:A:ILE:HG22 | 7        | 0.82          |
| (1,1520) | 1:100:A:ALA:HB3  | 1:111:A:ILE:HG23 | 7        | 0.82          |
| (1,10)   | 1:19:A:VAL:HG11  | 1:19:A:VAL:H     | 10       | 0.82          |
| (1,10)   | 1:19:A:VAL:HG12  | 1:19:A:VAL:H     | 10       | 0.82          |
| (1,10)   | 1:19:A:VAL:HG13  | 1:19:A:VAL:H     | 10       | 0.82          |
| (1,10)   | 1:19:A:VAL:HG21  | 1:19:A:VAL:H     | 10       | 0.82          |
| (1,10)   | 1:19:A:VAL:HG22  | 1:19:A:VAL:H     | 10       | 0.82          |
| (1,10)   | 1:19:A:VAL:HG23  | 1:19:A:VAL:H     | 10       | 0.82          |
| (2,719)  | 1:142:A:ILE:HG21 | 1:145:A:TYR:HA   | 3        | 0.81          |
| (2,719)  | 1:142:A:ILE:HG22 | 1:145:A:TYR:HA   | 3        | 0.81          |
| (2,719)  | 1:142:A:ILE:HG23 | 1:145:A:TYR:HA   | 3        | 0.81          |
| (2,466)  | 1:79:A:ILE:HG21  | 1:102:A:ILE:H    | 2        | 0.81          |
| (2,466)  | 1:79:A:ILE:HG22  | 1:102:A:ILE:H    | 2        | 0.81          |
| (2,466)  | 1:79:A:ILE:HG23  | 1:102:A:ILE:H    | 2        | 0.81          |
| (2,466)  | 1:79:A:ILE:HG21  | 1:102:A:ILE:H    | 5        | 0.81          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,466)  | 1:79:A:ILE:HG22 | 1:102:A:ILE:H    | 5        | 0.81          |
| (2,466)  | 1:79:A:ILE:HG23 | 1:102:A:ILE:H    | 5        | 0.81          |
| (1,1520) | 1:100:A:ALA:HB1 | 1:111:A:ILE:HG21 | 6        | 0.81          |
| (1,1520) | 1:100:A:ALA:HB1 | 1:111:A:ILE:HG22 | 6        | 0.81          |
| (1,1520) | 1:100:A:ALA:HB1 | 1:111:A:ILE:HG23 | 6        | 0.81          |
| (1,1520) | 1:100:A:ALA:HB2 | 1:111:A:ILE:HG21 | 6        | 0.81          |
| (1,1520) | 1:100:A:ALA:HB2 | 1:111:A:ILE:HG22 | 6        | 0.81          |
| (1,1520) | 1:100:A:ALA:HB2 | 1:111:A:ILE:HG23 | 6        | 0.81          |
| (1,1520) | 1:100:A:ALA:HB3 | 1:111:A:ILE:HG21 | 6        | 0.81          |
| (1,1520) | 1:100:A:ALA:HB3 | 1:111:A:ILE:HG22 | 6        | 0.81          |
| (1,1520) | 1:100:A:ALA:HB3 | 1:111:A:ILE:HG23 | 6        | 0.81          |
| (1,288)  | 1:36:A:ALA:HB1  | 1:37:A:GLY:H     | 2        | 0.81          |
| (1,288)  | 1:36:A:ALA:HB2  | 1:37:A:GLY:H     | 2        | 0.81          |
| (1,288)  | 1:36:A:ALA:HB3  | 1:37:A:GLY:H     | 2        | 0.81          |
| (1,206)  | 1:32:A:ILE:HA   | 1:32:A:ILE:HD11  | 8        | 0.81          |
| (1,206)  | 1:32:A:ILE:HA   | 1:32:A:ILE:HD12  | 8        | 0.81          |
| (1,206)  | 1:32:A:ILE:HA   | 1:32:A:ILE:HD13  | 8        | 0.81          |
| (2,518)  | 1:84:A:GLY:HA2  | 1:95:A:PHE:HE1   | 10       | 0.8           |
| (2,518)  | 1:84:A:GLY:HA2  | 1:95:A:PHE:HE2   | 10       | 0.8           |
| (2,518)  | 1:84:A:GLY:HA3  | 1:95:A:PHE:HE1   | 10       | 0.8           |
| (2,518)  | 1:84:A:GLY:HA3  | 1:95:A:PHE:HE2   | 10       | 0.8           |
| (2,467)  | 1:79:A:ILE:HG21 | 1:156:A:PHE:HA   | 1        | 0.8           |
| (2,467)  | 1:79:A:ILE:HG22 | 1:156:A:PHE:HA   | 1        | 0.8           |
| (2,467)  | 1:79:A:ILE:HG23 | 1:156:A:PHE:HA   | 1        | 0.8           |
| (2,386)  | 1:70:A:LEU:HD11 | 1:172:A:PRO:HD2  | 9        | 0.8           |
| (2,386)  | 1:70:A:LEU:HD12 | 1:172:A:PRO:HD2  | 9        | 0.8           |
| (2,386)  | 1:70:A:LEU:HD13 | 1:172:A:PRO:HD2  | 9        | 0.8           |
| (2,6)    | 1:16:A:ALA:HB1  | 1:17:A:GLN:H     | 1        | 0.8           |
| (2,6)    | 1:16:A:ALA:HB2  | 1:17:A:GLN:H     | 1        | 0.8           |
| (2,6)    | 1:16:A:ALA:HB3  | 1:17:A:GLN:H     | 1        | 0.8           |
| (2,6)    | 1:16:A:ALA:HB1  | 1:17:A:GLN:H     | 2        | 0.8           |
| (2,6)    | 1:16:A:ALA:HB2  | 1:17:A:GLN:H     | 2        | 0.8           |
| (2,6)    | 1:16:A:ALA:HB3  | 1:17:A:GLN:H     | 2        | 0.8           |
| (2,6)    | 1:16:A:ALA:HB1  | 1:17:A:GLN:H     | 3        | 0.8           |
| (2,6)    | 1:16:A:ALA:HB2  | 1:17:A:GLN:H     | 3        | 0.8           |
| (2,6)    | 1:16:A:ALA:HB3  | 1:17:A:GLN:H     | 3        | 0.8           |
| (2,6)    | 1:16:A:ALA:HB1  | 1:17:A:GLN:H     | 5        | 0.8           |
| (2,6)    | 1:16:A:ALA:HB2  | 1:17:A:GLN:H     | 5        | 0.8           |
| (2,6)    | 1:16:A:ALA:HB3  | 1:17:A:GLN:H     | 5        | 0.8           |
| (2,6)    | 1:16:A:ALA:HB1  | 1:17:A:GLN:H     | 6        | 0.8           |
| (2,6)    | 1:16:A:ALA:HB2  | 1:17:A:GLN:H     | 6        | 0.8           |
| (2,6)    | 1:16:A:ALA:HB3  | 1:17:A:GLN:H     | 6        | 0.8           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,6)    | 1:16:A:ALA:HB1  | 1:17:A:GLN:H    | 7        | 0.8           |
| (2,6)    | 1:16:A:ALA:HB2  | 1:17:A:GLN:H    | 7        | 0.8           |
| (2,6)    | 1:16:A:ALA:HB3  | 1:17:A:GLN:H    | 7        | 0.8           |
| (2,6)    | 1:16:A:ALA:HB1  | 1:17:A:GLN:H    | 8        | 0.8           |
| (2,6)    | 1:16:A:ALA:HB2  | 1:17:A:GLN:H    | 8        | 0.8           |
| (2,6)    | 1:16:A:ALA:HB3  | 1:17:A:GLN:H    | 8        | 0.8           |
| (2,6)    | 1:16:A:ALA:HB1  | 1:17:A:GLN:H    | 10       | 0.8           |
| (2,6)    | 1:16:A:ALA:HB2  | 1:17:A:GLN:H    | 10       | 0.8           |
| (2,6)    | 1:16:A:ALA:HB3  | 1:17:A:GLN:H    | 10       | 0.8           |
| (1,1241) | 1:81:A:ILE:HG21 | 1:156:A:PHE:HD1 | 1        | 0.8           |
| (1,1241) | 1:81:A:ILE:HG21 | 1:156:A:PHE:HD2 | 1        | 0.8           |
| (1,1241) | 1:81:A:ILE:HG22 | 1:156:A:PHE:HD1 | 1        | 0.8           |
| (1,1241) | 1:81:A:ILE:HG22 | 1:156:A:PHE:HD2 | 1        | 0.8           |
| (1,1241) | 1:81:A:ILE:HG23 | 1:156:A:PHE:HD1 | 1        | 0.8           |
| (1,1241) | 1:81:A:ILE:HG23 | 1:156:A:PHE:HD2 | 1        | 0.8           |
| (1,1215) | 1:81:A:ILE:HD11 | 1:100:A:ALA:HB1 | 2        | 0.8           |
| (1,1215) | 1:81:A:ILE:HD11 | 1:100:A:ALA:HB2 | 2        | 0.8           |
| (1,1215) | 1:81:A:ILE:HD11 | 1:100:A:ALA:HB3 | 2        | 0.8           |
| (1,1215) | 1:81:A:ILE:HD12 | 1:100:A:ALA:HB1 | 2        | 0.8           |
| (1,1215) | 1:81:A:ILE:HD12 | 1:100:A:ALA:HB2 | 2        | 0.8           |
| (1,1215) | 1:81:A:ILE:HD12 | 1:100:A:ALA:HB3 | 2        | 0.8           |
| (1,1215) | 1:81:A:ILE:HD13 | 1:100:A:ALA:HB1 | 2        | 0.8           |
| (1,1215) | 1:81:A:ILE:HD13 | 1:100:A:ALA:HB2 | 2        | 0.8           |
| (1,1215) | 1:81:A:ILE:HD13 | 1:100:A:ALA:HB3 | 2        | 0.8           |
| (1,489)  | 1:48:A:ILE:HG21 | 1:48:A:ILE:HD11 | 5        | 0.8           |
| (1,489)  | 1:48:A:ILE:HG21 | 1:48:A:ILE:HD12 | 5        | 0.8           |
| (1,489)  | 1:48:A:ILE:HG21 | 1:48:A:ILE:HD13 | 5        | 0.8           |
| (1,489)  | 1:48:A:ILE:HG22 | 1:48:A:ILE:HD11 | 5        | 0.8           |
| (1,489)  | 1:48:A:ILE:HG22 | 1:48:A:ILE:HD12 | 5        | 0.8           |
| (1,489)  | 1:48:A:ILE:HG22 | 1:48:A:ILE:HD13 | 5        | 0.8           |
| (1,489)  | 1:48:A:ILE:HG23 | 1:48:A:ILE:HD11 | 5        | 0.8           |
| (1,489)  | 1:48:A:ILE:HG23 | 1:48:A:ILE:HD12 | 5        | 0.8           |
| (1,489)  | 1:48:A:ILE:HG23 | 1:48:A:ILE:HD13 | 5        | 0.8           |
| (1,223)  | 1:32:A:ILE:HD11 | 1:160:A:TYR:HE1 | 6        | 0.8           |
| (1,223)  | 1:32:A:ILE:HD11 | 1:160:A:TYR:HE2 | 6        | 0.8           |
| (1,223)  | 1:32:A:ILE:HD12 | 1:160:A:TYR:HE1 | 6        | 0.8           |
| (1,223)  | 1:32:A:ILE:HD12 | 1:160:A:TYR:HE2 | 6        | 0.8           |
| (1,223)  | 1:32:A:ILE:HD13 | 1:160:A:TYR:HE1 | 6        | 0.8           |
| (1,223)  | 1:32:A:ILE:HD13 | 1:160:A:TYR:HE2 | 6        | 0.8           |
| (1,10)   | 1:19:A:VAL:HG11 | 1:19:A:VAL:H    | 2        | 0.8           |
| (1,10)   | 1:19:A:VAL:HG12 | 1:19:A:VAL:H    | 2        | 0.8           |
| (1,10)   | 1:19:A:VAL:HG13 | 1:19:A:VAL:H    | 2        | 0.8           |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,10)  | 1:19:A:VAL:HG21  | 1:19:A:VAL:H    | 2        | 0.8           |
| (1,10)  | 1:19:A:VAL:HG22  | 1:19:A:VAL:H    | 2        | 0.8           |
| (1,10)  | 1:19:A:VAL:HG23  | 1:19:A:VAL:H    | 2        | 0.8           |
| (2,719) | 1:142:A:ILE:HG21 | 1:145:A:TYR:HA  | 10       | 0.79          |
| (2,719) | 1:142:A:ILE:HG22 | 1:145:A:TYR:HA  | 10       | 0.79          |
| (2,719) | 1:142:A:ILE:HG23 | 1:145:A:TYR:HA  | 10       | 0.79          |
| (2,466) | 1:79:A:ILE:HG21  | 1:102:A:ILE:H   | 10       | 0.79          |
| (2,466) | 1:79:A:ILE:HG22  | 1:102:A:ILE:H   | 10       | 0.79          |
| (2,466) | 1:79:A:ILE:HG23  | 1:102:A:ILE:H   | 10       | 0.79          |
| (2,6)   | 1:16:A:ALA:HB1   | 1:17:A:GLN:H    | 4        | 0.79          |
| (2,6)   | 1:16:A:ALA:HB2   | 1:17:A:GLN:H    | 4        | 0.79          |
| (2,6)   | 1:16:A:ALA:HB3   | 1:17:A:GLN:H    | 4        | 0.79          |
| (2,4)   | 1:15:A:THR:HG21  | 1:16:A:ALA:H    | 9        | 0.79          |
| (2,4)   | 1:15:A:THR:HG22  | 1:16:A:ALA:H    | 9        | 0.79          |
| (2,4)   | 1:15:A:THR:HG23  | 1:16:A:ALA:H    | 9        | 0.79          |
| (1,579) | 1:51:A:ILE:HG21  | 1:53:A:ASP:HB2  | 6        | 0.79          |
| (1,579) | 1:51:A:ILE:HG21  | 1:53:A:ASP:HB3  | 6        | 0.79          |
| (1,579) | 1:51:A:ILE:HG22  | 1:53:A:ASP:HB2  | 6        | 0.79          |
| (1,579) | 1:51:A:ILE:HG22  | 1:53:A:ASP:HB3  | 6        | 0.79          |
| (1,579) | 1:51:A:ILE:HG23  | 1:53:A:ASP:HB2  | 6        | 0.79          |
| (1,579) | 1:51:A:ILE:HG23  | 1:53:A:ASP:HB3  | 6        | 0.79          |
| (1,489) | 1:48:A:ILE:HG21  | 1:48:A:ILE:HD11 | 10       | 0.79          |
| (1,489) | 1:48:A:ILE:HG21  | 1:48:A:ILE:HD12 | 10       | 0.79          |
| (1,489) | 1:48:A:ILE:HG21  | 1:48:A:ILE:HD13 | 10       | 0.79          |
| (1,489) | 1:48:A:ILE:HG22  | 1:48:A:ILE:HD11 | 10       | 0.79          |
| (1,489) | 1:48:A:ILE:HG22  | 1:48:A:ILE:HD12 | 10       | 0.79          |
| (1,489) | 1:48:A:ILE:HG22  | 1:48:A:ILE:HD13 | 10       | 0.79          |
| (1,489) | 1:48:A:ILE:HG23  | 1:48:A:ILE:HD11 | 10       | 0.79          |
| (1,489) | 1:48:A:ILE:HG23  | 1:48:A:ILE:HD12 | 10       | 0.79          |
| (1,489) | 1:48:A:ILE:HG23  | 1:48:A:ILE:HD13 | 10       | 0.79          |
| (1,288) | 1:36:A:ALA:HB1   | 1:37:A:GLY:H    | 4        | 0.79          |
| (1,288) | 1:36:A:ALA:HB2   | 1:37:A:GLY:H    | 4        | 0.79          |
| (1,288) | 1:36:A:ALA:HB3   | 1:37:A:GLY:H    | 4        | 0.79          |
| (2,719) | 1:142:A:ILE:HG21 | 1:145:A:TYR:HA  | 7        | 0.78          |
| (2,719) | 1:142:A:ILE:HG22 | 1:145:A:TYR:HA  | 7        | 0.78          |
| (2,719) | 1:142:A:ILE:HG23 | 1:145:A:TYR:HA  | 7        | 0.78          |
| (2,719) | 1:142:A:ILE:HG21 | 1:145:A:TYR:HA  | 8        | 0.78          |
| (2,719) | 1:142:A:ILE:HG22 | 1:145:A:TYR:HA  | 8        | 0.78          |
| (2,719) | 1:142:A:ILE:HG23 | 1:145:A:TYR:HA  | 8        | 0.78          |
| (2,518) | 1:84:A:GLY:HA2   | 1:95:A:PHE:HE1  | 8        | 0.78          |
| (2,518) | 1:84:A:GLY:HA2   | 1:95:A:PHE:HE2  | 8        | 0.78          |
| (2,518) | 1:84:A:GLY:HA3   | 1:95:A:PHE:HE1  | 8        | 0.78          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,518)  | 1:84:A:GLY:HA3  | 1:95:A:PHE:HE2   | 8        | 0.78          |
| (2,467)  | 1:79:A:ILE:HG21 | 1:156:A:PHE:HA   | 2        | 0.78          |
| (2,467)  | 1:79:A:ILE:HG22 | 1:156:A:PHE:HA   | 2        | 0.78          |
| (2,467)  | 1:79:A:ILE:HG23 | 1:156:A:PHE:HA   | 2        | 0.78          |
| (2,467)  | 1:79:A:ILE:HG21 | 1:156:A:PHE:HA   | 5        | 0.78          |
| (2,467)  | 1:79:A:ILE:HG22 | 1:156:A:PHE:HA   | 5        | 0.78          |
| (2,467)  | 1:79:A:ILE:HG23 | 1:156:A:PHE:HA   | 5        | 0.78          |
| (2,467)  | 1:79:A:ILE:HG21 | 1:156:A:PHE:HA   | 9        | 0.78          |
| (2,467)  | 1:79:A:ILE:HG22 | 1:156:A:PHE:HA   | 9        | 0.78          |
| (2,467)  | 1:79:A:ILE:HG23 | 1:156:A:PHE:HA   | 9        | 0.78          |
| (2,466)  | 1:79:A:ILE:HG21 | 1:102:A:ILE:H    | 3        | 0.78          |
| (2,466)  | 1:79:A:ILE:HG22 | 1:102:A:ILE:H    | 3        | 0.78          |
| (2,466)  | 1:79:A:ILE:HG23 | 1:102:A:ILE:H    | 3        | 0.78          |
| (2,365)  | 1:66:A:ASN:HB3  | 1:173:A:VAL:HG21 | 3        | 0.78          |
| (2,365)  | 1:66:A:ASN:HB3  | 1:173:A:VAL:HG22 | 3        | 0.78          |
| (2,365)  | 1:66:A:ASN:HB3  | 1:173:A:VAL:HG23 | 3        | 0.78          |
| (2,6)    | 1:16:A:ALA:HB1  | 1:17:A:GLN:H     | 9        | 0.78          |
| (2,6)    | 1:16:A:ALA:HB2  | 1:17:A:GLN:H     | 9        | 0.78          |
| (2,6)    | 1:16:A:ALA:HB3  | 1:17:A:GLN:H     | 9        | 0.78          |
| (1,1242) | 1:81:A:ILE:HG21 | 1:156:A:PHE:HE1  | 1        | 0.78          |
| (1,1242) | 1:81:A:ILE:HG21 | 1:156:A:PHE:HE2  | 1        | 0.78          |
| (1,1242) | 1:81:A:ILE:HG22 | 1:156:A:PHE:HE1  | 1        | 0.78          |
| (1,1242) | 1:81:A:ILE:HG22 | 1:156:A:PHE:HE2  | 1        | 0.78          |
| (1,1242) | 1:81:A:ILE:HG23 | 1:156:A:PHE:HE1  | 1        | 0.78          |
| (1,1242) | 1:81:A:ILE:HG23 | 1:156:A:PHE:HE2  | 1        | 0.78          |
| (1,489)  | 1:48:A:ILE:HG21 | 1:48:A:ILE:HD11  | 6        | 0.78          |
| (1,489)  | 1:48:A:ILE:HG21 | 1:48:A:ILE:HD12  | 6        | 0.78          |
| (1,489)  | 1:48:A:ILE:HG21 | 1:48:A:ILE:HD13  | 6        | 0.78          |
| (1,489)  | 1:48:A:ILE:HG22 | 1:48:A:ILE:HD11  | 6        | 0.78          |
| (1,489)  | 1:48:A:ILE:HG22 | 1:48:A:ILE:HD12  | 6        | 0.78          |
| (1,489)  | 1:48:A:ILE:HG22 | 1:48:A:ILE:HD13  | 6        | 0.78          |
| (1,489)  | 1:48:A:ILE:HG23 | 1:48:A:ILE:HD11  | 6        | 0.78          |
| (1,489)  | 1:48:A:ILE:HG23 | 1:48:A:ILE:HD12  | 6        | 0.78          |
| (1,489)  | 1:48:A:ILE:HG23 | 1:48:A:ILE:HD13  | 6        | 0.78          |
| (1,261)  | 1:33:A:THR:HG21 | 1:34:A:PRO:HD2   | 3        | 0.78          |
| (1,261)  | 1:33:A:THR:HG22 | 1:34:A:PRO:HD2   | 3        | 0.78          |
| (1,261)  | 1:33:A:THR:HG23 | 1:34:A:PRO:HD2   | 3        | 0.78          |
| (1,206)  | 1:32:A:ILE:HA   | 1:32:A:ILE:HD11  | 2        | 0.78          |
| (1,206)  | 1:32:A:ILE:HA   | 1:32:A:ILE:HD12  | 2        | 0.78          |
| (1,206)  | 1:32:A:ILE:HA   | 1:32:A:ILE:HD13  | 2        | 0.78          |
| (1,10)   | 1:19:A:VAL:HG11 | 1:19:A:VAL:H     | 6        | 0.78          |
| (1,10)   | 1:19:A:VAL:HG12 | 1:19:A:VAL:H     | 6        | 0.78          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,10)  | 1:19:A:VAL:HG13  | 1:19:A:VAL:H     | 6        | 0.78          |
| (1,10)  | 1:19:A:VAL:HG21  | 1:19:A:VAL:H     | 6        | 0.78          |
| (1,10)  | 1:19:A:VAL:HG22  | 1:19:A:VAL:H     | 6        | 0.78          |
| (1,10)  | 1:19:A:VAL:HG23  | 1:19:A:VAL:H     | 6        | 0.78          |
| (2,719) | 1:142:A:ILE:HG21 | 1:145:A:TYR:HA   | 1        | 0.77          |
| (2,719) | 1:142:A:ILE:HG22 | 1:145:A:TYR:HA   | 1        | 0.77          |
| (2,719) | 1:142:A:ILE:HG23 | 1:145:A:TYR:HA   | 1        | 0.77          |
| (2,719) | 1:142:A:ILE:HG21 | 1:145:A:TYR:HA   | 2        | 0.77          |
| (2,719) | 1:142:A:ILE:HG22 | 1:145:A:TYR:HA   | 2        | 0.77          |
| (2,719) | 1:142:A:ILE:HG23 | 1:145:A:TYR:HA   | 2        | 0.77          |
| (2,490) | 1:81:A:ILE:HD11  | 1:101:A:VAL:H    | 2        | 0.77          |
| (2,490) | 1:81:A:ILE:HD12  | 1:101:A:VAL:H    | 2        | 0.77          |
| (2,490) | 1:81:A:ILE:HD13  | 1:101:A:VAL:H    | 2        | 0.77          |
| (2,466) | 1:79:A:ILE:HG21  | 1:102:A:ILE:H    | 6        | 0.77          |
| (2,466) | 1:79:A:ILE:HG22  | 1:102:A:ILE:H    | 6        | 0.77          |
| (2,466) | 1:79:A:ILE:HG23  | 1:102:A:ILE:H    | 6        | 0.77          |
| (2,389) | 1:70:A:LEU:HD21  | 1:172:A:PRO:HD2  | 2        | 0.77          |
| (2,389) | 1:70:A:LEU:HD22  | 1:172:A:PRO:HD2  | 2        | 0.77          |
| (2,389) | 1:70:A:LEU:HD23  | 1:172:A:PRO:HD2  | 2        | 0.77          |
| (2,389) | 1:70:A:LEU:HD21  | 1:172:A:PRO:HD2  | 3        | 0.77          |
| (2,389) | 1:70:A:LEU:HD22  | 1:172:A:PRO:HD2  | 3        | 0.77          |
| (2,389) | 1:70:A:LEU:HD23  | 1:172:A:PRO:HD2  | 3        | 0.77          |
| (2,365) | 1:66:A:ASN:HB3   | 1:173:A:VAL:HG21 | 10       | 0.77          |
| (2,365) | 1:66:A:ASN:HB3   | 1:173:A:VAL:HG22 | 10       | 0.77          |
| (2,365) | 1:66:A:ASN:HB3   | 1:173:A:VAL:HG23 | 10       | 0.77          |
| (2,4)   | 1:15:A:THR:HG21  | 1:16:A:ALA:H     | 6        | 0.77          |
| (2,4)   | 1:15:A:THR:HG22  | 1:16:A:ALA:H     | 6        | 0.77          |
| (2,4)   | 1:15:A:THR:HG23  | 1:16:A:ALA:H     | 6        | 0.77          |
| (2,4)   | 1:15:A:THR:HG21  | 1:16:A:ALA:H     | 8        | 0.77          |
| (2,4)   | 1:15:A:THR:HG22  | 1:16:A:ALA:H     | 8        | 0.77          |
| (2,4)   | 1:15:A:THR:HG23  | 1:16:A:ALA:H     | 8        | 0.77          |
| (1,353) | 1:42:A:ASP:HB2   | 1:158:A:ALA:HB1  | 6        | 0.77          |
| (1,353) | 1:42:A:ASP:HB2   | 1:158:A:ALA:HB2  | 6        | 0.77          |
| (1,353) | 1:42:A:ASP:HB2   | 1:158:A:ALA:HB3  | 6        | 0.77          |
| (1,353) | 1:42:A:ASP:HB3   | 1:158:A:ALA:HB1  | 6        | 0.77          |
| (1,353) | 1:42:A:ASP:HB3   | 1:158:A:ALA:HB2  | 6        | 0.77          |
| (1,353) | 1:42:A:ASP:HB3   | 1:158:A:ALA:HB3  | 6        | 0.77          |
| (1,261) | 1:33:A:THR:HG21  | 1:34:A:PRO:HD2   | 6        | 0.77          |
| (1,261) | 1:33:A:THR:HG22  | 1:34:A:PRO:HD2   | 6        | 0.77          |
| (1,261) | 1:33:A:THR:HG23  | 1:34:A:PRO:HD2   | 6        | 0.77          |
| (1,206) | 1:32:A:ILE:HA    | 1:32:A:ILE:HD11  | 6        | 0.77          |
| (1,206) | 1:32:A:ILE:HA    | 1:32:A:ILE:HD12  | 6        | 0.77          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,206) | 1:32:A:ILE:HA    | 1:32:A:ILE:HD13  | 6        | 0.77          |
| (1,10)  | 1:19:A:VAL:HG11  | 1:19:A:VAL:H     | 1        | 0.77          |
| (1,10)  | 1:19:A:VAL:HG12  | 1:19:A:VAL:H     | 1        | 0.77          |
| (1,10)  | 1:19:A:VAL:HG13  | 1:19:A:VAL:H     | 1        | 0.77          |
| (1,10)  | 1:19:A:VAL:HG21  | 1:19:A:VAL:H     | 1        | 0.77          |
| (1,10)  | 1:19:A:VAL:HG22  | 1:19:A:VAL:H     | 1        | 0.77          |
| (1,10)  | 1:19:A:VAL:HG23  | 1:19:A:VAL:H     | 1        | 0.77          |
| (2,756) | 1:167:A:LEU:H    | 1:167:A:LEU:HD21 | 2        | 0.76          |
| (2,756) | 1:167:A:LEU:H    | 1:167:A:LEU:HD22 | 2        | 0.76          |
| (2,756) | 1:167:A:LEU:H    | 1:167:A:LEU:HD23 | 2        | 0.76          |
| (2,755) | 1:167:A:LEU:H    | 1:167:A:LEU:HD11 | 2        | 0.76          |
| (2,755) | 1:167:A:LEU:H    | 1:167:A:LEU:HD12 | 2        | 0.76          |
| (2,755) | 1:167:A:LEU:H    | 1:167:A:LEU:HD13 | 2        | 0.76          |
| (2,754) | 1:167:A:LEU:HD21 | 1:167:A:LEU:H    | 2        | 0.76          |
| (2,754) | 1:167:A:LEU:HD22 | 1:167:A:LEU:H    | 2        | 0.76          |
| (2,754) | 1:167:A:LEU:HD23 | 1:167:A:LEU:H    | 2        | 0.76          |
| (2,753) | 1:167:A:LEU:HD11 | 1:167:A:LEU:H    | 2        | 0.76          |
| (2,753) | 1:167:A:LEU:HD12 | 1:167:A:LEU:H    | 2        | 0.76          |
| (2,753) | 1:167:A:LEU:HD13 | 1:167:A:LEU:H    | 2        | 0.76          |
| (2,733) | 1:157:A:LYS:HE2  | 1:159:A:PHE:HD1  | 8        | 0.76          |
| (2,733) | 1:157:A:LYS:HE2  | 1:159:A:PHE:HD2  | 8        | 0.76          |
| (2,733) | 1:157:A:LYS:HE3  | 1:159:A:PHE:HD1  | 8        | 0.76          |
| (2,733) | 1:157:A:LYS:HE3  | 1:159:A:PHE:HD2  | 8        | 0.76          |
| (2,719) | 1:142:A:ILE:HG21 | 1:145:A:TYR:HA   | 6        | 0.76          |
| (2,719) | 1:142:A:ILE:HG22 | 1:145:A:TYR:HA   | 6        | 0.76          |
| (2,719) | 1:142:A:ILE:HG23 | 1:145:A:TYR:HA   | 6        | 0.76          |
| (2,517) | 1:84:A:GLY:HA2   | 1:85:A:TYR:HD1   | 2        | 0.76          |
| (2,517) | 1:84:A:GLY:HA2   | 1:85:A:TYR:HD2   | 2        | 0.76          |
| (2,517) | 1:84:A:GLY:HA3   | 1:85:A:TYR:HD1   | 2        | 0.76          |
| (2,517) | 1:84:A:GLY:HA3   | 1:85:A:TYR:HD2   | 2        | 0.76          |
| (2,467) | 1:79:A:ILE:HG21  | 1:156:A:PHE:HA   | 6        | 0.76          |
| (2,467) | 1:79:A:ILE:HG22  | 1:156:A:PHE:HA   | 6        | 0.76          |
| (2,467) | 1:79:A:ILE:HG23  | 1:156:A:PHE:HA   | 6        | 0.76          |
| (2,467) | 1:79:A:ILE:HG21  | 1:156:A:PHE:HA   | 7        | 0.76          |
| (2,467) | 1:79:A:ILE:HG22  | 1:156:A:PHE:HA   | 7        | 0.76          |
| (2,467) | 1:79:A:ILE:HG23  | 1:156:A:PHE:HA   | 7        | 0.76          |
| (2,389) | 1:70:A:LEU:HD21  | 1:172:A:PRO:HD2  | 4        | 0.76          |
| (2,389) | 1:70:A:LEU:HD22  | 1:172:A:PRO:HD2  | 4        | 0.76          |
| (2,389) | 1:70:A:LEU:HD23  | 1:172:A:PRO:HD2  | 4        | 0.76          |
| (2,389) | 1:70:A:LEU:HD21  | 1:172:A:PRO:HD2  | 10       | 0.76          |
| (2,389) | 1:70:A:LEU:HD22  | 1:172:A:PRO:HD2  | 10       | 0.76          |
| (2,389) | 1:70:A:LEU:HD23  | 1:172:A:PRO:HD2  | 10       | 0.76          |

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| Key     | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (2,365) | 1:66:A:ASN:HB3  | 1:173:A:VAL:HG21 | 5        | 0.76          |
| (2,365) | 1:66:A:ASN:HB3  | 1:173:A:VAL:HG22 | 5        | 0.76          |
| (2,365) | 1:66:A:ASN:HB3  | 1:173:A:VAL:HG23 | 5        | 0.76          |
| (2,365) | 1:66:A:ASN:HB3  | 1:173:A:VAL:HG21 | 7        | 0.76          |
| (2,365) | 1:66:A:ASN:HB3  | 1:173:A:VAL:HG22 | 7        | 0.76          |
| (2,365) | 1:66:A:ASN:HB3  | 1:173:A:VAL:HG23 | 7        | 0.76          |
| (2,7)   | 1:16:A:ALA:HB1  | 1:18:A:ALA:H     | 10       | 0.76          |
| (2,7)   | 1:16:A:ALA:HB2  | 1:18:A:ALA:H     | 10       | 0.76          |
| (2,7)   | 1:16:A:ALA:HB3  | 1:18:A:ALA:H     | 10       | 0.76          |
| (1,679) | 1:60:A:LEU:HD11 | 1:177:A:PHE:HD1  | 9        | 0.76          |
| (1,679) | 1:60:A:LEU:HD11 | 1:177:A:PHE:HD2  | 9        | 0.76          |
| (1,679) | 1:60:A:LEU:HD12 | 1:177:A:PHE:HD1  | 9        | 0.76          |
| (1,679) | 1:60:A:LEU:HD12 | 1:177:A:PHE:HD2  | 9        | 0.76          |
| (1,679) | 1:60:A:LEU:HD13 | 1:177:A:PHE:HD1  | 9        | 0.76          |
| (1,679) | 1:60:A:LEU:HD13 | 1:177:A:PHE:HD2  | 9        | 0.76          |
| (1,489) | 1:48:A:ILE:HG21 | 1:48:A:ILE:HD11  | 9        | 0.76          |
| (1,489) | 1:48:A:ILE:HG21 | 1:48:A:ILE:HD12  | 9        | 0.76          |
| (1,489) | 1:48:A:ILE:HG21 | 1:48:A:ILE:HD13  | 9        | 0.76          |
| (1,489) | 1:48:A:ILE:HG22 | 1:48:A:ILE:HD11  | 9        | 0.76          |
| (1,489) | 1:48:A:ILE:HG22 | 1:48:A:ILE:HD12  | 9        | 0.76          |
| (1,489) | 1:48:A:ILE:HG22 | 1:48:A:ILE:HD13  | 9        | 0.76          |
| (1,489) | 1:48:A:ILE:HG23 | 1:48:A:ILE:HD11  | 9        | 0.76          |
| (1,489) | 1:48:A:ILE:HG23 | 1:48:A:ILE:HD12  | 9        | 0.76          |
| (1,489) | 1:48:A:ILE:HG23 | 1:48:A:ILE:HD13  | 9        | 0.76          |
| (1,287) | 1:36:A:ALA:HB1  | 1:36:A:ALA:H     | 1        | 0.76          |
| (1,287) | 1:36:A:ALA:HB2  | 1:36:A:ALA:H     | 1        | 0.76          |
| (1,287) | 1:36:A:ALA:HB3  | 1:36:A:ALA:H     | 1        | 0.76          |
| (1,261) | 1:33:A:THR:HG21 | 1:34:A:PRO:HD2   | 1        | 0.76          |
| (1,261) | 1:33:A:THR:HG22 | 1:34:A:PRO:HD2   | 1        | 0.76          |
| (1,261) | 1:33:A:THR:HG23 | 1:34:A:PRO:HD2   | 1        | 0.76          |
| (1,261) | 1:33:A:THR:HG21 | 1:34:A:PRO:HD2   | 9        | 0.76          |
| (1,261) | 1:33:A:THR:HG22 | 1:34:A:PRO:HD2   | 9        | 0.76          |
| (1,261) | 1:33:A:THR:HG23 | 1:34:A:PRO:HD2   | 9        | 0.76          |
| (1,10)  | 1:19:A:VAL:HG11 | 1:19:A:VAL:H     | 3        | 0.76          |
| (1,10)  | 1:19:A:VAL:HG12 | 1:19:A:VAL:H     | 3        | 0.76          |
| (1,10)  | 1:19:A:VAL:HG13 | 1:19:A:VAL:H     | 3        | 0.76          |
| (1,10)  | 1:19:A:VAL:HG21 | 1:19:A:VAL:H     | 3        | 0.76          |
| (1,10)  | 1:19:A:VAL:HG22 | 1:19:A:VAL:H     | 3        | 0.76          |
| (1,10)  | 1:19:A:VAL:HG23 | 1:19:A:VAL:H     | 3        | 0.76          |
| (2,765) | 1:169:A:ASP:H   | 1:171:A:LEU:HD11 | 6        | 0.75          |
| (2,765) | 1:169:A:ASP:H   | 1:171:A:LEU:HD12 | 6        | 0.75          |
| (2,765) | 1:169:A:ASP:H   | 1:171:A:LEU:HD13 | 6        | 0.75          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (2,517)  | 1:84:A:GLY:HA2   | 1:85:A:TYR:HD1  | 6        | 0.75          |
| (2,517)  | 1:84:A:GLY:HA2   | 1:85:A:TYR:HD2  | 6        | 0.75          |
| (2,517)  | 1:84:A:GLY:HA3   | 1:85:A:TYR:HD1  | 6        | 0.75          |
| (2,517)  | 1:84:A:GLY:HA3   | 1:85:A:TYR:HD2  | 6        | 0.75          |
| (2,490)  | 1:81:A:ILE:HD11  | 1:101:A:VAL:H   | 7        | 0.75          |
| (2,490)  | 1:81:A:ILE:HD12  | 1:101:A:VAL:H   | 7        | 0.75          |
| (2,490)  | 1:81:A:ILE:HD13  | 1:101:A:VAL:H   | 7        | 0.75          |
| (2,194)  | 1:38:A:ALA:HB1   | 1:39:A:GLN:HE21 | 2        | 0.75          |
| (2,194)  | 1:38:A:ALA:HB2   | 1:39:A:GLN:HE21 | 2        | 0.75          |
| (2,194)  | 1:38:A:ALA:HB3   | 1:39:A:GLN:HE21 | 2        | 0.75          |
| (2,94)   | 1:23:A:ILE:HD11  | 1:53:A:ASP:H    | 7        | 0.75          |
| (2,94)   | 1:23:A:ILE:HD12  | 1:53:A:ASP:H    | 7        | 0.75          |
| (2,94)   | 1:23:A:ILE:HD13  | 1:53:A:ASP:H    | 7        | 0.75          |
| (2,5)    | 1:16:A:ALA:HB1   | 1:17:A:GLN:HE21 | 6        | 0.75          |
| (2,5)    | 1:16:A:ALA:HB2   | 1:17:A:GLN:HE21 | 6        | 0.75          |
| (2,5)    | 1:16:A:ALA:HB3   | 1:17:A:GLN:HE21 | 6        | 0.75          |
| (1,2357) | 1:173:A:VAL:HG21 | 1:175:A:PHE:HE1 | 2        | 0.75          |
| (1,2357) | 1:173:A:VAL:HG21 | 1:175:A:PHE:HE2 | 2        | 0.75          |
| (1,2357) | 1:173:A:VAL:HG22 | 1:175:A:PHE:HE1 | 2        | 0.75          |
| (1,2357) | 1:173:A:VAL:HG22 | 1:175:A:PHE:HE2 | 2        | 0.75          |
| (1,2357) | 1:173:A:VAL:HG23 | 1:175:A:PHE:HE1 | 2        | 0.75          |
| (1,2357) | 1:173:A:VAL:HG23 | 1:175:A:PHE:HE2 | 2        | 0.75          |
| (1,1457) | 1:92:A:LEU:HD11  | 1:93:A:GLY:H    | 8        | 0.75          |
| (1,1457) | 1:92:A:LEU:HD12  | 1:93:A:GLY:H    | 8        | 0.75          |
| (1,1457) | 1:92:A:LEU:HD13  | 1:93:A:GLY:H    | 8        | 0.75          |
| (1,679)  | 1:60:A:LEU:HD11  | 1:177:A:PHE:HD1 | 2        | 0.75          |
| (1,679)  | 1:60:A:LEU:HD11  | 1:177:A:PHE:HD2 | 2        | 0.75          |
| (1,679)  | 1:60:A:LEU:HD12  | 1:177:A:PHE:HD1 | 2        | 0.75          |
| (1,679)  | 1:60:A:LEU:HD12  | 1:177:A:PHE:HD2 | 2        | 0.75          |
| (1,679)  | 1:60:A:LEU:HD13  | 1:177:A:PHE:HD1 | 2        | 0.75          |
| (1,679)  | 1:60:A:LEU:HD13  | 1:177:A:PHE:HD2 | 2        | 0.75          |
| (1,679)  | 1:60:A:LEU:HD11  | 1:177:A:PHE:HD1 | 10       | 0.75          |
| (1,679)  | 1:60:A:LEU:HD11  | 1:177:A:PHE:HD2 | 10       | 0.75          |
| (1,679)  | 1:60:A:LEU:HD12  | 1:177:A:PHE:HD1 | 10       | 0.75          |
| (1,679)  | 1:60:A:LEU:HD12  | 1:177:A:PHE:HD2 | 10       | 0.75          |
| (1,679)  | 1:60:A:LEU:HD13  | 1:177:A:PHE:HD1 | 10       | 0.75          |
| (1,679)  | 1:60:A:LEU:HD13  | 1:177:A:PHE:HD2 | 10       | 0.75          |
| (1,6)    | 1:18:A:ALA:HB1   | 1:19:A:VAL:H    | 2        | 0.75          |
| (1,6)    | 1:18:A:ALA:HB2   | 1:19:A:VAL:H    | 2        | 0.75          |
| (1,6)    | 1:18:A:ALA:HB3   | 1:19:A:VAL:H    | 2        | 0.75          |
| (1,2357) | 1:173:A:VAL:HG21 | 1:175:A:PHE:HE1 | 5        | 0.74          |
| (1,2357) | 1:173:A:VAL:HG21 | 1:175:A:PHE:HE2 | 5        | 0.74          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2357) | 1:173:A:VAL:HG22 | 1:175:A:PHE:HE1  | 5        | 0.74          |
| (1,2357) | 1:173:A:VAL:HG22 | 1:175:A:PHE:HE2  | 5        | 0.74          |
| (1,2357) | 1:173:A:VAL:HG23 | 1:175:A:PHE:HE1  | 5        | 0.74          |
| (1,2357) | 1:173:A:VAL:HG23 | 1:175:A:PHE:HE2  | 5        | 0.74          |
| (1,2357) | 1:173:A:VAL:HG21 | 1:175:A:PHE:HE1  | 7        | 0.74          |
| (1,2357) | 1:173:A:VAL:HG21 | 1:175:A:PHE:HE2  | 7        | 0.74          |
| (1,2357) | 1:173:A:VAL:HG22 | 1:175:A:PHE:HE1  | 7        | 0.74          |
| (1,2357) | 1:173:A:VAL:HG22 | 1:175:A:PHE:HE2  | 7        | 0.74          |
| (1,2357) | 1:173:A:VAL:HG23 | 1:175:A:PHE:HE1  | 7        | 0.74          |
| (1,2357) | 1:173:A:VAL:HG23 | 1:175:A:PHE:HE2  | 7        | 0.74          |
| (1,2010) | 1:142:A:ILE:HD11 | 1:145:A:TYR:HD1  | 5        | 0.74          |
| (1,2010) | 1:142:A:ILE:HD11 | 1:145:A:TYR:HD2  | 5        | 0.74          |
| (1,2010) | 1:142:A:ILE:HD12 | 1:145:A:TYR:HD1  | 5        | 0.74          |
| (1,2010) | 1:142:A:ILE:HD12 | 1:145:A:TYR:HD2  | 5        | 0.74          |
| (1,2010) | 1:142:A:ILE:HD13 | 1:145:A:TYR:HD1  | 5        | 0.74          |
| (1,2010) | 1:142:A:ILE:HD13 | 1:145:A:TYR:HD2  | 5        | 0.74          |
| (1,1215) | 1:81:A:ILE:HD11  | 1:100:A:ALA:HB1  | 7        | 0.74          |
| (1,1215) | 1:81:A:ILE:HD11  | 1:100:A:ALA:HB2  | 7        | 0.74          |
| (1,1215) | 1:81:A:ILE:HD11  | 1:100:A:ALA:HB3  | 7        | 0.74          |
| (1,1215) | 1:81:A:ILE:HD12  | 1:100:A:ALA:HB1  | 7        | 0.74          |
| (1,1215) | 1:81:A:ILE:HD12  | 1:100:A:ALA:HB2  | 7        | 0.74          |
| (1,1215) | 1:81:A:ILE:HD12  | 1:100:A:ALA:HB3  | 7        | 0.74          |
| (1,1215) | 1:81:A:ILE:HD13  | 1:100:A:ALA:HB1  | 7        | 0.74          |
| (1,1215) | 1:81:A:ILE:HD13  | 1:100:A:ALA:HB2  | 7        | 0.74          |
| (1,1215) | 1:81:A:ILE:HD13  | 1:100:A:ALA:HB3  | 7        | 0.74          |
| (1,261)  | 1:33:A:THR:HG21  | 1:34:A:PRO:HD2   | 5        | 0.74          |
| (1,261)  | 1:33:A:THR:HG22  | 1:34:A:PRO:HD2   | 5        | 0.74          |
| (1,261)  | 1:33:A:THR:HG23  | 1:34:A:PRO:HD2   | 5        | 0.74          |
| (1,261)  | 1:33:A:THR:HG21  | 1:34:A:PRO:HD2   | 10       | 0.74          |
| (1,261)  | 1:33:A:THR:HG22  | 1:34:A:PRO:HD2   | 10       | 0.74          |
| (1,261)  | 1:33:A:THR:HG23  | 1:34:A:PRO:HD2   | 10       | 0.74          |
| (2,520)  | 1:84:A:GLY:HA2   | 1:155:A:ASN:HD21 | 1        | 0.73          |
| (2,520)  | 1:84:A:GLY:HA2   | 1:155:A:ASN:HD22 | 1        | 0.73          |
| (2,520)  | 1:84:A:GLY:HA3   | 1:155:A:ASN:HD21 | 1        | 0.73          |
| (2,520)  | 1:84:A:GLY:HA3   | 1:155:A:ASN:HD22 | 1        | 0.73          |
| (2,520)  | 1:84:A:GLY:HA2   | 1:155:A:ASN:HD21 | 4        | 0.73          |
| (2,520)  | 1:84:A:GLY:HA2   | 1:155:A:ASN:HD22 | 4        | 0.73          |
| (2,520)  | 1:84:A:GLY:HA3   | 1:155:A:ASN:HD21 | 4        | 0.73          |
| (2,520)  | 1:84:A:GLY:HA3   | 1:155:A:ASN:HD22 | 4        | 0.73          |
| (2,467)  | 1:79:A:ILE:HG21  | 1:156:A:PHE:HA   | 3        | 0.73          |
| (2,467)  | 1:79:A:ILE:HG22  | 1:156:A:PHE:HA   | 3        | 0.73          |
| (2,467)  | 1:79:A:ILE:HG23  | 1:156:A:PHE:HA   | 3        | 0.73          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,365)  | 1:66:A:ASN:HB3   | 1:173:A:VAL:HG21 | 4        | 0.73          |
| (2,365)  | 1:66:A:ASN:HB3   | 1:173:A:VAL:HG22 | 4        | 0.73          |
| (2,365)  | 1:66:A:ASN:HB3   | 1:173:A:VAL:HG23 | 4        | 0.73          |
| (2,4)    | 1:15:A:THR:HG21  | 1:16:A:ALA:H     | 4        | 0.73          |
| (2,4)    | 1:15:A:THR:HG22  | 1:16:A:ALA:H     | 4        | 0.73          |
| (2,4)    | 1:15:A:THR:HG23  | 1:16:A:ALA:H     | 4        | 0.73          |
| (1,2357) | 1:173:A:VAL:HG21 | 1:175:A:PHE:HE1  | 3        | 0.73          |
| (1,2357) | 1:173:A:VAL:HG21 | 1:175:A:PHE:HE2  | 3        | 0.73          |
| (1,2357) | 1:173:A:VAL:HG22 | 1:175:A:PHE:HE1  | 3        | 0.73          |
| (1,2357) | 1:173:A:VAL:HG22 | 1:175:A:PHE:HE2  | 3        | 0.73          |
| (1,2357) | 1:173:A:VAL:HG23 | 1:175:A:PHE:HE1  | 3        | 0.73          |
| (1,2357) | 1:173:A:VAL:HG23 | 1:175:A:PHE:HE2  | 3        | 0.73          |
| (1,2357) | 1:173:A:VAL:HG21 | 1:175:A:PHE:HE1  | 4        | 0.73          |
| (1,2357) | 1:173:A:VAL:HG21 | 1:175:A:PHE:HE2  | 4        | 0.73          |
| (1,2357) | 1:173:A:VAL:HG22 | 1:175:A:PHE:HE1  | 4        | 0.73          |
| (1,2357) | 1:173:A:VAL:HG22 | 1:175:A:PHE:HE2  | 4        | 0.73          |
| (1,2357) | 1:173:A:VAL:HG23 | 1:175:A:PHE:HE1  | 4        | 0.73          |
| (1,2357) | 1:173:A:VAL:HG23 | 1:175:A:PHE:HE2  | 4        | 0.73          |
| (1,2357) | 1:173:A:VAL:HG21 | 1:175:A:PHE:HE1  | 8        | 0.73          |
| (1,2357) | 1:173:A:VAL:HG21 | 1:175:A:PHE:HE2  | 8        | 0.73          |
| (1,2357) | 1:173:A:VAL:HG22 | 1:175:A:PHE:HE1  | 8        | 0.73          |
| (1,2357) | 1:173:A:VAL:HG22 | 1:175:A:PHE:HE2  | 8        | 0.73          |
| (1,2357) | 1:173:A:VAL:HG23 | 1:175:A:PHE:HE1  | 8        | 0.73          |
| (1,2357) | 1:173:A:VAL:HG23 | 1:175:A:PHE:HE2  | 8        | 0.73          |
| (1,2357) | 1:173:A:VAL:HG21 | 1:175:A:PHE:HE1  | 9        | 0.73          |
| (1,2357) | 1:173:A:VAL:HG21 | 1:175:A:PHE:HE2  | 9        | 0.73          |
| (1,2357) | 1:173:A:VAL:HG22 | 1:175:A:PHE:HE1  | 9        | 0.73          |
| (1,2357) | 1:173:A:VAL:HG22 | 1:175:A:PHE:HE2  | 9        | 0.73          |
| (1,2357) | 1:173:A:VAL:HG23 | 1:175:A:PHE:HE1  | 9        | 0.73          |
| (1,2357) | 1:173:A:VAL:HG23 | 1:175:A:PHE:HE2  | 9        | 0.73          |
| (1,2357) | 1:173:A:VAL:HG21 | 1:175:A:PHE:HE1  | 10       | 0.73          |
| (1,2357) | 1:173:A:VAL:HG21 | 1:175:A:PHE:HE2  | 10       | 0.73          |
| (1,2357) | 1:173:A:VAL:HG22 | 1:175:A:PHE:HE1  | 10       | 0.73          |
| (1,2357) | 1:173:A:VAL:HG22 | 1:175:A:PHE:HE2  | 10       | 0.73          |
| (1,2357) | 1:173:A:VAL:HG23 | 1:175:A:PHE:HE1  | 10       | 0.73          |
| (1,2357) | 1:173:A:VAL:HG23 | 1:175:A:PHE:HE2  | 10       | 0.73          |
| (1,2324) | 1:171:A:LEU:HD21 | 1:171:A:LEU:H    | 8        | 0.73          |
| (1,2324) | 1:171:A:LEU:HD22 | 1:171:A:LEU:H    | 8        | 0.73          |
| (1,2324) | 1:171:A:LEU:HD23 | 1:171:A:LEU:H    | 8        | 0.73          |
| (1,282)  | 1:35:A:ALA:HB1   | 1:36:A:ALA:H     | 10       | 0.73          |
| (1,282)  | 1:35:A:ALA:HB2   | 1:36:A:ALA:H     | 10       | 0.73          |
| (1,282)  | 1:35:A:ALA:HB3   | 1:36:A:ALA:H     | 10       | 0.73          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,206)  | 1:32:A:ILE:HA    | 1:32:A:ILE:HD11 | 5        | 0.73          |
| (1,206)  | 1:32:A:ILE:HA    | 1:32:A:ILE:HD12 | 5        | 0.73          |
| (1,206)  | 1:32:A:ILE:HA    | 1:32:A:ILE:HD13 | 5        | 0.73          |
| (1,206)  | 1:32:A:ILE:HA    | 1:32:A:ILE:HD11 | 9        | 0.73          |
| (1,206)  | 1:32:A:ILE:HA    | 1:32:A:ILE:HD12 | 9        | 0.73          |
| (1,206)  | 1:32:A:ILE:HA    | 1:32:A:ILE:HD13 | 9        | 0.73          |
| (2,518)  | 1:84:A:GLY:HA2   | 1:95:A:PHE:HE1  | 1        | 0.72          |
| (2,518)  | 1:84:A:GLY:HA2   | 1:95:A:PHE:HE2  | 1        | 0.72          |
| (2,518)  | 1:84:A:GLY:HA3   | 1:95:A:PHE:HE1  | 1        | 0.72          |
| (2,518)  | 1:84:A:GLY:HA3   | 1:95:A:PHE:HE2  | 1        | 0.72          |
| (2,517)  | 1:84:A:GLY:HA2   | 1:85:A:TYR:HD1  | 7        | 0.72          |
| (2,517)  | 1:84:A:GLY:HA2   | 1:85:A:TYR:HD2  | 7        | 0.72          |
| (2,517)  | 1:84:A:GLY:HA3   | 1:85:A:TYR:HD1  | 7        | 0.72          |
| (2,517)  | 1:84:A:GLY:HA3   | 1:85:A:TYR:HD2  | 7        | 0.72          |
| (1,2357) | 1:173:A:VAL:HG21 | 1:175:A:PHE:HE1 | 1        | 0.72          |
| (1,2357) | 1:173:A:VAL:HG21 | 1:175:A:PHE:HE2 | 1        | 0.72          |
| (1,2357) | 1:173:A:VAL:HG22 | 1:175:A:PHE:HE1 | 1        | 0.72          |
| (1,2357) | 1:173:A:VAL:HG22 | 1:175:A:PHE:HE2 | 1        | 0.72          |
| (1,2357) | 1:173:A:VAL:HG23 | 1:175:A:PHE:HE1 | 1        | 0.72          |
| (1,2357) | 1:173:A:VAL:HG23 | 1:175:A:PHE:HE2 | 1        | 0.72          |
| (1,2032) | 1:143:A:ILE:HG21 | 1:144:A:VAL:H   | 4        | 0.72          |
| (1,2032) | 1:143:A:ILE:HG22 | 1:144:A:VAL:H   | 4        | 0.72          |
| (1,2032) | 1:143:A:ILE:HG23 | 1:144:A:VAL:H   | 4        | 0.72          |
| (1,2032) | 1:143:A:ILE:HG21 | 1:144:A:VAL:H   | 5        | 0.72          |
| (1,2032) | 1:143:A:ILE:HG22 | 1:144:A:VAL:H   | 5        | 0.72          |
| (1,2032) | 1:143:A:ILE:HG23 | 1:144:A:VAL:H   | 5        | 0.72          |
| (1,1030) | 1:74:A:PHE:HE1   | 1:162:A:ALA:HB1 | 6        | 0.72          |
| (1,1030) | 1:74:A:PHE:HE1   | 1:162:A:ALA:HB2 | 6        | 0.72          |
| (1,1030) | 1:74:A:PHE:HE1   | 1:162:A:ALA:HB3 | 6        | 0.72          |
| (1,1030) | 1:74:A:PHE:HE2   | 1:162:A:ALA:HB1 | 6        | 0.72          |
| (1,1030) | 1:74:A:PHE:HE2   | 1:162:A:ALA:HB2 | 6        | 0.72          |
| (1,1030) | 1:74:A:PHE:HE2   | 1:162:A:ALA:HB3 | 6        | 0.72          |
| (1,288)  | 1:36:A:ALA:HB1   | 1:37:A:GLY:H    | 5        | 0.72          |
| (1,288)  | 1:36:A:ALA:HB2   | 1:37:A:GLY:H    | 5        | 0.72          |
| (1,288)  | 1:36:A:ALA:HB3   | 1:37:A:GLY:H    | 5        | 0.72          |
| (1,145)  | 1:28:A:HIS:HE1   | 1:48:A:ILE:HD11 | 1        | 0.72          |
| (1,145)  | 1:28:A:HIS:HE1   | 1:48:A:ILE:HD12 | 1        | 0.72          |
| (1,145)  | 1:28:A:HIS:HE1   | 1:48:A:ILE:HD13 | 1        | 0.72          |
| (1,145)  | 1:28:A:HIS:HE1   | 1:48:A:ILE:HD11 | 7        | 0.72          |
| (1,145)  | 1:28:A:HIS:HE1   | 1:48:A:ILE:HD12 | 7        | 0.72          |
| (1,145)  | 1:28:A:HIS:HE1   | 1:48:A:ILE:HD13 | 7        | 0.72          |
| (2,614)  | 1:118:A:ILE:HG21 | 1:151:A:VAL:HA  | 8        | 0.71          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,614)  | 1:118:A:ILE:HG22 | 1:151:A:VAL:HA   | 8        | 0.71          |
| (2,614)  | 1:118:A:ILE:HG23 | 1:151:A:VAL:HA   | 8        | 0.71          |
| (2,467)  | 1:79:A:ILE:HG21  | 1:156:A:PHE:HA   | 8        | 0.71          |
| (2,467)  | 1:79:A:ILE:HG22  | 1:156:A:PHE:HA   | 8        | 0.71          |
| (2,467)  | 1:79:A:ILE:HG23  | 1:156:A:PHE:HA   | 8        | 0.71          |
| (1,288)  | 1:36:A:ALA:HB1   | 1:37:A:GLY:H     | 6        | 0.71          |
| (1,288)  | 1:36:A:ALA:HB2   | 1:37:A:GLY:H     | 6        | 0.71          |
| (1,288)  | 1:36:A:ALA:HB3   | 1:37:A:GLY:H     | 6        | 0.71          |
| (1,261)  | 1:33:A:THR:HG21  | 1:34:A:PRO:HD2   | 7        | 0.71          |
| (1,261)  | 1:33:A:THR:HG22  | 1:34:A:PRO:HD2   | 7        | 0.71          |
| (1,261)  | 1:33:A:THR:HG23  | 1:34:A:PRO:HD2   | 7        | 0.71          |
| (1,206)  | 1:32:A:ILE:HA    | 1:32:A:ILE:HD11  | 1        | 0.71          |
| (1,206)  | 1:32:A:ILE:HA    | 1:32:A:ILE:HD12  | 1        | 0.71          |
| (1,206)  | 1:32:A:ILE:HA    | 1:32:A:ILE:HD13  | 1        | 0.71          |
| (1,145)  | 1:28:A:HIS:HE1   | 1:48:A:ILE:HD11  | 4        | 0.71          |
| (1,145)  | 1:28:A:HIS:HE1   | 1:48:A:ILE:HD12  | 4        | 0.71          |
| (1,145)  | 1:28:A:HIS:HE1   | 1:48:A:ILE:HD13  | 4        | 0.71          |
| (1,6)    | 1:18:A:ALA:HB1   | 1:19:A:VAL:H     | 1        | 0.71          |
| (1,6)    | 1:18:A:ALA:HB2   | 1:19:A:VAL:H     | 1        | 0.71          |
| (1,6)    | 1:18:A:ALA:HB3   | 1:19:A:VAL:H     | 1        | 0.71          |
| (2,365)  | 1:66:A:ASN:HB3   | 1:173:A:VAL:HG21 | 2        | 0.7           |
| (2,365)  | 1:66:A:ASN:HB3   | 1:173:A:VAL:HG22 | 2        | 0.7           |
| (2,365)  | 1:66:A:ASN:HB3   | 1:173:A:VAL:HG23 | 2        | 0.7           |
| (2,7)    | 1:16:A:ALA:HB1   | 1:18:A:ALA:H     | 9        | 0.7           |
| (2,7)    | 1:16:A:ALA:HB2   | 1:18:A:ALA:H     | 9        | 0.7           |
| (2,7)    | 1:16:A:ALA:HB3   | 1:18:A:ALA:H     | 9        | 0.7           |
| (1,2354) | 1:173:A:VAL:HG11 | 1:175:A:PHE:HE1  | 3        | 0.7           |
| (1,2354) | 1:173:A:VAL:HG11 | 1:175:A:PHE:HE2  | 3        | 0.7           |
| (1,2354) | 1:173:A:VAL:HG12 | 1:175:A:PHE:HE1  | 3        | 0.7           |
| (1,2354) | 1:173:A:VAL:HG12 | 1:175:A:PHE:HE2  | 3        | 0.7           |
| (1,2354) | 1:173:A:VAL:HG13 | 1:175:A:PHE:HE1  | 3        | 0.7           |
| (1,2354) | 1:173:A:VAL:HG13 | 1:175:A:PHE:HE2  | 3        | 0.7           |
| (1,1548) | 1:102:A:ILE:HG21 | 1:109:A:ALA:HB1  | 10       | 0.7           |
| (1,1548) | 1:102:A:ILE:HG21 | 1:109:A:ALA:HB2  | 10       | 0.7           |
| (1,1548) | 1:102:A:ILE:HG21 | 1:109:A:ALA:HB3  | 10       | 0.7           |
| (1,1548) | 1:102:A:ILE:HG22 | 1:109:A:ALA:HB1  | 10       | 0.7           |
| (1,1548) | 1:102:A:ILE:HG22 | 1:109:A:ALA:HB2  | 10       | 0.7           |
| (1,1548) | 1:102:A:ILE:HG22 | 1:109:A:ALA:HB3  | 10       | 0.7           |
| (1,1548) | 1:102:A:ILE:HG23 | 1:109:A:ALA:HB1  | 10       | 0.7           |
| (1,1548) | 1:102:A:ILE:HG23 | 1:109:A:ALA:HB2  | 10       | 0.7           |
| (1,1548) | 1:102:A:ILE:HG23 | 1:109:A:ALA:HB3  | 10       | 0.7           |
| (1,1215) | 1:81:A:ILE:HD11  | 1:100:A:ALA:HB1  | 3        | 0.7           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1215) | 1:81:A:ILE:HD11 | 1:100:A:ALA:HB2 | 3        | 0.7           |
| (1,1215) | 1:81:A:ILE:HD11 | 1:100:A:ALA:HB3 | 3        | 0.7           |
| (1,1215) | 1:81:A:ILE:HD12 | 1:100:A:ALA:HB1 | 3        | 0.7           |
| (1,1215) | 1:81:A:ILE:HD12 | 1:100:A:ALA:HB2 | 3        | 0.7           |
| (1,1215) | 1:81:A:ILE:HD12 | 1:100:A:ALA:HB3 | 3        | 0.7           |
| (1,1215) | 1:81:A:ILE:HD13 | 1:100:A:ALA:HB1 | 3        | 0.7           |
| (1,1215) | 1:81:A:ILE:HD13 | 1:100:A:ALA:HB2 | 3        | 0.7           |
| (1,1215) | 1:81:A:ILE:HD13 | 1:100:A:ALA:HB3 | 3        | 0.7           |
| (1,1215) | 1:81:A:ILE:HD11 | 1:100:A:ALA:HB1 | 9        | 0.7           |
| (1,1215) | 1:81:A:ILE:HD11 | 1:100:A:ALA:HB2 | 9        | 0.7           |
| (1,1215) | 1:81:A:ILE:HD11 | 1:100:A:ALA:HB3 | 9        | 0.7           |
| (1,1215) | 1:81:A:ILE:HD12 | 1:100:A:ALA:HB1 | 9        | 0.7           |
| (1,1215) | 1:81:A:ILE:HD12 | 1:100:A:ALA:HB2 | 9        | 0.7           |
| (1,1215) | 1:81:A:ILE:HD12 | 1:100:A:ALA:HB3 | 9        | 0.7           |
| (1,1215) | 1:81:A:ILE:HD13 | 1:100:A:ALA:HB1 | 9        | 0.7           |
| (1,1215) | 1:81:A:ILE:HD13 | 1:100:A:ALA:HB2 | 9        | 0.7           |
| (1,1215) | 1:81:A:ILE:HD13 | 1:100:A:ALA:HB3 | 9        | 0.7           |
| (1,489)  | 1:48:A:ILE:HG21 | 1:48:A:ILE:HD11 | 7        | 0.7           |
| (1,489)  | 1:48:A:ILE:HG21 | 1:48:A:ILE:HD12 | 7        | 0.7           |
| (1,489)  | 1:48:A:ILE:HG21 | 1:48:A:ILE:HD13 | 7        | 0.7           |
| (1,489)  | 1:48:A:ILE:HG22 | 1:48:A:ILE:HD11 | 7        | 0.7           |
| (1,489)  | 1:48:A:ILE:HG22 | 1:48:A:ILE:HD12 | 7        | 0.7           |
| (1,489)  | 1:48:A:ILE:HG22 | 1:48:A:ILE:HD13 | 7        | 0.7           |
| (1,489)  | 1:48:A:ILE:HG23 | 1:48:A:ILE:HD11 | 7        | 0.7           |
| (1,489)  | 1:48:A:ILE:HG23 | 1:48:A:ILE:HD12 | 7        | 0.7           |
| (1,489)  | 1:48:A:ILE:HG23 | 1:48:A:ILE:HD13 | 7        | 0.7           |
| (1,242)  | 1:32:A:ILE:HG21 | 1:160:A:TYR:HE1 | 1        | 0.7           |
| (1,242)  | 1:32:A:ILE:HG21 | 1:160:A:TYR:HE2 | 1        | 0.7           |
| (1,242)  | 1:32:A:ILE:HG22 | 1:160:A:TYR:HE1 | 1        | 0.7           |
| (1,242)  | 1:32:A:ILE:HG22 | 1:160:A:TYR:HE2 | 1        | 0.7           |
| (1,242)  | 1:32:A:ILE:HG23 | 1:160:A:TYR:HE1 | 1        | 0.7           |
| (1,242)  | 1:32:A:ILE:HG23 | 1:160:A:TYR:HE2 | 1        | 0.7           |
| (1,145)  | 1:28:A:HIS:HE1  | 1:48:A:ILE:HD11 | 3        | 0.7           |
| (1,145)  | 1:28:A:HIS:HE1  | 1:48:A:ILE:HD12 | 3        | 0.7           |
| (1,145)  | 1:28:A:HIS:HE1  | 1:48:A:ILE:HD13 | 3        | 0.7           |
| (1,145)  | 1:28:A:HIS:HE1  | 1:48:A:ILE:HD11 | 8        | 0.7           |
| (1,145)  | 1:28:A:HIS:HE1  | 1:48:A:ILE:HD12 | 8        | 0.7           |
| (1,145)  | 1:28:A:HIS:HE1  | 1:48:A:ILE:HD13 | 8        | 0.7           |
| (1,145)  | 1:28:A:HIS:HE1  | 1:48:A:ILE:HD11 | 9        | 0.7           |
| (1,145)  | 1:28:A:HIS:HE1  | 1:48:A:ILE:HD12 | 9        | 0.7           |
| (1,145)  | 1:28:A:HIS:HE1  | 1:48:A:ILE:HD13 | 9        | 0.7           |
| (1,145)  | 1:28:A:HIS:HE1  | 1:48:A:ILE:HD11 | 10       | 0.7           |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,145)  | 1:28:A:HIS:HE1  | 1:48:A:ILE:HD12  | 10       | 0.7           |
| (1,145)  | 1:28:A:HIS:HE1  | 1:48:A:ILE:HD13  | 10       | 0.7           |
| (1,6)    | 1:18:A:ALA:HB1  | 1:19:A:VAL:H     | 3        | 0.7           |
| (1,6)    | 1:18:A:ALA:HB2  | 1:19:A:VAL:H     | 3        | 0.7           |
| (1,6)    | 1:18:A:ALA:HB3  | 1:19:A:VAL:H     | 3        | 0.7           |
| (1,6)    | 1:18:A:ALA:HB1  | 1:19:A:VAL:H     | 5        | 0.7           |
| (1,6)    | 1:18:A:ALA:HB2  | 1:19:A:VAL:H     | 5        | 0.7           |
| (1,6)    | 1:18:A:ALA:HB3  | 1:19:A:VAL:H     | 5        | 0.7           |
| (1,6)    | 1:18:A:ALA:HB1  | 1:19:A:VAL:H     | 8        | 0.7           |
| (1,6)    | 1:18:A:ALA:HB2  | 1:19:A:VAL:H     | 8        | 0.7           |
| (1,6)    | 1:18:A:ALA:HB3  | 1:19:A:VAL:H     | 8        | 0.7           |
| (1,6)    | 1:18:A:ALA:HB1  | 1:19:A:VAL:H     | 9        | 0.7           |
| (1,6)    | 1:18:A:ALA:HB2  | 1:19:A:VAL:H     | 9        | 0.7           |
| (1,6)    | 1:18:A:ALA:HB3  | 1:19:A:VAL:H     | 9        | 0.7           |
| (2,520)  | 1:84:A:GLY:HA2  | 1:155:A:ASN:HD21 | 5        | 0.69          |
| (2,520)  | 1:84:A:GLY:HA2  | 1:155:A:ASN:HD22 | 5        | 0.69          |
| (2,520)  | 1:84:A:GLY:HA3  | 1:155:A:ASN:HD21 | 5        | 0.69          |
| (2,520)  | 1:84:A:GLY:HA3  | 1:155:A:ASN:HD22 | 5        | 0.69          |
| (1,1243) | 1:81:A:ILE:HG21 | 1:156:A:PHE:HZ   | 4        | 0.69          |
| (1,1243) | 1:81:A:ILE:HG22 | 1:156:A:PHE:HZ   | 4        | 0.69          |
| (1,1243) | 1:81:A:ILE:HG23 | 1:156:A:PHE:HZ   | 4        | 0.69          |
| (1,992)  | 1:73:A:TYR:HE1  | 1:171:A:LEU:HD21 | 10       | 0.69          |
| (1,992)  | 1:73:A:TYR:HE1  | 1:171:A:LEU:HD22 | 10       | 0.69          |
| (1,992)  | 1:73:A:TYR:HE1  | 1:171:A:LEU:HD23 | 10       | 0.69          |
| (1,992)  | 1:73:A:TYR:HE2  | 1:171:A:LEU:HD21 | 10       | 0.69          |
| (1,992)  | 1:73:A:TYR:HE2  | 1:171:A:LEU:HD22 | 10       | 0.69          |
| (1,992)  | 1:73:A:TYR:HE2  | 1:171:A:LEU:HD23 | 10       | 0.69          |
| (1,756)  | 1:63:A:THR:HG21 | 1:108:A:SER:HB2  | 10       | 0.69          |
| (1,756)  | 1:63:A:THR:HG21 | 1:108:A:SER:HB3  | 10       | 0.69          |
| (1,756)  | 1:63:A:THR:HG22 | 1:108:A:SER:HB2  | 10       | 0.69          |
| (1,756)  | 1:63:A:THR:HG22 | 1:108:A:SER:HB3  | 10       | 0.69          |
| (1,756)  | 1:63:A:THR:HG23 | 1:108:A:SER:HB2  | 10       | 0.69          |
| (1,756)  | 1:63:A:THR:HG23 | 1:108:A:SER:HB3  | 10       | 0.69          |
| (1,261)  | 1:33:A:THR:HG21 | 1:34:A:PRO:HD2   | 2        | 0.69          |
| (1,261)  | 1:33:A:THR:HG22 | 1:34:A:PRO:HD2   | 2        | 0.69          |
| (1,261)  | 1:33:A:THR:HG23 | 1:34:A:PRO:HD2   | 2        | 0.69          |
| (1,261)  | 1:33:A:THR:HG21 | 1:34:A:PRO:HD2   | 8        | 0.69          |
| (1,261)  | 1:33:A:THR:HG22 | 1:34:A:PRO:HD2   | 8        | 0.69          |
| (1,261)  | 1:33:A:THR:HG23 | 1:34:A:PRO:HD2   | 8        | 0.69          |
| (1,145)  | 1:28:A:HIS:HE1  | 1:48:A:ILE:HD11  | 6        | 0.69          |
| (1,145)  | 1:28:A:HIS:HE1  | 1:48:A:ILE:HD12  | 6        | 0.69          |
| (1,145)  | 1:28:A:HIS:HE1  | 1:48:A:ILE:HD13  | 6        | 0.69          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,6)    | 1:18:A:ALA:HB1   | 1:19:A:VAL:H     | 6        | 0.69          |
| (1,6)    | 1:18:A:ALA:HB2   | 1:19:A:VAL:H     | 6        | 0.69          |
| (1,6)    | 1:18:A:ALA:HB3   | 1:19:A:VAL:H     | 6        | 0.69          |
| (2,733)  | 1:157:A:LYS:HE2  | 1:159:A:PHE:HD1  | 6        | 0.68          |
| (2,733)  | 1:157:A:LYS:HE2  | 1:159:A:PHE:HD2  | 6        | 0.68          |
| (2,733)  | 1:157:A:LYS:HE3  | 1:159:A:PHE:HD1  | 6        | 0.68          |
| (2,733)  | 1:157:A:LYS:HE3  | 1:159:A:PHE:HD2  | 6        | 0.68          |
| (2,184)  | 1:37:A:GLY:H     | 1:38:A:ALA:HB1   | 9        | 0.68          |
| (2,184)  | 1:37:A:GLY:H     | 1:38:A:ALA:HB2   | 9        | 0.68          |
| (2,184)  | 1:37:A:GLY:H     | 1:38:A:ALA:HB3   | 9        | 0.68          |
| (1,2078) | 1:151:A:VAL:HG11 | 1:151:A:VAL:HG21 | 2        | 0.68          |
| (1,2078) | 1:151:A:VAL:HG11 | 1:151:A:VAL:HG22 | 2        | 0.68          |
| (1,2078) | 1:151:A:VAL:HG11 | 1:151:A:VAL:HG23 | 2        | 0.68          |
| (1,2078) | 1:151:A:VAL:HG12 | 1:151:A:VAL:HG21 | 2        | 0.68          |
| (1,2078) | 1:151:A:VAL:HG12 | 1:151:A:VAL:HG22 | 2        | 0.68          |
| (1,2078) | 1:151:A:VAL:HG12 | 1:151:A:VAL:HG23 | 2        | 0.68          |
| (1,2078) | 1:151:A:VAL:HG13 | 1:151:A:VAL:HG21 | 2        | 0.68          |
| (1,2078) | 1:151:A:VAL:HG13 | 1:151:A:VAL:HG22 | 2        | 0.68          |
| (1,2078) | 1:151:A:VAL:HG13 | 1:151:A:VAL:HG23 | 2        | 0.68          |
| (1,2078) | 1:151:A:VAL:HG11 | 1:151:A:VAL:HG21 | 8        | 0.68          |
| (1,2078) | 1:151:A:VAL:HG11 | 1:151:A:VAL:HG22 | 8        | 0.68          |
| (1,2078) | 1:151:A:VAL:HG11 | 1:151:A:VAL:HG23 | 8        | 0.68          |
| (1,2078) | 1:151:A:VAL:HG12 | 1:151:A:VAL:HG21 | 8        | 0.68          |
| (1,2078) | 1:151:A:VAL:HG12 | 1:151:A:VAL:HG22 | 8        | 0.68          |
| (1,2078) | 1:151:A:VAL:HG12 | 1:151:A:VAL:HG23 | 8        | 0.68          |
| (1,2078) | 1:151:A:VAL:HG13 | 1:151:A:VAL:HG21 | 8        | 0.68          |
| (1,2078) | 1:151:A:VAL:HG13 | 1:151:A:VAL:HG22 | 8        | 0.68          |
| (1,2078) | 1:151:A:VAL:HG13 | 1:151:A:VAL:HG23 | 8        | 0.68          |
| (1,1457) | 1:92:A:LEU:HD11  | 1:93:A:GLY:H     | 4        | 0.68          |
| (1,1457) | 1:92:A:LEU:HD12  | 1:93:A:GLY:H     | 4        | 0.68          |
| (1,1457) | 1:92:A:LEU:HD13  | 1:93:A:GLY:H     | 4        | 0.68          |
| (1,756)  | 1:63:A:THR:HG21  | 1:108:A:SER:HB2  | 1        | 0.68          |
| (1,756)  | 1:63:A:THR:HG21  | 1:108:A:SER:HB3  | 1        | 0.68          |
| (1,756)  | 1:63:A:THR:HG22  | 1:108:A:SER:HB2  | 1        | 0.68          |
| (1,756)  | 1:63:A:THR:HG22  | 1:108:A:SER:HB3  | 1        | 0.68          |
| (1,756)  | 1:63:A:THR:HG23  | 1:108:A:SER:HB2  | 1        | 0.68          |
| (1,756)  | 1:63:A:THR:HG23  | 1:108:A:SER:HB3  | 1        | 0.68          |
| (1,756)  | 1:63:A:THR:HG21  | 1:108:A:SER:HB2  | 2        | 0.68          |
| (1,756)  | 1:63:A:THR:HG21  | 1:108:A:SER:HB3  | 2        | 0.68          |
| (1,756)  | 1:63:A:THR:HG22  | 1:108:A:SER:HB2  | 2        | 0.68          |
| (1,756)  | 1:63:A:THR:HG22  | 1:108:A:SER:HB3  | 2        | 0.68          |
| (1,756)  | 1:63:A:THR:HG23  | 1:108:A:SER:HB2  | 2        | 0.68          |

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| Key     | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,756) | 1:63:A:THR:HG23 | 1:108:A:SER:HB3  | 2        | 0.68          |
| (1,756) | 1:63:A:THR:HG21 | 1:108:A:SER:HB2  | 3        | 0.68          |
| (1,756) | 1:63:A:THR:HG21 | 1:108:A:SER:HB3  | 3        | 0.68          |
| (1,756) | 1:63:A:THR:HG22 | 1:108:A:SER:HB2  | 3        | 0.68          |
| (1,756) | 1:63:A:THR:HG22 | 1:108:A:SER:HB3  | 3        | 0.68          |
| (1,756) | 1:63:A:THR:HG23 | 1:108:A:SER:HB2  | 3        | 0.68          |
| (1,756) | 1:63:A:THR:HG23 | 1:108:A:SER:HB3  | 3        | 0.68          |
| (1,756) | 1:63:A:THR:HG21 | 1:108:A:SER:HB2  | 7        | 0.68          |
| (1,756) | 1:63:A:THR:HG21 | 1:108:A:SER:HB3  | 7        | 0.68          |
| (1,756) | 1:63:A:THR:HG22 | 1:108:A:SER:HB2  | 7        | 0.68          |
| (1,756) | 1:63:A:THR:HG22 | 1:108:A:SER:HB3  | 7        | 0.68          |
| (1,756) | 1:63:A:THR:HG23 | 1:108:A:SER:HB2  | 7        | 0.68          |
| (1,756) | 1:63:A:THR:HG23 | 1:108:A:SER:HB3  | 7        | 0.68          |
| (1,756) | 1:63:A:THR:HG21 | 1:108:A:SER:HB2  | 8        | 0.68          |
| (1,756) | 1:63:A:THR:HG21 | 1:108:A:SER:HB3  | 8        | 0.68          |
| (1,756) | 1:63:A:THR:HG22 | 1:108:A:SER:HB2  | 8        | 0.68          |
| (1,756) | 1:63:A:THR:HG22 | 1:108:A:SER:HB3  | 8        | 0.68          |
| (1,756) | 1:63:A:THR:HG23 | 1:108:A:SER:HB2  | 8        | 0.68          |
| (1,756) | 1:63:A:THR:HG23 | 1:108:A:SER:HB3  | 8        | 0.68          |
| (1,489) | 1:48:A:ILE:HG21 | 1:48:A:ILE:HD11  | 1        | 0.68          |
| (1,489) | 1:48:A:ILE:HG21 | 1:48:A:ILE:HD12  | 1        | 0.68          |
| (1,489) | 1:48:A:ILE:HG21 | 1:48:A:ILE:HD13  | 1        | 0.68          |
| (1,489) | 1:48:A:ILE:HG22 | 1:48:A:ILE:HD11  | 1        | 0.68          |
| (1,489) | 1:48:A:ILE:HG22 | 1:48:A:ILE:HD12  | 1        | 0.68          |
| (1,489) | 1:48:A:ILE:HG22 | 1:48:A:ILE:HD13  | 1        | 0.68          |
| (1,489) | 1:48:A:ILE:HG23 | 1:48:A:ILE:HD11  | 1        | 0.68          |
| (1,489) | 1:48:A:ILE:HG23 | 1:48:A:ILE:HD12  | 1        | 0.68          |
| (1,489) | 1:48:A:ILE:HG23 | 1:48:A:ILE:HD13  | 1        | 0.68          |
| (1,489) | 1:48:A:ILE:HG21 | 1:48:A:ILE:HD11  | 2        | 0.68          |
| (1,489) | 1:48:A:ILE:HG21 | 1:48:A:ILE:HD12  | 2        | 0.68          |
| (1,489) | 1:48:A:ILE:HG21 | 1:48:A:ILE:HD13  | 2        | 0.68          |
| (1,489) | 1:48:A:ILE:HG22 | 1:48:A:ILE:HD11  | 2        | 0.68          |
| (1,489) | 1:48:A:ILE:HG22 | 1:48:A:ILE:HD12  | 2        | 0.68          |
| (1,489) | 1:48:A:ILE:HG22 | 1:48:A:ILE:HD13  | 2        | 0.68          |
| (1,489) | 1:48:A:ILE:HG23 | 1:48:A:ILE:HD11  | 2        | 0.68          |
| (1,489) | 1:48:A:ILE:HG23 | 1:48:A:ILE:HD12  | 2        | 0.68          |
| (1,489) | 1:48:A:ILE:HG23 | 1:48:A:ILE:HD13  | 2        | 0.68          |
| (2,520) | 1:84:A:GLY:HA2  | 1:155:A:ASN:HD21 | 6        | 0.67          |
| (2,520) | 1:84:A:GLY:HA2  | 1:155:A:ASN:HD22 | 6        | 0.67          |
| (2,520) | 1:84:A:GLY:HA3  | 1:155:A:ASN:HD21 | 6        | 0.67          |
| (2,520) | 1:84:A:GLY:HA3  | 1:155:A:ASN:HD22 | 6        | 0.67          |
| (2,520) | 1:84:A:GLY:HA2  | 1:155:A:ASN:HD21 | 10       | 0.67          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,520)  | 1:84:A:GLY:HA2   | 1:155:A:ASN:HD22 | 10       | 0.67          |
| (2,520)  | 1:84:A:GLY:HA3   | 1:155:A:ASN:HD21 | 10       | 0.67          |
| (2,520)  | 1:84:A:GLY:HA3   | 1:155:A:ASN:HD22 | 10       | 0.67          |
| (2,3)    | 1:13:A:THR:HG21  | 1:17:A:GLN:HE21  | 8        | 0.67          |
| (2,3)    | 1:13:A:THR:HG22  | 1:17:A:GLN:HE21  | 8        | 0.67          |
| (2,3)    | 1:13:A:THR:HG23  | 1:17:A:GLN:HE21  | 8        | 0.67          |
| (1,2304) | 1:170:A:SER:HA   | 1:171:A:LEU:HD21 | 1        | 0.67          |
| (1,2304) | 1:170:A:SER:HA   | 1:171:A:LEU:HD22 | 1        | 0.67          |
| (1,2304) | 1:170:A:SER:HA   | 1:171:A:LEU:HD23 | 1        | 0.67          |
| (1,2032) | 1:143:A:ILE:HG21 | 1:144:A:VAL:H    | 1        | 0.67          |
| (1,2032) | 1:143:A:ILE:HG22 | 1:144:A:VAL:H    | 1        | 0.67          |
| (1,2032) | 1:143:A:ILE:HG23 | 1:144:A:VAL:H    | 1        | 0.67          |
| (1,1243) | 1:81:A:ILE:HG21  | 1:156:A:PHE:HZ   | 3        | 0.67          |
| (1,1243) | 1:81:A:ILE:HG22  | 1:156:A:PHE:HZ   | 3        | 0.67          |
| (1,1243) | 1:81:A:ILE:HG23  | 1:156:A:PHE:HZ   | 3        | 0.67          |
| (1,1243) | 1:81:A:ILE:HG21  | 1:156:A:PHE:HZ   | 5        | 0.67          |
| (1,1243) | 1:81:A:ILE:HG22  | 1:156:A:PHE:HZ   | 5        | 0.67          |
| (1,1243) | 1:81:A:ILE:HG23  | 1:156:A:PHE:HZ   | 5        | 0.67          |
| (1,1243) | 1:81:A:ILE:HG21  | 1:156:A:PHE:HZ   | 6        | 0.67          |
| (1,1243) | 1:81:A:ILE:HG22  | 1:156:A:PHE:HZ   | 6        | 0.67          |
| (1,1243) | 1:81:A:ILE:HG23  | 1:156:A:PHE:HZ   | 6        | 0.67          |
| (1,1091) | 1:77:A:LEU:HD11  | 1:103:A:SER:HA   | 4        | 0.67          |
| (1,1091) | 1:77:A:LEU:HD12  | 1:103:A:SER:HA   | 4        | 0.67          |
| (1,1091) | 1:77:A:LEU:HD13  | 1:103:A:SER:HA   | 4        | 0.67          |
| (1,1091) | 1:77:A:LEU:HD21  | 1:103:A:SER:HA   | 4        | 0.67          |
| (1,1091) | 1:77:A:LEU:HD22  | 1:103:A:SER:HA   | 4        | 0.67          |
| (1,1091) | 1:77:A:LEU:HD23  | 1:103:A:SER:HA   | 4        | 0.67          |
| (1,1068) | 1:76:A:TYR:HE1   | 1:78:A:GLN:HG2   | 10       | 0.67          |
| (1,1068) | 1:76:A:TYR:HE1   | 1:78:A:GLN:HG3   | 10       | 0.67          |
| (1,1068) | 1:76:A:TYR:HE2   | 1:78:A:GLN:HG2   | 10       | 0.67          |
| (1,1068) | 1:76:A:TYR:HE2   | 1:78:A:GLN:HG3   | 10       | 0.67          |
| (1,261)  | 1:33:A:THR:HG21  | 1:34:A:PRO:HD2   | 4        | 0.67          |
| (1,261)  | 1:33:A:THR:HG22  | 1:34:A:PRO:HD2   | 4        | 0.67          |
| (1,261)  | 1:33:A:THR:HG23  | 1:34:A:PRO:HD2   | 4        | 0.67          |
| (1,170)  | 1:29:A:LEU:HD21  | 1:175:A:PHE:HD1  | 1        | 0.67          |
| (1,170)  | 1:29:A:LEU:HD21  | 1:175:A:PHE:HD2  | 1        | 0.67          |
| (1,170)  | 1:29:A:LEU:HD22  | 1:175:A:PHE:HD1  | 1        | 0.67          |
| (1,170)  | 1:29:A:LEU:HD22  | 1:175:A:PHE:HD2  | 1        | 0.67          |
| (1,170)  | 1:29:A:LEU:HD23  | 1:175:A:PHE:HD1  | 1        | 0.67          |
| (1,170)  | 1:29:A:LEU:HD23  | 1:175:A:PHE:HD2  | 1        | 0.67          |
| (2,719)  | 1:142:A:ILE:HG21 | 1:145:A:TYR:HA   | 9        | 0.66          |
| (2,719)  | 1:142:A:ILE:HG22 | 1:145:A:TYR:HA   | 9        | 0.66          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,719)  | 1:142:A:ILE:HG23 | 1:145:A:TYR:HA   | 9        | 0.66          |
| (1,2304) | 1:170:A:SER:HA   | 1:171:A:LEU:HD21 | 7        | 0.66          |
| (1,2304) | 1:170:A:SER:HA   | 1:171:A:LEU:HD22 | 7        | 0.66          |
| (1,2304) | 1:170:A:SER:HA   | 1:171:A:LEU:HD23 | 7        | 0.66          |
| (1,2303) | 1:170:A:SER:HA   | 1:171:A:LEU:HD11 | 6        | 0.66          |
| (1,2303) | 1:170:A:SER:HA   | 1:171:A:LEU:HD12 | 6        | 0.66          |
| (1,2303) | 1:170:A:SER:HA   | 1:171:A:LEU:HD13 | 6        | 0.66          |
| (1,2245) | 1:162:A:ALA:HB1  | 1:168:A:PHE:HE1  | 10       | 0.66          |
| (1,2245) | 1:162:A:ALA:HB1  | 1:168:A:PHE:HE2  | 10       | 0.66          |
| (1,2245) | 1:162:A:ALA:HB2  | 1:168:A:PHE:HE1  | 10       | 0.66          |
| (1,2245) | 1:162:A:ALA:HB2  | 1:168:A:PHE:HE2  | 10       | 0.66          |
| (1,2245) | 1:162:A:ALA:HB3  | 1:168:A:PHE:HE1  | 10       | 0.66          |
| (1,2245) | 1:162:A:ALA:HB3  | 1:168:A:PHE:HE2  | 10       | 0.66          |
| (1,2078) | 1:151:A:VAL:HG11 | 1:151:A:VAL:HG21 | 3        | 0.66          |
| (1,2078) | 1:151:A:VAL:HG11 | 1:151:A:VAL:HG22 | 3        | 0.66          |
| (1,2078) | 1:151:A:VAL:HG11 | 1:151:A:VAL:HG23 | 3        | 0.66          |
| (1,2078) | 1:151:A:VAL:HG12 | 1:151:A:VAL:HG21 | 3        | 0.66          |
| (1,2078) | 1:151:A:VAL:HG12 | 1:151:A:VAL:HG22 | 3        | 0.66          |
| (1,2078) | 1:151:A:VAL:HG12 | 1:151:A:VAL:HG23 | 3        | 0.66          |
| (1,2078) | 1:151:A:VAL:HG13 | 1:151:A:VAL:HG21 | 3        | 0.66          |
| (1,2078) | 1:151:A:VAL:HG13 | 1:151:A:VAL:HG22 | 3        | 0.66          |
| (1,2078) | 1:151:A:VAL:HG13 | 1:151:A:VAL:HG23 | 3        | 0.66          |
| (1,2078) | 1:151:A:VAL:HG11 | 1:151:A:VAL:HG21 | 4        | 0.66          |
| (1,2078) | 1:151:A:VAL:HG11 | 1:151:A:VAL:HG22 | 4        | 0.66          |
| (1,2078) | 1:151:A:VAL:HG11 | 1:151:A:VAL:HG23 | 4        | 0.66          |
| (1,2078) | 1:151:A:VAL:HG12 | 1:151:A:VAL:HG21 | 4        | 0.66          |
| (1,2078) | 1:151:A:VAL:HG12 | 1:151:A:VAL:HG22 | 4        | 0.66          |
| (1,2078) | 1:151:A:VAL:HG12 | 1:151:A:VAL:HG23 | 4        | 0.66          |
| (1,2078) | 1:151:A:VAL:HG13 | 1:151:A:VAL:HG21 | 4        | 0.66          |
| (1,2078) | 1:151:A:VAL:HG13 | 1:151:A:VAL:HG22 | 4        | 0.66          |
| (1,2078) | 1:151:A:VAL:HG13 | 1:151:A:VAL:HG23 | 4        | 0.66          |
| (1,2078) | 1:151:A:VAL:HG11 | 1:151:A:VAL:HG21 | 7        | 0.66          |
| (1,2078) | 1:151:A:VAL:HG11 | 1:151:A:VAL:HG22 | 7        | 0.66          |
| (1,2078) | 1:151:A:VAL:HG11 | 1:151:A:VAL:HG23 | 7        | 0.66          |
| (1,2078) | 1:151:A:VAL:HG12 | 1:151:A:VAL:HG21 | 7        | 0.66          |
| (1,2078) | 1:151:A:VAL:HG12 | 1:151:A:VAL:HG22 | 7        | 0.66          |
| (1,2078) | 1:151:A:VAL:HG12 | 1:151:A:VAL:HG23 | 7        | 0.66          |
| (1,2078) | 1:151:A:VAL:HG13 | 1:151:A:VAL:HG21 | 7        | 0.66          |
| (1,2078) | 1:151:A:VAL:HG13 | 1:151:A:VAL:HG22 | 7        | 0.66          |
| (1,2078) | 1:151:A:VAL:HG13 | 1:151:A:VAL:HG23 | 7        | 0.66          |
| (1,2078) | 1:151:A:VAL:HG11 | 1:151:A:VAL:HG21 | 9        | 0.66          |
| (1,2078) | 1:151:A:VAL:HG11 | 1:151:A:VAL:HG22 | 9        | 0.66          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2078) | 1:151:A:VAL:HG11 | 1:151:A:VAL:HG23 | 9        | 0.66          |
| (1,2078) | 1:151:A:VAL:HG12 | 1:151:A:VAL:HG21 | 9        | 0.66          |
| (1,2078) | 1:151:A:VAL:HG12 | 1:151:A:VAL:HG22 | 9        | 0.66          |
| (1,2078) | 1:151:A:VAL:HG12 | 1:151:A:VAL:HG23 | 9        | 0.66          |
| (1,2078) | 1:151:A:VAL:HG13 | 1:151:A:VAL:HG21 | 9        | 0.66          |
| (1,2078) | 1:151:A:VAL:HG13 | 1:151:A:VAL:HG22 | 9        | 0.66          |
| (1,2078) | 1:151:A:VAL:HG13 | 1:151:A:VAL:HG23 | 9        | 0.66          |
| (1,2032) | 1:143:A:ILE:HG21 | 1:144:A:VAL:H    | 7        | 0.66          |
| (1,2032) | 1:143:A:ILE:HG22 | 1:144:A:VAL:H    | 7        | 0.66          |
| (1,2032) | 1:143:A:ILE:HG23 | 1:144:A:VAL:H    | 7        | 0.66          |
| (1,2016) | 1:142:A:ILE:HG21 | 1:145:A:TYR:HD1  | 5        | 0.66          |
| (1,2016) | 1:142:A:ILE:HG21 | 1:145:A:TYR:HD2  | 5        | 0.66          |
| (1,2016) | 1:142:A:ILE:HG22 | 1:145:A:TYR:HD1  | 5        | 0.66          |
| (1,2016) | 1:142:A:ILE:HG22 | 1:145:A:TYR:HD2  | 5        | 0.66          |
| (1,2016) | 1:142:A:ILE:HG23 | 1:145:A:TYR:HD1  | 5        | 0.66          |
| (1,2016) | 1:142:A:ILE:HG23 | 1:145:A:TYR:HD2  | 5        | 0.66          |
| (1,1548) | 1:102:A:ILE:HG21 | 1:109:A:ALA:HB1  | 7        | 0.66          |
| (1,1548) | 1:102:A:ILE:HG21 | 1:109:A:ALA:HB2  | 7        | 0.66          |
| (1,1548) | 1:102:A:ILE:HG21 | 1:109:A:ALA:HB3  | 7        | 0.66          |
| (1,1548) | 1:102:A:ILE:HG22 | 1:109:A:ALA:HB1  | 7        | 0.66          |
| (1,1548) | 1:102:A:ILE:HG22 | 1:109:A:ALA:HB2  | 7        | 0.66          |
| (1,1548) | 1:102:A:ILE:HG22 | 1:109:A:ALA:HB3  | 7        | 0.66          |
| (1,1548) | 1:102:A:ILE:HG23 | 1:109:A:ALA:HB1  | 7        | 0.66          |
| (1,1548) | 1:102:A:ILE:HG23 | 1:109:A:ALA:HB2  | 7        | 0.66          |
| (1,1548) | 1:102:A:ILE:HG23 | 1:109:A:ALA:HB3  | 7        | 0.66          |
| (1,1548) | 1:102:A:ILE:HG21 | 1:109:A:ALA:HB1  | 9        | 0.66          |
| (1,1548) | 1:102:A:ILE:HG21 | 1:109:A:ALA:HB2  | 9        | 0.66          |
| (1,1548) | 1:102:A:ILE:HG21 | 1:109:A:ALA:HB3  | 9        | 0.66          |
| (1,1548) | 1:102:A:ILE:HG22 | 1:109:A:ALA:HB1  | 9        | 0.66          |
| (1,1548) | 1:102:A:ILE:HG22 | 1:109:A:ALA:HB2  | 9        | 0.66          |
| (1,1548) | 1:102:A:ILE:HG22 | 1:109:A:ALA:HB3  | 9        | 0.66          |
| (1,1548) | 1:102:A:ILE:HG23 | 1:109:A:ALA:HB1  | 9        | 0.66          |
| (1,1548) | 1:102:A:ILE:HG23 | 1:109:A:ALA:HB2  | 9        | 0.66          |
| (1,1548) | 1:102:A:ILE:HG23 | 1:109:A:ALA:HB3  | 9        | 0.66          |
| (1,1243) | 1:81:A:ILE:HG21  | 1:156:A:PHE:HZ   | 8        | 0.66          |
| (1,1243) | 1:81:A:ILE:HG22  | 1:156:A:PHE:HZ   | 8        | 0.66          |
| (1,1243) | 1:81:A:ILE:HG23  | 1:156:A:PHE:HZ   | 8        | 0.66          |
| (1,1243) | 1:81:A:ILE:HG21  | 1:156:A:PHE:HZ   | 9        | 0.66          |
| (1,1243) | 1:81:A:ILE:HG22  | 1:156:A:PHE:HZ   | 9        | 0.66          |
| (1,1243) | 1:81:A:ILE:HG23  | 1:156:A:PHE:HZ   | 9        | 0.66          |
| (1,287)  | 1:36:A:ALA:HB1   | 1:36:A:ALA:H     | 6        | 0.66          |
| (1,287)  | 1:36:A:ALA:HB2   | 1:36:A:ALA:H     | 6        | 0.66          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,287)  | 1:36:A:ALA:HB3   | 1:36:A:ALA:H     | 6        | 0.66          |
| (2,718)  | 1:142:A:ILE:HD11 | 1:145:A:TYR:HE1  | 5        | 0.65          |
| (2,718)  | 1:142:A:ILE:HD11 | 1:145:A:TYR:HE2  | 5        | 0.65          |
| (2,718)  | 1:142:A:ILE:HD12 | 1:145:A:TYR:HE1  | 5        | 0.65          |
| (2,718)  | 1:142:A:ILE:HD12 | 1:145:A:TYR:HE2  | 5        | 0.65          |
| (2,718)  | 1:142:A:ILE:HD13 | 1:145:A:TYR:HE1  | 5        | 0.65          |
| (2,718)  | 1:142:A:ILE:HD13 | 1:145:A:TYR:HE2  | 5        | 0.65          |
| (2,520)  | 1:84:A:GLY:HA2   | 1:155:A:ASN:HD21 | 8        | 0.65          |
| (2,520)  | 1:84:A:GLY:HA2   | 1:155:A:ASN:HD22 | 8        | 0.65          |
| (2,520)  | 1:84:A:GLY:HA3   | 1:155:A:ASN:HD21 | 8        | 0.65          |
| (2,520)  | 1:84:A:GLY:HA3   | 1:155:A:ASN:HD22 | 8        | 0.65          |
| (2,520)  | 1:84:A:GLY:HA2   | 1:155:A:ASN:HD21 | 9        | 0.65          |
| (2,520)  | 1:84:A:GLY:HA2   | 1:155:A:ASN:HD22 | 9        | 0.65          |
| (2,520)  | 1:84:A:GLY:HA3   | 1:155:A:ASN:HD21 | 9        | 0.65          |
| (2,520)  | 1:84:A:GLY:HA3   | 1:155:A:ASN:HD22 | 9        | 0.65          |
| (2,490)  | 1:81:A:ILE:HD11  | 1:101:A:VAL:H    | 3        | 0.65          |
| (2,490)  | 1:81:A:ILE:HD12  | 1:101:A:VAL:H    | 3        | 0.65          |
| (2,490)  | 1:81:A:ILE:HD13  | 1:101:A:VAL:H    | 3        | 0.65          |
| (1,2304) | 1:170:A:SER:HA   | 1:171:A:LEU:HD21 | 9        | 0.65          |
| (1,2304) | 1:170:A:SER:HA   | 1:171:A:LEU:HD22 | 9        | 0.65          |
| (1,2304) | 1:170:A:SER:HA   | 1:171:A:LEU:HD23 | 9        | 0.65          |
| (1,2245) | 1:162:A:ALA:HB1  | 1:168:A:PHE:HE1  | 3        | 0.65          |
| (1,2245) | 1:162:A:ALA:HB1  | 1:168:A:PHE:HE2  | 3        | 0.65          |
| (1,2245) | 1:162:A:ALA:HB2  | 1:168:A:PHE:HE1  | 3        | 0.65          |
| (1,2245) | 1:162:A:ALA:HB2  | 1:168:A:PHE:HE2  | 3        | 0.65          |
| (1,2245) | 1:162:A:ALA:HB3  | 1:168:A:PHE:HE1  | 3        | 0.65          |
| (1,2245) | 1:162:A:ALA:HB3  | 1:168:A:PHE:HE2  | 3        | 0.65          |
| (1,2245) | 1:162:A:ALA:HB1  | 1:168:A:PHE:HE1  | 5        | 0.65          |
| (1,2245) | 1:162:A:ALA:HB1  | 1:168:A:PHE:HE2  | 5        | 0.65          |
| (1,2245) | 1:162:A:ALA:HB2  | 1:168:A:PHE:HE1  | 5        | 0.65          |
| (1,2245) | 1:162:A:ALA:HB2  | 1:168:A:PHE:HE2  | 5        | 0.65          |
| (1,2245) | 1:162:A:ALA:HB3  | 1:168:A:PHE:HE1  | 5        | 0.65          |
| (1,2245) | 1:162:A:ALA:HB3  | 1:168:A:PHE:HE2  | 5        | 0.65          |
| (1,2245) | 1:162:A:ALA:HB1  | 1:168:A:PHE:HE1  | 9        | 0.65          |
| (1,2245) | 1:162:A:ALA:HB1  | 1:168:A:PHE:HE2  | 9        | 0.65          |
| (1,2245) | 1:162:A:ALA:HB2  | 1:168:A:PHE:HE1  | 9        | 0.65          |
| (1,2245) | 1:162:A:ALA:HB2  | 1:168:A:PHE:HE2  | 9        | 0.65          |
| (1,2245) | 1:162:A:ALA:HB3  | 1:168:A:PHE:HE1  | 9        | 0.65          |
| (1,2245) | 1:162:A:ALA:HB3  | 1:168:A:PHE:HE2  | 9        | 0.65          |
| (1,2078) | 1:151:A:VAL:HG11 | 1:151:A:VAL:HG21 | 5        | 0.65          |
| (1,2078) | 1:151:A:VAL:HG11 | 1:151:A:VAL:HG22 | 5        | 0.65          |
| (1,2078) | 1:151:A:VAL:HG11 | 1:151:A:VAL:HG23 | 5        | 0.65          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2078) | 1:151:A:VAL:HG12 | 1:151:A:VAL:HG21 | 5        | 0.65          |
| (1,2078) | 1:151:A:VAL:HG12 | 1:151:A:VAL:HG22 | 5        | 0.65          |
| (1,2078) | 1:151:A:VAL:HG12 | 1:151:A:VAL:HG23 | 5        | 0.65          |
| (1,2078) | 1:151:A:VAL:HG13 | 1:151:A:VAL:HG21 | 5        | 0.65          |
| (1,2078) | 1:151:A:VAL:HG13 | 1:151:A:VAL:HG22 | 5        | 0.65          |
| (1,2078) | 1:151:A:VAL:HG13 | 1:151:A:VAL:HG23 | 5        | 0.65          |
| (1,2032) | 1:143:A:ILE:HG21 | 1:144:A:VAL:H    | 8        | 0.65          |
| (1,2032) | 1:143:A:ILE:HG22 | 1:144:A:VAL:H    | 8        | 0.65          |
| (1,2032) | 1:143:A:ILE:HG23 | 1:144:A:VAL:H    | 8        | 0.65          |
| (1,1788) | 1:125:A:LYS:HB2  | 1:125:A:LYS:HE2  | 7        | 0.65          |
| (1,1788) | 1:125:A:LYS:HB2  | 1:125:A:LYS:HE3  | 7        | 0.65          |
| (1,1788) | 1:125:A:LYS:HB3  | 1:125:A:LYS:HE2  | 7        | 0.65          |
| (1,1788) | 1:125:A:LYS:HB3  | 1:125:A:LYS:HE3  | 7        | 0.65          |
| (1,1548) | 1:102:A:ILE:HG21 | 1:109:A:ALA:HB1  | 8        | 0.65          |
| (1,1548) | 1:102:A:ILE:HG21 | 1:109:A:ALA:HB2  | 8        | 0.65          |
| (1,1548) | 1:102:A:ILE:HG21 | 1:109:A:ALA:HB3  | 8        | 0.65          |
| (1,1548) | 1:102:A:ILE:HG22 | 1:109:A:ALA:HB1  | 8        | 0.65          |
| (1,1548) | 1:102:A:ILE:HG22 | 1:109:A:ALA:HB2  | 8        | 0.65          |
| (1,1548) | 1:102:A:ILE:HG22 | 1:109:A:ALA:HB3  | 8        | 0.65          |
| (1,1548) | 1:102:A:ILE:HG23 | 1:109:A:ALA:HB1  | 8        | 0.65          |
| (1,1548) | 1:102:A:ILE:HG23 | 1:109:A:ALA:HB2  | 8        | 0.65          |
| (1,1548) | 1:102:A:ILE:HG23 | 1:109:A:ALA:HB3  | 8        | 0.65          |
| (1,1243) | 1:81:A:ILE:HG21  | 1:156:A:PHE:HZ   | 7        | 0.65          |
| (1,1243) | 1:81:A:ILE:HG22  | 1:156:A:PHE:HZ   | 7        | 0.65          |
| (1,1243) | 1:81:A:ILE:HG23  | 1:156:A:PHE:HZ   | 7        | 0.65          |
| (1,1243) | 1:81:A:ILE:HG21  | 1:156:A:PHE:HZ   | 10       | 0.65          |
| (1,1243) | 1:81:A:ILE:HG22  | 1:156:A:PHE:HZ   | 10       | 0.65          |
| (1,1243) | 1:81:A:ILE:HG23  | 1:156:A:PHE:HZ   | 10       | 0.65          |
| (1,1215) | 1:81:A:ILE:HD11  | 1:100:A:ALA:HB1  | 6        | 0.65          |
| (1,1215) | 1:81:A:ILE:HD11  | 1:100:A:ALA:HB2  | 6        | 0.65          |
| (1,1215) | 1:81:A:ILE:HD11  | 1:100:A:ALA:HB3  | 6        | 0.65          |
| (1,1215) | 1:81:A:ILE:HD12  | 1:100:A:ALA:HB1  | 6        | 0.65          |
| (1,1215) | 1:81:A:ILE:HD12  | 1:100:A:ALA:HB2  | 6        | 0.65          |
| (1,1215) | 1:81:A:ILE:HD12  | 1:100:A:ALA:HB3  | 6        | 0.65          |
| (1,1215) | 1:81:A:ILE:HD13  | 1:100:A:ALA:HB1  | 6        | 0.65          |
| (1,1215) | 1:81:A:ILE:HD13  | 1:100:A:ALA:HB2  | 6        | 0.65          |
| (1,1215) | 1:81:A:ILE:HD13  | 1:100:A:ALA:HB3  | 6        | 0.65          |
| (1,756)  | 1:63:A:THR:HG21  | 1:108:A:SER:HB2  | 5        | 0.65          |
| (1,756)  | 1:63:A:THR:HG21  | 1:108:A:SER:HB3  | 5        | 0.65          |
| (1,756)  | 1:63:A:THR:HG22  | 1:108:A:SER:HB2  | 5        | 0.65          |
| (1,756)  | 1:63:A:THR:HG22  | 1:108:A:SER:HB3  | 5        | 0.65          |
| (1,756)  | 1:63:A:THR:HG23  | 1:108:A:SER:HB2  | 5        | 0.65          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,756)  | 1:63:A:THR:HG23  | 1:108:A:SER:HB3 | 5        | 0.65          |
| (1,756)  | 1:63:A:THR:HG21  | 1:108:A:SER:HB2 | 6        | 0.65          |
| (1,756)  | 1:63:A:THR:HG21  | 1:108:A:SER:HB3 | 6        | 0.65          |
| (1,756)  | 1:63:A:THR:HG22  | 1:108:A:SER:HB2 | 6        | 0.65          |
| (1,756)  | 1:63:A:THR:HG22  | 1:108:A:SER:HB3 | 6        | 0.65          |
| (1,756)  | 1:63:A:THR:HG23  | 1:108:A:SER:HB2 | 6        | 0.65          |
| (1,756)  | 1:63:A:THR:HG23  | 1:108:A:SER:HB3 | 6        | 0.65          |
| (1,489)  | 1:48:A:ILE:HG21  | 1:48:A:ILE:HD11 | 4        | 0.65          |
| (1,489)  | 1:48:A:ILE:HG21  | 1:48:A:ILE:HD12 | 4        | 0.65          |
| (1,489)  | 1:48:A:ILE:HG21  | 1:48:A:ILE:HD13 | 4        | 0.65          |
| (1,489)  | 1:48:A:ILE:HG22  | 1:48:A:ILE:HD11 | 4        | 0.65          |
| (1,489)  | 1:48:A:ILE:HG22  | 1:48:A:ILE:HD12 | 4        | 0.65          |
| (1,489)  | 1:48:A:ILE:HG22  | 1:48:A:ILE:HD13 | 4        | 0.65          |
| (1,489)  | 1:48:A:ILE:HG23  | 1:48:A:ILE:HD11 | 4        | 0.65          |
| (1,489)  | 1:48:A:ILE:HG23  | 1:48:A:ILE:HD12 | 4        | 0.65          |
| (1,489)  | 1:48:A:ILE:HG23  | 1:48:A:ILE:HD13 | 4        | 0.65          |
| (1,489)  | 1:48:A:ILE:HG21  | 1:48:A:ILE:HD11 | 8        | 0.65          |
| (1,489)  | 1:48:A:ILE:HG21  | 1:48:A:ILE:HD12 | 8        | 0.65          |
| (1,489)  | 1:48:A:ILE:HG21  | 1:48:A:ILE:HD13 | 8        | 0.65          |
| (1,489)  | 1:48:A:ILE:HG22  | 1:48:A:ILE:HD11 | 8        | 0.65          |
| (1,489)  | 1:48:A:ILE:HG22  | 1:48:A:ILE:HD12 | 8        | 0.65          |
| (1,489)  | 1:48:A:ILE:HG22  | 1:48:A:ILE:HD13 | 8        | 0.65          |
| (1,489)  | 1:48:A:ILE:HG23  | 1:48:A:ILE:HD11 | 8        | 0.65          |
| (1,489)  | 1:48:A:ILE:HG23  | 1:48:A:ILE:HD12 | 8        | 0.65          |
| (1,489)  | 1:48:A:ILE:HG23  | 1:48:A:ILE:HD13 | 8        | 0.65          |
| (2,389)  | 1:70:A:LEU:HD21  | 1:172:A:PRO:HD2 | 8        | 0.64          |
| (2,389)  | 1:70:A:LEU:HD22  | 1:172:A:PRO:HD2 | 8        | 0.64          |
| (2,389)  | 1:70:A:LEU:HD23  | 1:172:A:PRO:HD2 | 8        | 0.64          |
| (1,2245) | 1:162:A:ALA:HB1  | 1:168:A:PHE:HE1 | 6        | 0.64          |
| (1,2245) | 1:162:A:ALA:HB1  | 1:168:A:PHE:HE2 | 6        | 0.64          |
| (1,2245) | 1:162:A:ALA:HB2  | 1:168:A:PHE:HE1 | 6        | 0.64          |
| (1,2245) | 1:162:A:ALA:HB2  | 1:168:A:PHE:HE2 | 6        | 0.64          |
| (1,2245) | 1:162:A:ALA:HB3  | 1:168:A:PHE:HE1 | 6        | 0.64          |
| (1,2245) | 1:162:A:ALA:HB3  | 1:168:A:PHE:HE2 | 6        | 0.64          |
| (1,2010) | 1:142:A:ILE:HD11 | 1:145:A:TYR:HD1 | 10       | 0.64          |
| (1,2010) | 1:142:A:ILE:HD11 | 1:145:A:TYR:HD2 | 10       | 0.64          |
| (1,2010) | 1:142:A:ILE:HD12 | 1:145:A:TYR:HD1 | 10       | 0.64          |
| (1,2010) | 1:142:A:ILE:HD12 | 1:145:A:TYR:HD2 | 10       | 0.64          |
| (1,2010) | 1:142:A:ILE:HD13 | 1:145:A:TYR:HD1 | 10       | 0.64          |
| (1,2010) | 1:142:A:ILE:HD13 | 1:145:A:TYR:HD2 | 10       | 0.64          |
| (1,923)  | 1:70:A:LEU:HD11  | 1:71:A:LYS:H    | 2        | 0.64          |
| (1,923)  | 1:70:A:LEU:HD12  | 1:71:A:LYS:H    | 2        | 0.64          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,923)  | 1:70:A:LEU:HD13  | 1:71:A:LYS:H     | 2        | 0.64          |
| (1,287)  | 1:36:A:ALA:HB1   | 1:36:A:ALA:H     | 5        | 0.64          |
| (1,287)  | 1:36:A:ALA:HB2   | 1:36:A:ALA:H     | 5        | 0.64          |
| (1,287)  | 1:36:A:ALA:HB3   | 1:36:A:ALA:H     | 5        | 0.64          |
| (1,145)  | 1:28:A:HIS:HE1   | 1:48:A:ILE:HD11  | 2        | 0.64          |
| (1,145)  | 1:28:A:HIS:HE1   | 1:48:A:ILE:HD12  | 2        | 0.64          |
| (1,145)  | 1:28:A:HIS:HE1   | 1:48:A:ILE:HD13  | 2        | 0.64          |
| (2,389)  | 1:70:A:LEU:HD21  | 1:172:A:PRO:HD2  | 5        | 0.63          |
| (2,389)  | 1:70:A:LEU:HD22  | 1:172:A:PRO:HD2  | 5        | 0.63          |
| (2,389)  | 1:70:A:LEU:HD23  | 1:172:A:PRO:HD2  | 5        | 0.63          |
| (2,380)  | 1:69:A:GLN:HE22  | 1:73:A:TYR:HE1   | 5        | 0.63          |
| (2,380)  | 1:69:A:GLN:HE22  | 1:73:A:TYR:HE2   | 5        | 0.63          |
| (1,2354) | 1:173:A:VAL:HG11 | 1:175:A:PHE:HE1  | 10       | 0.63          |
| (1,2354) | 1:173:A:VAL:HG11 | 1:175:A:PHE:HE2  | 10       | 0.63          |
| (1,2354) | 1:173:A:VAL:HG12 | 1:175:A:PHE:HE1  | 10       | 0.63          |
| (1,2354) | 1:173:A:VAL:HG12 | 1:175:A:PHE:HE2  | 10       | 0.63          |
| (1,2354) | 1:173:A:VAL:HG13 | 1:175:A:PHE:HE1  | 10       | 0.63          |
| (1,2354) | 1:173:A:VAL:HG13 | 1:175:A:PHE:HE2  | 10       | 0.63          |
| (1,2078) | 1:151:A:VAL:HG11 | 1:151:A:VAL:HG21 | 1        | 0.63          |
| (1,2078) | 1:151:A:VAL:HG11 | 1:151:A:VAL:HG22 | 1        | 0.63          |
| (1,2078) | 1:151:A:VAL:HG11 | 1:151:A:VAL:HG23 | 1        | 0.63          |
| (1,2078) | 1:151:A:VAL:HG12 | 1:151:A:VAL:HG21 | 1        | 0.63          |
| (1,2078) | 1:151:A:VAL:HG12 | 1:151:A:VAL:HG22 | 1        | 0.63          |
| (1,2078) | 1:151:A:VAL:HG12 | 1:151:A:VAL:HG23 | 1        | 0.63          |
| (1,2078) | 1:151:A:VAL:HG13 | 1:151:A:VAL:HG21 | 1        | 0.63          |
| (1,2078) | 1:151:A:VAL:HG13 | 1:151:A:VAL:HG22 | 1        | 0.63          |
| (1,2078) | 1:151:A:VAL:HG13 | 1:151:A:VAL:HG23 | 1        | 0.63          |
| (1,1940) | 1:135:A:VAL:HG11 | 1:155:A:ASN:HD21 | 9        | 0.63          |
| (1,1940) | 1:135:A:VAL:HG11 | 1:155:A:ASN:HD22 | 9        | 0.63          |
| (1,1940) | 1:135:A:VAL:HG12 | 1:155:A:ASN:HD21 | 9        | 0.63          |
| (1,1940) | 1:135:A:VAL:HG12 | 1:155:A:ASN:HD22 | 9        | 0.63          |
| (1,1940) | 1:135:A:VAL:HG13 | 1:155:A:ASN:HD21 | 9        | 0.63          |
| (1,1940) | 1:135:A:VAL:HG13 | 1:155:A:ASN:HD22 | 9        | 0.63          |
| (1,1884) | 1:134:A:TRP:HA   | 1:143:A:ILE:HD11 | 5        | 0.63          |
| (1,1884) | 1:134:A:TRP:HA   | 1:143:A:ILE:HD12 | 5        | 0.63          |
| (1,1884) | 1:134:A:TRP:HA   | 1:143:A:ILE:HD13 | 5        | 0.63          |
| (1,1777) | 1:121:A:LEU:HD21 | 1:121:A:LEU:H    | 2        | 0.63          |
| (1,1777) | 1:121:A:LEU:HD22 | 1:121:A:LEU:H    | 2        | 0.63          |
| (1,1777) | 1:121:A:LEU:HD23 | 1:121:A:LEU:H    | 2        | 0.63          |
| (1,1777) | 1:121:A:LEU:HD21 | 1:121:A:LEU:H    | 9        | 0.63          |
| (1,1777) | 1:121:A:LEU:HD22 | 1:121:A:LEU:H    | 9        | 0.63          |
| (1,1777) | 1:121:A:LEU:HD23 | 1:121:A:LEU:H    | 9        | 0.63          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1548) | 1:102:A:ILE:HG21 | 1:109:A:ALA:HB1  | 1        | 0.63          |
| (1,1548) | 1:102:A:ILE:HG21 | 1:109:A:ALA:HB2  | 1        | 0.63          |
| (1,1548) | 1:102:A:ILE:HG21 | 1:109:A:ALA:HB3  | 1        | 0.63          |
| (1,1548) | 1:102:A:ILE:HG22 | 1:109:A:ALA:HB1  | 1        | 0.63          |
| (1,1548) | 1:102:A:ILE:HG22 | 1:109:A:ALA:HB2  | 1        | 0.63          |
| (1,1548) | 1:102:A:ILE:HG22 | 1:109:A:ALA:HB3  | 1        | 0.63          |
| (1,1548) | 1:102:A:ILE:HG23 | 1:109:A:ALA:HB1  | 1        | 0.63          |
| (1,1548) | 1:102:A:ILE:HG23 | 1:109:A:ALA:HB2  | 1        | 0.63          |
| (1,1548) | 1:102:A:ILE:HG23 | 1:109:A:ALA:HB3  | 1        | 0.63          |
| (1,1215) | 1:81:A:ILE:HD11  | 1:100:A:ALA:HB1  | 10       | 0.63          |
| (1,1215) | 1:81:A:ILE:HD11  | 1:100:A:ALA:HB2  | 10       | 0.63          |
| (1,1215) | 1:81:A:ILE:HD11  | 1:100:A:ALA:HB3  | 10       | 0.63          |
| (1,1215) | 1:81:A:ILE:HD12  | 1:100:A:ALA:HB1  | 10       | 0.63          |
| (1,1215) | 1:81:A:ILE:HD12  | 1:100:A:ALA:HB2  | 10       | 0.63          |
| (1,1215) | 1:81:A:ILE:HD12  | 1:100:A:ALA:HB3  | 10       | 0.63          |
| (1,1215) | 1:81:A:ILE:HD13  | 1:100:A:ALA:HB1  | 10       | 0.63          |
| (1,1215) | 1:81:A:ILE:HD13  | 1:100:A:ALA:HB2  | 10       | 0.63          |
| (1,1215) | 1:81:A:ILE:HD13  | 1:100:A:ALA:HB3  | 10       | 0.63          |
| (1,991)  | 1:73:A:TYR:HE1   | 1:171:A:LEU:HD11 | 3        | 0.63          |
| (1,991)  | 1:73:A:TYR:HE1   | 1:171:A:LEU:HD12 | 3        | 0.63          |
| (1,991)  | 1:73:A:TYR:HE1   | 1:171:A:LEU:HD13 | 3        | 0.63          |
| (1,991)  | 1:73:A:TYR:HE2   | 1:171:A:LEU:HD11 | 3        | 0.63          |
| (1,991)  | 1:73:A:TYR:HE2   | 1:171:A:LEU:HD12 | 3        | 0.63          |
| (1,991)  | 1:73:A:TYR:HE2   | 1:171:A:LEU:HD13 | 3        | 0.63          |
| (1,599)  | 1:53:A:ASP:H     | 1:55:A:VAL:HG11  | 8        | 0.63          |
| (1,599)  | 1:53:A:ASP:H     | 1:55:A:VAL:HG12  | 8        | 0.63          |
| (1,599)  | 1:53:A:ASP:H     | 1:55:A:VAL:HG13  | 8        | 0.63          |
| (1,6)    | 1:18:A:ALA:HB1   | 1:19:A:VAL:H     | 4        | 0.63          |
| (1,6)    | 1:18:A:ALA:HB2   | 1:19:A:VAL:H     | 4        | 0.63          |
| (1,6)    | 1:18:A:ALA:HB3   | 1:19:A:VAL:H     | 4        | 0.63          |
| (2,632)  | 1:122:A:TYR:HD1  | 1:125:A:LYS:H    | 4        | 0.62          |
| (2,632)  | 1:122:A:TYR:HD2  | 1:125:A:LYS:H    | 4        | 0.62          |
| (2,490)  | 1:81:A:ILE:HD11  | 1:101:A:VAL:H    | 9        | 0.62          |
| (2,490)  | 1:81:A:ILE:HD12  | 1:101:A:VAL:H    | 9        | 0.62          |
| (2,490)  | 1:81:A:ILE:HD13  | 1:101:A:VAL:H    | 9        | 0.62          |
| (2,184)  | 1:37:A:GLY:H     | 1:38:A:ALA:HB1   | 3        | 0.62          |
| (2,184)  | 1:37:A:GLY:H     | 1:38:A:ALA:HB2   | 3        | 0.62          |
| (2,184)  | 1:37:A:GLY:H     | 1:38:A:ALA:HB3   | 3        | 0.62          |
| (1,2354) | 1:173:A:VAL:HG11 | 1:175:A:PHE:HE1  | 5        | 0.62          |
| (1,2354) | 1:173:A:VAL:HG11 | 1:175:A:PHE:HE2  | 5        | 0.62          |
| (1,2354) | 1:173:A:VAL:HG12 | 1:175:A:PHE:HE1  | 5        | 0.62          |
| (1,2354) | 1:173:A:VAL:HG12 | 1:175:A:PHE:HE2  | 5        | 0.62          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2354) | 1:173:A:VAL:HG13 | 1:175:A:PHE:HE1  | 5        | 0.62          |
| (1,2354) | 1:173:A:VAL:HG13 | 1:175:A:PHE:HE2  | 5        | 0.62          |
| (1,2304) | 1:170:A:SER:HA   | 1:171:A:LEU:HD21 | 6        | 0.62          |
| (1,2304) | 1:170:A:SER:HA   | 1:171:A:LEU:HD22 | 6        | 0.62          |
| (1,2304) | 1:170:A:SER:HA   | 1:171:A:LEU:HD23 | 6        | 0.62          |
| (1,1777) | 1:121:A:LEU:HD21 | 1:121:A:LEU:H    | 3        | 0.62          |
| (1,1777) | 1:121:A:LEU:HD22 | 1:121:A:LEU:H    | 3        | 0.62          |
| (1,1777) | 1:121:A:LEU:HD23 | 1:121:A:LEU:H    | 3        | 0.62          |
| (1,1777) | 1:121:A:LEU:HD21 | 1:121:A:LEU:H    | 4        | 0.62          |
| (1,1777) | 1:121:A:LEU:HD22 | 1:121:A:LEU:H    | 4        | 0.62          |
| (1,1777) | 1:121:A:LEU:HD23 | 1:121:A:LEU:H    | 4        | 0.62          |
| (1,1777) | 1:121:A:LEU:HD21 | 1:121:A:LEU:H    | 5        | 0.62          |
| (1,1777) | 1:121:A:LEU:HD22 | 1:121:A:LEU:H    | 5        | 0.62          |
| (1,1777) | 1:121:A:LEU:HD23 | 1:121:A:LEU:H    | 5        | 0.62          |
| (1,1243) | 1:81:A:ILE:HG21  | 1:156:A:PHE:HZ   | 2        | 0.62          |
| (1,1243) | 1:81:A:ILE:HG22  | 1:156:A:PHE:HZ   | 2        | 0.62          |
| (1,1243) | 1:81:A:ILE:HG23  | 1:156:A:PHE:HZ   | 2        | 0.62          |
| (1,991)  | 1:73:A:TYR:HE1   | 1:171:A:LEU:HD11 | 5        | 0.62          |
| (1,991)  | 1:73:A:TYR:HE1   | 1:171:A:LEU:HD12 | 5        | 0.62          |
| (1,991)  | 1:73:A:TYR:HE1   | 1:171:A:LEU:HD13 | 5        | 0.62          |
| (1,991)  | 1:73:A:TYR:HE2   | 1:171:A:LEU:HD11 | 5        | 0.62          |
| (1,991)  | 1:73:A:TYR:HE2   | 1:171:A:LEU:HD12 | 5        | 0.62          |
| (1,991)  | 1:73:A:TYR:HE2   | 1:171:A:LEU:HD13 | 5        | 0.62          |
| (1,599)  | 1:53:A:ASP:H     | 1:55:A:VAL:HG11  | 10       | 0.62          |
| (1,599)  | 1:53:A:ASP:H     | 1:55:A:VAL:HG12  | 10       | 0.62          |
| (1,599)  | 1:53:A:ASP:H     | 1:55:A:VAL:HG13  | 10       | 0.62          |
| (1,223)  | 1:32:A:ILE:HD11  | 1:160:A:TYR:HE1  | 2        | 0.62          |
| (1,223)  | 1:32:A:ILE:HD11  | 1:160:A:TYR:HE2  | 2        | 0.62          |
| (1,223)  | 1:32:A:ILE:HD12  | 1:160:A:TYR:HE1  | 2        | 0.62          |
| (1,223)  | 1:32:A:ILE:HD12  | 1:160:A:TYR:HE2  | 2        | 0.62          |
| (1,223)  | 1:32:A:ILE:HD13  | 1:160:A:TYR:HE1  | 2        | 0.62          |
| (1,223)  | 1:32:A:ILE:HD13  | 1:160:A:TYR:HE2  | 2        | 0.62          |
| (2,733)  | 1:157:A:LYS:HE2  | 1:159:A:PHE:HD1  | 9        | 0.61          |
| (2,733)  | 1:157:A:LYS:HE2  | 1:159:A:PHE:HD2  | 9        | 0.61          |
| (2,733)  | 1:157:A:LYS:HE3  | 1:159:A:PHE:HD1  | 9        | 0.61          |
| (2,733)  | 1:157:A:LYS:HE3  | 1:159:A:PHE:HD2  | 9        | 0.61          |
| (2,614)  | 1:118:A:ILE:HG21 | 1:151:A:VAL:HA   | 5        | 0.61          |
| (2,614)  | 1:118:A:ILE:HG22 | 1:151:A:VAL:HA   | 5        | 0.61          |
| (2,614)  | 1:118:A:ILE:HG23 | 1:151:A:VAL:HA   | 5        | 0.61          |
| (2,520)  | 1:84:A:GLY:HA2   | 1:155:A:ASN:HD21 | 2        | 0.61          |
| (2,520)  | 1:84:A:GLY:HA2   | 1:155:A:ASN:HD22 | 2        | 0.61          |
| (2,520)  | 1:84:A:GLY:HA3   | 1:155:A:ASN:HD21 | 2        | 0.61          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,520)  | 1:84:A:GLY:HA3   | 1:155:A:ASN:HD22 | 2        | 0.61          |
| (2,194)  | 1:38:A:ALA:HB1   | 1:39:A:GLN:HE21  | 3        | 0.61          |
| (2,194)  | 1:38:A:ALA:HB2   | 1:39:A:GLN:HE21  | 3        | 0.61          |
| (2,194)  | 1:38:A:ALA:HB3   | 1:39:A:GLN:HE21  | 3        | 0.61          |
| (1,2245) | 1:162:A:ALA:HB1  | 1:168:A:PHE:HE1  | 7        | 0.61          |
| (1,2245) | 1:162:A:ALA:HB1  | 1:168:A:PHE:HE2  | 7        | 0.61          |
| (1,2245) | 1:162:A:ALA:HB2  | 1:168:A:PHE:HE1  | 7        | 0.61          |
| (1,2245) | 1:162:A:ALA:HB2  | 1:168:A:PHE:HE2  | 7        | 0.61          |
| (1,2245) | 1:162:A:ALA:HB3  | 1:168:A:PHE:HE1  | 7        | 0.61          |
| (1,2245) | 1:162:A:ALA:HB3  | 1:168:A:PHE:HE2  | 7        | 0.61          |
| (1,1884) | 1:134:A:TRP:HA   | 1:143:A:ILE:HD11 | 4        | 0.61          |
| (1,1884) | 1:134:A:TRP:HA   | 1:143:A:ILE:HD12 | 4        | 0.61          |
| (1,1884) | 1:134:A:TRP:HA   | 1:143:A:ILE:HD13 | 4        | 0.61          |
| (1,1548) | 1:102:A:ILE:HG21 | 1:109:A:ALA:HB1  | 5        | 0.61          |
| (1,1548) | 1:102:A:ILE:HG21 | 1:109:A:ALA:HB2  | 5        | 0.61          |
| (1,1548) | 1:102:A:ILE:HG21 | 1:109:A:ALA:HB3  | 5        | 0.61          |
| (1,1548) | 1:102:A:ILE:HG22 | 1:109:A:ALA:HB1  | 5        | 0.61          |
| (1,1548) | 1:102:A:ILE:HG22 | 1:109:A:ALA:HB2  | 5        | 0.61          |
| (1,1548) | 1:102:A:ILE:HG22 | 1:109:A:ALA:HB3  | 5        | 0.61          |
| (1,1548) | 1:102:A:ILE:HG23 | 1:109:A:ALA:HB1  | 5        | 0.61          |
| (1,1548) | 1:102:A:ILE:HG23 | 1:109:A:ALA:HB2  | 5        | 0.61          |
| (1,1548) | 1:102:A:ILE:HG23 | 1:109:A:ALA:HB3  | 5        | 0.61          |
| (1,1342) | 1:85:A:TYR:HE1   | 1:143:A:ILE:HG21 | 3        | 0.61          |
| (1,1342) | 1:85:A:TYR:HE1   | 1:143:A:ILE:HG22 | 3        | 0.61          |
| (1,1342) | 1:85:A:TYR:HE1   | 1:143:A:ILE:HG23 | 3        | 0.61          |
| (1,1342) | 1:85:A:TYR:HE2   | 1:143:A:ILE:HG21 | 3        | 0.61          |
| (1,1342) | 1:85:A:TYR:HE2   | 1:143:A:ILE:HG22 | 3        | 0.61          |
| (1,1342) | 1:85:A:TYR:HE2   | 1:143:A:ILE:HG23 | 3        | 0.61          |
| (1,1274) | 1:82:A:THR:HG21  | 1:96:A:SER:HB3   | 10       | 0.61          |
| (1,1274) | 1:82:A:THR:HG22  | 1:96:A:SER:HB3   | 10       | 0.61          |
| (1,1274) | 1:82:A:THR:HG23  | 1:96:A:SER:HB3   | 10       | 0.61          |
| (1,756)  | 1:63:A:THR:HG21  | 1:108:A:SER:HB2  | 4        | 0.61          |
| (1,756)  | 1:63:A:THR:HG21  | 1:108:A:SER:HB3  | 4        | 0.61          |
| (1,756)  | 1:63:A:THR:HG22  | 1:108:A:SER:HB2  | 4        | 0.61          |
| (1,756)  | 1:63:A:THR:HG22  | 1:108:A:SER:HB3  | 4        | 0.61          |
| (1,756)  | 1:63:A:THR:HG23  | 1:108:A:SER:HB2  | 4        | 0.61          |
| (1,756)  | 1:63:A:THR:HG23  | 1:108:A:SER:HB3  | 4        | 0.61          |
| (1,139)  | 1:28:A:HIS:HD2   | 1:46:A:TYR:HE1   | 1        | 0.61          |
| (1,139)  | 1:28:A:HIS:HD2   | 1:46:A:TYR:HE2   | 1        | 0.61          |
| (1,139)  | 1:28:A:HIS:HD2   | 1:46:A:TYR:HE1   | 7        | 0.61          |
| (1,139)  | 1:28:A:HIS:HD2   | 1:46:A:TYR:HE2   | 7        | 0.61          |
| (2,656)  | 1:125:A:LYS:HB2  | 1:126:A:THR:H    | 7        | 0.6           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,656)  | 1:125:A:LYS:HB3  | 1:126:A:THR:H    | 7        | 0.6           |
| (2,614)  | 1:118:A:ILE:HG21 | 1:151:A:VAL:HA   | 1        | 0.6           |
| (2,614)  | 1:118:A:ILE:HG22 | 1:151:A:VAL:HA   | 1        | 0.6           |
| (2,614)  | 1:118:A:ILE:HG23 | 1:151:A:VAL:HA   | 1        | 0.6           |
| (2,239)  | 1:46:A:TYR:HB3   | 1:155:A:ASN:HD21 | 3        | 0.6           |
| (2,239)  | 1:46:A:TYR:HB3   | 1:155:A:ASN:HD22 | 3        | 0.6           |
| (2,94)   | 1:23:A:ILE:HD11  | 1:53:A:ASP:H     | 8        | 0.6           |
| (2,94)   | 1:23:A:ILE:HD12  | 1:53:A:ASP:H     | 8        | 0.6           |
| (2,94)   | 1:23:A:ILE:HD13  | 1:53:A:ASP:H     | 8        | 0.6           |
| (1,2324) | 1:171:A:LEU:HD21 | 1:171:A:LEU:H    | 6        | 0.6           |
| (1,2324) | 1:171:A:LEU:HD22 | 1:171:A:LEU:H    | 6        | 0.6           |
| (1,2324) | 1:171:A:LEU:HD23 | 1:171:A:LEU:H    | 6        | 0.6           |
| (1,2078) | 1:151:A:VAL:HG11 | 1:151:A:VAL:HG21 | 6        | 0.6           |
| (1,2078) | 1:151:A:VAL:HG11 | 1:151:A:VAL:HG22 | 6        | 0.6           |
| (1,2078) | 1:151:A:VAL:HG11 | 1:151:A:VAL:HG23 | 6        | 0.6           |
| (1,2078) | 1:151:A:VAL:HG12 | 1:151:A:VAL:HG21 | 6        | 0.6           |
| (1,2078) | 1:151:A:VAL:HG12 | 1:151:A:VAL:HG22 | 6        | 0.6           |
| (1,2078) | 1:151:A:VAL:HG12 | 1:151:A:VAL:HG23 | 6        | 0.6           |
| (1,2078) | 1:151:A:VAL:HG13 | 1:151:A:VAL:HG21 | 6        | 0.6           |
| (1,2078) | 1:151:A:VAL:HG13 | 1:151:A:VAL:HG22 | 6        | 0.6           |
| (1,2078) | 1:151:A:VAL:HG13 | 1:151:A:VAL:HG23 | 6        | 0.6           |
| (1,2078) | 1:151:A:VAL:HG11 | 1:151:A:VAL:HG21 | 10       | 0.6           |
| (1,2078) | 1:151:A:VAL:HG11 | 1:151:A:VAL:HG22 | 10       | 0.6           |
| (1,2078) | 1:151:A:VAL:HG11 | 1:151:A:VAL:HG23 | 10       | 0.6           |
| (1,2078) | 1:151:A:VAL:HG12 | 1:151:A:VAL:HG21 | 10       | 0.6           |
| (1,2078) | 1:151:A:VAL:HG12 | 1:151:A:VAL:HG22 | 10       | 0.6           |
| (1,2078) | 1:151:A:VAL:HG12 | 1:151:A:VAL:HG23 | 10       | 0.6           |
| (1,2078) | 1:151:A:VAL:HG13 | 1:151:A:VAL:HG21 | 10       | 0.6           |
| (1,2078) | 1:151:A:VAL:HG13 | 1:151:A:VAL:HG22 | 10       | 0.6           |
| (1,2078) | 1:151:A:VAL:HG13 | 1:151:A:VAL:HG23 | 10       | 0.6           |
| (1,1758) | 1:119:A:ALA:HB1  | 1:151:A:VAL:H    | 1        | 0.6           |
| (1,1758) | 1:119:A:ALA:HB2  | 1:151:A:VAL:H    | 1        | 0.6           |
| (1,1758) | 1:119:A:ALA:HB3  | 1:151:A:VAL:H    | 1        | 0.6           |
| (1,1758) | 1:119:A:ALA:HB1  | 1:151:A:VAL:H    | 4        | 0.6           |
| (1,1758) | 1:119:A:ALA:HB2  | 1:151:A:VAL:H    | 4        | 0.6           |
| (1,1758) | 1:119:A:ALA:HB3  | 1:151:A:VAL:H    | 4        | 0.6           |
| (1,1758) | 1:119:A:ALA:HB1  | 1:151:A:VAL:H    | 5        | 0.6           |
| (1,1758) | 1:119:A:ALA:HB2  | 1:151:A:VAL:H    | 5        | 0.6           |
| (1,1758) | 1:119:A:ALA:HB3  | 1:151:A:VAL:H    | 5        | 0.6           |
| (1,1758) | 1:119:A:ALA:HB1  | 1:151:A:VAL:H    | 7        | 0.6           |
| (1,1758) | 1:119:A:ALA:HB2  | 1:151:A:VAL:H    | 7        | 0.6           |
| (1,1758) | 1:119:A:ALA:HB3  | 1:151:A:VAL:H    | 7        | 0.6           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1206) | 1:81:A:ILE:HA   | 1:81:A:ILE:HG21 | 1        | 0.6           |
| (1,1206) | 1:81:A:ILE:HA   | 1:81:A:ILE:HG22 | 1        | 0.6           |
| (1,1206) | 1:81:A:ILE:HA   | 1:81:A:ILE:HG23 | 1        | 0.6           |
| (1,1206) | 1:81:A:ILE:HA   | 1:81:A:ILE:HG21 | 2        | 0.6           |
| (1,1206) | 1:81:A:ILE:HA   | 1:81:A:ILE:HG22 | 2        | 0.6           |
| (1,1206) | 1:81:A:ILE:HA   | 1:81:A:ILE:HG23 | 2        | 0.6           |
| (1,1206) | 1:81:A:ILE:HA   | 1:81:A:ILE:HG21 | 4        | 0.6           |
| (1,1206) | 1:81:A:ILE:HA   | 1:81:A:ILE:HG22 | 4        | 0.6           |
| (1,1206) | 1:81:A:ILE:HA   | 1:81:A:ILE:HG23 | 4        | 0.6           |
| (1,1206) | 1:81:A:ILE:HA   | 1:81:A:ILE:HG21 | 10       | 0.6           |
| (1,1206) | 1:81:A:ILE:HA   | 1:81:A:ILE:HG22 | 10       | 0.6           |
| (1,1206) | 1:81:A:ILE:HA   | 1:81:A:ILE:HG23 | 10       | 0.6           |
| (1,1088) | 1:77:A:LEU:HD11 | 1:78:A:GLN:H    | 8        | 0.6           |
| (1,1088) | 1:77:A:LEU:HD12 | 1:78:A:GLN:H    | 8        | 0.6           |
| (1,1088) | 1:77:A:LEU:HD13 | 1:78:A:GLN:H    | 8        | 0.6           |
| (1,1088) | 1:77:A:LEU:HD21 | 1:78:A:GLN:H    | 8        | 0.6           |
| (1,1088) | 1:77:A:LEU:HD22 | 1:78:A:GLN:H    | 8        | 0.6           |
| (1,1088) | 1:77:A:LEU:HD23 | 1:78:A:GLN:H    | 8        | 0.6           |
| (1,923)  | 1:70:A:LEU:HD11 | 1:71:A:LYS:H    | 1        | 0.6           |
| (1,923)  | 1:70:A:LEU:HD12 | 1:71:A:LYS:H    | 1        | 0.6           |
| (1,923)  | 1:70:A:LEU:HD13 | 1:71:A:LYS:H    | 1        | 0.6           |
| (1,650)  | 1:58:A:VAL:HG11 | 1:58:A:VAL:H    | 3        | 0.6           |
| (1,650)  | 1:58:A:VAL:HG12 | 1:58:A:VAL:H    | 3        | 0.6           |
| (1,650)  | 1:58:A:VAL:HG13 | 1:58:A:VAL:H    | 3        | 0.6           |
| (1,650)  | 1:58:A:VAL:HG21 | 1:58:A:VAL:H    | 3        | 0.6           |
| (1,650)  | 1:58:A:VAL:HG22 | 1:58:A:VAL:H    | 3        | 0.6           |
| (1,650)  | 1:58:A:VAL:HG23 | 1:58:A:VAL:H    | 3        | 0.6           |
| (1,650)  | 1:58:A:VAL:HG11 | 1:58:A:VAL:H    | 5        | 0.6           |
| (1,650)  | 1:58:A:VAL:HG12 | 1:58:A:VAL:H    | 5        | 0.6           |
| (1,650)  | 1:58:A:VAL:HG13 | 1:58:A:VAL:H    | 5        | 0.6           |
| (1,650)  | 1:58:A:VAL:HG21 | 1:58:A:VAL:H    | 5        | 0.6           |
| (1,650)  | 1:58:A:VAL:HG22 | 1:58:A:VAL:H    | 5        | 0.6           |
| (1,650)  | 1:58:A:VAL:HG23 | 1:58:A:VAL:H    | 5        | 0.6           |
| (2,656)  | 1:125:A:LYS:HB2 | 1:126:A:THR:H   | 1        | 0.59          |
| (2,656)  | 1:125:A:LYS:HB3 | 1:126:A:THR:H   | 1        | 0.59          |
| (2,656)  | 1:125:A:LYS:HB2 | 1:126:A:THR:H   | 8        | 0.59          |
| (2,656)  | 1:125:A:LYS:HB3 | 1:126:A:THR:H   | 8        | 0.59          |
| (2,535)  | 1:85:A:TYR:HE1  | 1:153:A:ILE:H   | 2        | 0.59          |
| (2,535)  | 1:85:A:TYR:HE2  | 1:153:A:ILE:H   | 2        | 0.59          |
| (2,4)    | 1:15:A:THR:HG21 | 1:16:A:ALA:H    | 2        | 0.59          |
| (2,4)    | 1:15:A:THR:HG22 | 1:16:A:ALA:H    | 2        | 0.59          |
| (2,4)    | 1:15:A:THR:HG23 | 1:16:A:ALA:H    | 2        | 0.59          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2355) | 1:173:A:VAL:HG21 | 1:173:A:VAL:H    | 6        | 0.59          |
| (1,2355) | 1:173:A:VAL:HG22 | 1:173:A:VAL:H    | 6        | 0.59          |
| (1,2355) | 1:173:A:VAL:HG23 | 1:173:A:VAL:H    | 6        | 0.59          |
| (1,2324) | 1:171:A:LEU:HD21 | 1:171:A:LEU:H    | 1        | 0.59          |
| (1,2324) | 1:171:A:LEU:HD22 | 1:171:A:LEU:H    | 1        | 0.59          |
| (1,2324) | 1:171:A:LEU:HD23 | 1:171:A:LEU:H    | 1        | 0.59          |
| (1,2287) | 1:168:A:PHE:HD1  | 1:169:A:ASP:H    | 2        | 0.59          |
| (1,2287) | 1:168:A:PHE:HD2  | 1:169:A:ASP:H    | 2        | 0.59          |
| (1,2032) | 1:143:A:ILE:HG21 | 1:144:A:VAL:H    | 2        | 0.59          |
| (1,2032) | 1:143:A:ILE:HG22 | 1:144:A:VAL:H    | 2        | 0.59          |
| (1,2032) | 1:143:A:ILE:HG23 | 1:144:A:VAL:H    | 2        | 0.59          |
| (1,1818) | 1:131:A:THR:HG21 | 1:131:A:THR:H    | 3        | 0.59          |
| (1,1818) | 1:131:A:THR:HG22 | 1:131:A:THR:H    | 3        | 0.59          |
| (1,1818) | 1:131:A:THR:HG23 | 1:131:A:THR:H    | 3        | 0.59          |
| (1,1758) | 1:119:A:ALA:HB1  | 1:151:A:VAL:H    | 2        | 0.59          |
| (1,1758) | 1:119:A:ALA:HB2  | 1:151:A:VAL:H    | 2        | 0.59          |
| (1,1758) | 1:119:A:ALA:HB3  | 1:151:A:VAL:H    | 2        | 0.59          |
| (1,1758) | 1:119:A:ALA:HB1  | 1:151:A:VAL:H    | 3        | 0.59          |
| (1,1758) | 1:119:A:ALA:HB2  | 1:151:A:VAL:H    | 3        | 0.59          |
| (1,1758) | 1:119:A:ALA:HB3  | 1:151:A:VAL:H    | 3        | 0.59          |
| (1,1342) | 1:85:A:TYR:HE1   | 1:143:A:ILE:HG21 | 10       | 0.59          |
| (1,1342) | 1:85:A:TYR:HE1   | 1:143:A:ILE:HG22 | 10       | 0.59          |
| (1,1342) | 1:85:A:TYR:HE1   | 1:143:A:ILE:HG23 | 10       | 0.59          |
| (1,1342) | 1:85:A:TYR:HE2   | 1:143:A:ILE:HG21 | 10       | 0.59          |
| (1,1342) | 1:85:A:TYR:HE2   | 1:143:A:ILE:HG22 | 10       | 0.59          |
| (1,1342) | 1:85:A:TYR:HE2   | 1:143:A:ILE:HG23 | 10       | 0.59          |
| (1,1275) | 1:82:A:THR:HG21  | 1:96:A:SER:HB2   | 1        | 0.59          |
| (1,1275) | 1:82:A:THR:HG22  | 1:96:A:SER:HB2   | 1        | 0.59          |
| (1,1275) | 1:82:A:THR:HG23  | 1:96:A:SER:HB2   | 1        | 0.59          |
| (1,1275) | 1:82:A:THR:HG21  | 1:96:A:SER:HB2   | 4        | 0.59          |
| (1,1275) | 1:82:A:THR:HG22  | 1:96:A:SER:HB2   | 4        | 0.59          |
| (1,1275) | 1:82:A:THR:HG23  | 1:96:A:SER:HB2   | 4        | 0.59          |
| (1,1215) | 1:81:A:ILE:HD11  | 1:100:A:ALA:HB1  | 1        | 0.59          |
| (1,1215) | 1:81:A:ILE:HD11  | 1:100:A:ALA:HB2  | 1        | 0.59          |
| (1,1215) | 1:81:A:ILE:HD11  | 1:100:A:ALA:HB3  | 1        | 0.59          |
| (1,1215) | 1:81:A:ILE:HD12  | 1:100:A:ALA:HB1  | 1        | 0.59          |
| (1,1215) | 1:81:A:ILE:HD12  | 1:100:A:ALA:HB2  | 1        | 0.59          |
| (1,1215) | 1:81:A:ILE:HD12  | 1:100:A:ALA:HB3  | 1        | 0.59          |
| (1,1215) | 1:81:A:ILE:HD13  | 1:100:A:ALA:HB1  | 1        | 0.59          |
| (1,1215) | 1:81:A:ILE:HD13  | 1:100:A:ALA:HB2  | 1        | 0.59          |
| (1,1215) | 1:81:A:ILE:HD13  | 1:100:A:ALA:HB3  | 1        | 0.59          |
| (1,1206) | 1:81:A:ILE:HA    | 1:81:A:ILE:HG21  | 7        | 0.59          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1206) | 1:81:A:ILE:HA   | 1:81:A:ILE:HG22  | 7        | 0.59          |
| (1,1206) | 1:81:A:ILE:HA   | 1:81:A:ILE:HG23  | 7        | 0.59          |
| (1,1206) | 1:81:A:ILE:HA   | 1:81:A:ILE:HG21  | 8        | 0.59          |
| (1,1206) | 1:81:A:ILE:HA   | 1:81:A:ILE:HG22  | 8        | 0.59          |
| (1,1206) | 1:81:A:ILE:HA   | 1:81:A:ILE:HG23  | 8        | 0.59          |
| (1,1206) | 1:81:A:ILE:HA   | 1:81:A:ILE:HG21  | 9        | 0.59          |
| (1,1206) | 1:81:A:ILE:HA   | 1:81:A:ILE:HG22  | 9        | 0.59          |
| (1,1206) | 1:81:A:ILE:HA   | 1:81:A:ILE:HG23  | 9        | 0.59          |
| (1,923)  | 1:70:A:LEU:HD11 | 1:71:A:LYS:H     | 7        | 0.59          |
| (1,923)  | 1:70:A:LEU:HD12 | 1:71:A:LYS:H     | 7        | 0.59          |
| (1,923)  | 1:70:A:LEU:HD13 | 1:71:A:LYS:H     | 7        | 0.59          |
| (1,508)  | 1:48:A:ILE:HG21 | 1:153:A:ILE:HG13 | 8        | 0.59          |
| (1,508)  | 1:48:A:ILE:HG22 | 1:153:A:ILE:HG13 | 8        | 0.59          |
| (1,508)  | 1:48:A:ILE:HG23 | 1:153:A:ILE:HG13 | 8        | 0.59          |
| (1,489)  | 1:48:A:ILE:HG21 | 1:48:A:ILE:HD11  | 3        | 0.59          |
| (1,489)  | 1:48:A:ILE:HG21 | 1:48:A:ILE:HD12  | 3        | 0.59          |
| (1,489)  | 1:48:A:ILE:HG21 | 1:48:A:ILE:HD13  | 3        | 0.59          |
| (1,489)  | 1:48:A:ILE:HG22 | 1:48:A:ILE:HD11  | 3        | 0.59          |
| (1,489)  | 1:48:A:ILE:HG22 | 1:48:A:ILE:HD12  | 3        | 0.59          |
| (1,489)  | 1:48:A:ILE:HG22 | 1:48:A:ILE:HD13  | 3        | 0.59          |
| (1,489)  | 1:48:A:ILE:HG23 | 1:48:A:ILE:HD11  | 3        | 0.59          |
| (1,489)  | 1:48:A:ILE:HG23 | 1:48:A:ILE:HD12  | 3        | 0.59          |
| (1,489)  | 1:48:A:ILE:HG23 | 1:48:A:ILE:HD13  | 3        | 0.59          |
| (1,287)  | 1:36:A:ALA:HB1  | 1:36:A:ALA:H     | 8        | 0.59          |
| (1,287)  | 1:36:A:ALA:HB2  | 1:36:A:ALA:H     | 8        | 0.59          |
| (1,287)  | 1:36:A:ALA:HB3  | 1:36:A:ALA:H     | 8        | 0.59          |
| (1,282)  | 1:35:A:ALA:HB1  | 1:36:A:ALA:H     | 1        | 0.59          |
| (1,282)  | 1:35:A:ALA:HB2  | 1:36:A:ALA:H     | 1        | 0.59          |
| (1,282)  | 1:35:A:ALA:HB3  | 1:36:A:ALA:H     | 1        | 0.59          |
| (2,766)  | 1:169:A:ASP:H   | 1:171:A:LEU:HD21 | 2        | 0.58          |
| (2,766)  | 1:169:A:ASP:H   | 1:171:A:LEU:HD22 | 2        | 0.58          |
| (2,766)  | 1:169:A:ASP:H   | 1:171:A:LEU:HD23 | 2        | 0.58          |
| (2,473)  | 1:80:A:GLN:HB2  | 1:101:A:VAL:HA   | 9        | 0.58          |
| (2,473)  | 1:80:A:GLN:HB3  | 1:101:A:VAL:HA   | 9        | 0.58          |
| (2,467)  | 1:79:A:ILE:HG21 | 1:156:A:PHE:HA   | 10       | 0.58          |
| (2,467)  | 1:79:A:ILE:HG22 | 1:156:A:PHE:HA   | 10       | 0.58          |
| (2,467)  | 1:79:A:ILE:HG23 | 1:156:A:PHE:HA   | 10       | 0.58          |
| (1,2284) | 1:168:A:PHE:HB2 | 1:171:A:LEU:HD11 | 6        | 0.58          |
| (1,2284) | 1:168:A:PHE:HB2 | 1:171:A:LEU:HD12 | 6        | 0.58          |
| (1,2284) | 1:168:A:PHE:HB2 | 1:171:A:LEU:HD13 | 6        | 0.58          |
| (1,1884) | 1:134:A:TRP:HA  | 1:143:A:ILE:HD11 | 8        | 0.58          |
| (1,1884) | 1:134:A:TRP:HA  | 1:143:A:ILE:HD12 | 8        | 0.58          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1884) | 1:134:A:TRP:HA   | 1:143:A:ILE:HD13 | 8        | 0.58          |
| (1,1758) | 1:119:A:ALA:HB1  | 1:151:A:VAL:H    | 10       | 0.58          |
| (1,1758) | 1:119:A:ALA:HB2  | 1:151:A:VAL:H    | 10       | 0.58          |
| (1,1758) | 1:119:A:ALA:HB3  | 1:151:A:VAL:H    | 10       | 0.58          |
| (1,1548) | 1:102:A:ILE:HG21 | 1:109:A:ALA:HB1  | 2        | 0.58          |
| (1,1548) | 1:102:A:ILE:HG21 | 1:109:A:ALA:HB2  | 2        | 0.58          |
| (1,1548) | 1:102:A:ILE:HG21 | 1:109:A:ALA:HB3  | 2        | 0.58          |
| (1,1548) | 1:102:A:ILE:HG22 | 1:109:A:ALA:HB1  | 2        | 0.58          |
| (1,1548) | 1:102:A:ILE:HG22 | 1:109:A:ALA:HB2  | 2        | 0.58          |
| (1,1548) | 1:102:A:ILE:HG22 | 1:109:A:ALA:HB3  | 2        | 0.58          |
| (1,1548) | 1:102:A:ILE:HG23 | 1:109:A:ALA:HB1  | 2        | 0.58          |
| (1,1548) | 1:102:A:ILE:HG23 | 1:109:A:ALA:HB2  | 2        | 0.58          |
| (1,1548) | 1:102:A:ILE:HG23 | 1:109:A:ALA:HB3  | 2        | 0.58          |
| (1,1522) | 1:100:A:ALA:H    | 1:111:A:ILE:HD11 | 3        | 0.58          |
| (1,1522) | 1:100:A:ALA:H    | 1:111:A:ILE:HD12 | 3        | 0.58          |
| (1,1522) | 1:100:A:ALA:H    | 1:111:A:ILE:HD13 | 3        | 0.58          |
| (1,1274) | 1:82:A:THR:HG21  | 1:96:A:SER:HB3   | 5        | 0.58          |
| (1,1274) | 1:82:A:THR:HG22  | 1:96:A:SER:HB3   | 5        | 0.58          |
| (1,1274) | 1:82:A:THR:HG23  | 1:96:A:SER:HB3   | 5        | 0.58          |
| (1,1206) | 1:81:A:ILE:HA    | 1:81:A:ILE:HG21  | 3        | 0.58          |
| (1,1206) | 1:81:A:ILE:HA    | 1:81:A:ILE:HG22  | 3        | 0.58          |
| (1,1206) | 1:81:A:ILE:HA    | 1:81:A:ILE:HG23  | 3        | 0.58          |
| (1,1206) | 1:81:A:ILE:HA    | 1:81:A:ILE:HG21  | 5        | 0.58          |
| (1,1206) | 1:81:A:ILE:HA    | 1:81:A:ILE:HG22  | 5        | 0.58          |
| (1,1206) | 1:81:A:ILE:HA    | 1:81:A:ILE:HG23  | 5        | 0.58          |
| (1,1206) | 1:81:A:ILE:HA    | 1:81:A:ILE:HG21  | 6        | 0.58          |
| (1,1206) | 1:81:A:ILE:HA    | 1:81:A:ILE:HG22  | 6        | 0.58          |
| (1,1206) | 1:81:A:ILE:HA    | 1:81:A:ILE:HG23  | 6        | 0.58          |
| (1,1097) | 1:77:A:LEU:HD11  | 1:160:A:TYR:HB3  | 1        | 0.58          |
| (1,1097) | 1:77:A:LEU:HD12  | 1:160:A:TYR:HB3  | 1        | 0.58          |
| (1,1097) | 1:77:A:LEU:HD13  | 1:160:A:TYR:HB3  | 1        | 0.58          |
| (1,1097) | 1:77:A:LEU:HD21  | 1:160:A:TYR:HB3  | 1        | 0.58          |
| (1,1097) | 1:77:A:LEU:HD22  | 1:160:A:TYR:HB3  | 1        | 0.58          |
| (1,1097) | 1:77:A:LEU:HD23  | 1:160:A:TYR:HB3  | 1        | 0.58          |
| (1,1097) | 1:77:A:LEU:HD11  | 1:160:A:TYR:HB3  | 2        | 0.58          |
| (1,1097) | 1:77:A:LEU:HD12  | 1:160:A:TYR:HB3  | 2        | 0.58          |
| (1,1097) | 1:77:A:LEU:HD13  | 1:160:A:TYR:HB3  | 2        | 0.58          |
| (1,1097) | 1:77:A:LEU:HD21  | 1:160:A:TYR:HB3  | 2        | 0.58          |
| (1,1097) | 1:77:A:LEU:HD22  | 1:160:A:TYR:HB3  | 2        | 0.58          |
| (1,1097) | 1:77:A:LEU:HD23  | 1:160:A:TYR:HB3  | 2        | 0.58          |
| (1,756)  | 1:63:A:THR:HG21  | 1:108:A:SER:HB2  | 9        | 0.58          |
| (1,756)  | 1:63:A:THR:HG21  | 1:108:A:SER:HB3  | 9        | 0.58          |

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| Key     | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,756) | 1:63:A:THR:HG22 | 1:108:A:SER:HB2  | 9        | 0.58          |
| (1,756) | 1:63:A:THR:HG22 | 1:108:A:SER:HB3  | 9        | 0.58          |
| (1,756) | 1:63:A:THR:HG23 | 1:108:A:SER:HB2  | 9        | 0.58          |
| (1,756) | 1:63:A:THR:HG23 | 1:108:A:SER:HB3  | 9        | 0.58          |
| (1,508) | 1:48:A:ILE:HG21 | 1:153:A:ILE:HG13 | 3        | 0.58          |
| (1,508) | 1:48:A:ILE:HG22 | 1:153:A:ILE:HG13 | 3        | 0.58          |
| (1,508) | 1:48:A:ILE:HG23 | 1:153:A:ILE:HG13 | 3        | 0.58          |
| (3,8)   | 1:111:A:ILE:HA  | 1:111:A:ILE:HG21 | 5        | 0.57          |
| (3,8)   | 1:111:A:ILE:HA  | 1:111:A:ILE:HG22 | 5        | 0.57          |
| (3,8)   | 1:111:A:ILE:HA  | 1:111:A:ILE:HG23 | 5        | 0.57          |
| (3,8)   | 1:111:A:ILE:HA  | 1:111:A:ILE:HG21 | 6        | 0.57          |
| (3,8)   | 1:111:A:ILE:HA  | 1:111:A:ILE:HG22 | 6        | 0.57          |
| (3,8)   | 1:111:A:ILE:HA  | 1:111:A:ILE:HG23 | 6        | 0.57          |
| (2,656) | 1:125:A:LYS:HB2 | 1:126:A:THR:H    | 4        | 0.57          |
| (2,656) | 1:125:A:LYS:HB3 | 1:126:A:THR:H    | 4        | 0.57          |
| (2,656) | 1:125:A:LYS:HB2 | 1:126:A:THR:H    | 6        | 0.57          |
| (2,656) | 1:125:A:LYS:HB3 | 1:126:A:THR:H    | 6        | 0.57          |
| (2,520) | 1:84:A:GLY:HA2  | 1:155:A:ASN:HD21 | 7        | 0.57          |
| (2,520) | 1:84:A:GLY:HA2  | 1:155:A:ASN:HD22 | 7        | 0.57          |
| (2,520) | 1:84:A:GLY:HA3  | 1:155:A:ASN:HD21 | 7        | 0.57          |
| (2,520) | 1:84:A:GLY:HA3  | 1:155:A:ASN:HD22 | 7        | 0.57          |
| (2,507) | 1:82:A:THR:H    | 1:156:A:PHE:HD1  | 1        | 0.57          |
| (2,507) | 1:82:A:THR:H    | 1:156:A:PHE:HD2  | 1        | 0.57          |
| (2,473) | 1:80:A:GLN:HB2  | 1:101:A:VAL:HA   | 1        | 0.57          |
| (2,473) | 1:80:A:GLN:HB3  | 1:101:A:VAL:HA   | 1        | 0.57          |
| (2,473) | 1:80:A:GLN:HB2  | 1:101:A:VAL:HA   | 6        | 0.57          |
| (2,473) | 1:80:A:GLN:HB3  | 1:101:A:VAL:HA   | 6        | 0.57          |
| (2,473) | 1:80:A:GLN:HB2  | 1:101:A:VAL:HA   | 10       | 0.57          |
| (2,473) | 1:80:A:GLN:HB3  | 1:101:A:VAL:HA   | 10       | 0.57          |
| (2,467) | 1:79:A:ILE:HG21 | 1:156:A:PHE:HA   | 4        | 0.57          |
| (2,467) | 1:79:A:ILE:HG22 | 1:156:A:PHE:HA   | 4        | 0.57          |
| (2,467) | 1:79:A:ILE:HG23 | 1:156:A:PHE:HA   | 4        | 0.57          |
| (2,380) | 1:69:A:GLN:HE22 | 1:73:A:TYR:HE1   | 3        | 0.57          |
| (2,380) | 1:69:A:GLN:HE22 | 1:73:A:TYR:HE2   | 3        | 0.57          |
| (2,380) | 1:69:A:GLN:HE22 | 1:73:A:TYR:HE1   | 6        | 0.57          |
| (2,380) | 1:69:A:GLN:HE22 | 1:73:A:TYR:HE2   | 6        | 0.57          |
| (2,239) | 1:46:A:TYR:HB3  | 1:155:A:ASN:HD21 | 1        | 0.57          |
| (2,239) | 1:46:A:TYR:HB3  | 1:155:A:ASN:HD22 | 1        | 0.57          |
| (2,239) | 1:46:A:TYR:HB3  | 1:155:A:ASN:HD21 | 4        | 0.57          |
| (2,239) | 1:46:A:TYR:HB3  | 1:155:A:ASN:HD22 | 4        | 0.57          |
| (2,239) | 1:46:A:TYR:HB3  | 1:155:A:ASN:HD21 | 6        | 0.57          |
| (2,239) | 1:46:A:TYR:HB3  | 1:155:A:ASN:HD22 | 6        | 0.57          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,239)  | 1:46:A:TYR:HB3   | 1:155:A:ASN:HD21 | 8        | 0.57          |
| (2,239)  | 1:46:A:TYR:HB3   | 1:155:A:ASN:HD22 | 8        | 0.57          |
| (2,239)  | 1:46:A:TYR:HB3   | 1:155:A:ASN:HD21 | 10       | 0.57          |
| (2,239)  | 1:46:A:TYR:HB3   | 1:155:A:ASN:HD22 | 10       | 0.57          |
| (2,7)    | 1:16:A:ALA:HB1   | 1:18:A:ALA:H     | 7        | 0.57          |
| (2,7)    | 1:16:A:ALA:HB2   | 1:18:A:ALA:H     | 7        | 0.57          |
| (2,7)    | 1:16:A:ALA:HB3   | 1:18:A:ALA:H     | 7        | 0.57          |
| (1,2324) | 1:171:A:LEU:HD21 | 1:171:A:LEU:H    | 3        | 0.57          |
| (1,2324) | 1:171:A:LEU:HD22 | 1:171:A:LEU:H    | 3        | 0.57          |
| (1,2324) | 1:171:A:LEU:HD23 | 1:171:A:LEU:H    | 3        | 0.57          |
| (1,2324) | 1:171:A:LEU:HD21 | 1:171:A:LEU:H    | 7        | 0.57          |
| (1,2324) | 1:171:A:LEU:HD22 | 1:171:A:LEU:H    | 7        | 0.57          |
| (1,2324) | 1:171:A:LEU:HD23 | 1:171:A:LEU:H    | 7        | 0.57          |
| (1,991)  | 1:73:A:TYR:HE1   | 1:171:A:LEU:HD11 | 8        | 0.57          |
| (1,991)  | 1:73:A:TYR:HE1   | 1:171:A:LEU:HD12 | 8        | 0.57          |
| (1,991)  | 1:73:A:TYR:HE1   | 1:171:A:LEU:HD13 | 8        | 0.57          |
| (1,991)  | 1:73:A:TYR:HE2   | 1:171:A:LEU:HD11 | 8        | 0.57          |
| (1,991)  | 1:73:A:TYR:HE2   | 1:171:A:LEU:HD12 | 8        | 0.57          |
| (1,991)  | 1:73:A:TYR:HE2   | 1:171:A:LEU:HD13 | 8        | 0.57          |
| (1,508)  | 1:48:A:ILE:HG21  | 1:153:A:ILE:HG13 | 2        | 0.57          |
| (1,508)  | 1:48:A:ILE:HG22  | 1:153:A:ILE:HG13 | 2        | 0.57          |
| (1,508)  | 1:48:A:ILE:HG23  | 1:153:A:ILE:HG13 | 2        | 0.57          |
| (1,296)  | 1:38:A:ALA:HB1   | 1:39:A:GLN:H     | 9        | 0.57          |
| (1,296)  | 1:38:A:ALA:HB2   | 1:39:A:GLN:H     | 9        | 0.57          |
| (1,296)  | 1:38:A:ALA:HB3   | 1:39:A:GLN:H     | 9        | 0.57          |
| (1,282)  | 1:35:A:ALA:HB1   | 1:36:A:ALA:H     | 6        | 0.57          |
| (1,282)  | 1:35:A:ALA:HB2   | 1:36:A:ALA:H     | 6        | 0.57          |
| (1,282)  | 1:35:A:ALA:HB3   | 1:36:A:ALA:H     | 6        | 0.57          |
| (1,166)  | 1:29:A:LEU:HD11  | 1:175:A:PHE:H    | 1        | 0.57          |
| (1,166)  | 1:29:A:LEU:HD12  | 1:175:A:PHE:H    | 1        | 0.57          |
| (1,166)  | 1:29:A:LEU:HD13  | 1:175:A:PHE:H    | 1        | 0.57          |
| (3,8)    | 1:111:A:ILE:HA   | 1:111:A:ILE:HG21 | 4        | 0.56          |
| (3,8)    | 1:111:A:ILE:HA   | 1:111:A:ILE:HG22 | 4        | 0.56          |
| (3,8)    | 1:111:A:ILE:HA   | 1:111:A:ILE:HG23 | 4        | 0.56          |
| (3,8)    | 1:111:A:ILE:HA   | 1:111:A:ILE:HG21 | 7        | 0.56          |
| (3,8)    | 1:111:A:ILE:HA   | 1:111:A:ILE:HG22 | 7        | 0.56          |
| (3,8)    | 1:111:A:ILE:HA   | 1:111:A:ILE:HG23 | 7        | 0.56          |
| (2,733)  | 1:157:A:LYS:HE2  | 1:159:A:PHE:HD1  | 3        | 0.56          |
| (2,733)  | 1:157:A:LYS:HE2  | 1:159:A:PHE:HD2  | 3        | 0.56          |
| (2,733)  | 1:157:A:LYS:HE3  | 1:159:A:PHE:HD1  | 3        | 0.56          |
| (2,733)  | 1:157:A:LYS:HE3  | 1:159:A:PHE:HD2  | 3        | 0.56          |
| (2,733)  | 1:157:A:LYS:HE2  | 1:159:A:PHE:HD1  | 7        | 0.56          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,733)  | 1:157:A:LYS:HE2  | 1:159:A:PHE:HD2  | 7        | 0.56          |
| (2,733)  | 1:157:A:LYS:HE3  | 1:159:A:PHE:HD1  | 7        | 0.56          |
| (2,733)  | 1:157:A:LYS:HE3  | 1:159:A:PHE:HD2  | 7        | 0.56          |
| (2,721)  | 1:144:A:VAL:HA   | 1:145:A:TYR:HD1  | 6        | 0.56          |
| (2,721)  | 1:144:A:VAL:HA   | 1:145:A:TYR:HD2  | 6        | 0.56          |
| (2,656)  | 1:125:A:LYS:HB2  | 1:126:A:THR:H    | 2        | 0.56          |
| (2,656)  | 1:125:A:LYS:HB3  | 1:126:A:THR:H    | 2        | 0.56          |
| (2,656)  | 1:125:A:LYS:HB2  | 1:126:A:THR:H    | 9        | 0.56          |
| (2,656)  | 1:125:A:LYS:HB3  | 1:126:A:THR:H    | 9        | 0.56          |
| (2,618)  | 1:119:A:ALA:HB1  | 1:149:A:LYS:H    | 6        | 0.56          |
| (2,618)  | 1:119:A:ALA:HB2  | 1:149:A:LYS:H    | 6        | 0.56          |
| (2,618)  | 1:119:A:ALA:HB3  | 1:149:A:LYS:H    | 6        | 0.56          |
| (2,535)  | 1:85:A:TYR:HE1   | 1:153:A:ILE:H    | 4        | 0.56          |
| (2,535)  | 1:85:A:TYR:HE2   | 1:153:A:ILE:H    | 4        | 0.56          |
| (2,535)  | 1:85:A:TYR:HE1   | 1:153:A:ILE:H    | 6        | 0.56          |
| (2,535)  | 1:85:A:TYR:HE2   | 1:153:A:ILE:H    | 6        | 0.56          |
| (2,535)  | 1:85:A:TYR:HE1   | 1:153:A:ILE:H    | 10       | 0.56          |
| (2,535)  | 1:85:A:TYR:HE2   | 1:153:A:ILE:H    | 10       | 0.56          |
| (2,518)  | 1:84:A:GLY:HA2   | 1:95:A:PHE:HE1   | 7        | 0.56          |
| (2,518)  | 1:84:A:GLY:HA2   | 1:95:A:PHE:HE2   | 7        | 0.56          |
| (2,518)  | 1:84:A:GLY:HA3   | 1:95:A:PHE:HE1   | 7        | 0.56          |
| (2,518)  | 1:84:A:GLY:HA3   | 1:95:A:PHE:HE2   | 7        | 0.56          |
| (2,473)  | 1:80:A:GLN:HB2   | 1:101:A:VAL:HA   | 3        | 0.56          |
| (2,473)  | 1:80:A:GLN:HB3   | 1:101:A:VAL:HA   | 3        | 0.56          |
| (2,365)  | 1:66:A:ASN:HB3   | 1:173:A:VAL:HG21 | 8        | 0.56          |
| (2,365)  | 1:66:A:ASN:HB3   | 1:173:A:VAL:HG22 | 8        | 0.56          |
| (2,365)  | 1:66:A:ASN:HB3   | 1:173:A:VAL:HG23 | 8        | 0.56          |
| (2,7)    | 1:16:A:ALA:HB1   | 1:18:A:ALA:H     | 4        | 0.56          |
| (2,7)    | 1:16:A:ALA:HB2   | 1:18:A:ALA:H     | 4        | 0.56          |
| (2,7)    | 1:16:A:ALA:HB3   | 1:18:A:ALA:H     | 4        | 0.56          |
| (1,2245) | 1:162:A:ALA:HB1  | 1:168:A:PHE:HE1  | 4        | 0.56          |
| (1,2245) | 1:162:A:ALA:HB1  | 1:168:A:PHE:HE2  | 4        | 0.56          |
| (1,2245) | 1:162:A:ALA:HB2  | 1:168:A:PHE:HE1  | 4        | 0.56          |
| (1,2245) | 1:162:A:ALA:HB2  | 1:168:A:PHE:HE2  | 4        | 0.56          |
| (1,2245) | 1:162:A:ALA:HB3  | 1:168:A:PHE:HE1  | 4        | 0.56          |
| (1,2245) | 1:162:A:ALA:HB3  | 1:168:A:PHE:HE2  | 4        | 0.56          |
| (1,1747) | 1:118:A:ILE:HD11 | 1:118:A:ILE:H    | 9        | 0.56          |
| (1,1747) | 1:118:A:ILE:HD12 | 1:118:A:ILE:H    | 9        | 0.56          |
| (1,1747) | 1:118:A:ILE:HD13 | 1:118:A:ILE:H    | 9        | 0.56          |
| (1,1548) | 1:102:A:ILE:HG21 | 1:109:A:ALA:HB1  | 3        | 0.56          |
| (1,1548) | 1:102:A:ILE:HG21 | 1:109:A:ALA:HB2  | 3        | 0.56          |
| (1,1548) | 1:102:A:ILE:HG21 | 1:109:A:ALA:HB3  | 3        | 0.56          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1548) | 1:102:A:ILE:HG22 | 1:109:A:ALA:HB1  | 3        | 0.56          |
| (1,1548) | 1:102:A:ILE:HG22 | 1:109:A:ALA:HB2  | 3        | 0.56          |
| (1,1548) | 1:102:A:ILE:HG22 | 1:109:A:ALA:HB3  | 3        | 0.56          |
| (1,1548) | 1:102:A:ILE:HG23 | 1:109:A:ALA:HB1  | 3        | 0.56          |
| (1,1548) | 1:102:A:ILE:HG23 | 1:109:A:ALA:HB2  | 3        | 0.56          |
| (1,1548) | 1:102:A:ILE:HG23 | 1:109:A:ALA:HB3  | 3        | 0.56          |
| (1,1215) | 1:81:A:ILE:HD11  | 1:100:A:ALA:HB1  | 4        | 0.56          |
| (1,1215) | 1:81:A:ILE:HD11  | 1:100:A:ALA:HB2  | 4        | 0.56          |
| (1,1215) | 1:81:A:ILE:HD11  | 1:100:A:ALA:HB3  | 4        | 0.56          |
| (1,1215) | 1:81:A:ILE:HD12  | 1:100:A:ALA:HB1  | 4        | 0.56          |
| (1,1215) | 1:81:A:ILE:HD12  | 1:100:A:ALA:HB2  | 4        | 0.56          |
| (1,1215) | 1:81:A:ILE:HD12  | 1:100:A:ALA:HB3  | 4        | 0.56          |
| (1,1215) | 1:81:A:ILE:HD13  | 1:100:A:ALA:HB1  | 4        | 0.56          |
| (1,1215) | 1:81:A:ILE:HD13  | 1:100:A:ALA:HB2  | 4        | 0.56          |
| (1,1215) | 1:81:A:ILE:HD13  | 1:100:A:ALA:HB3  | 4        | 0.56          |
| (1,1103) | 1:77:A:LEU:H     | 1:104:A:LEU:HD11 | 10       | 0.56          |
| (1,1103) | 1:77:A:LEU:H     | 1:104:A:LEU:HD12 | 10       | 0.56          |
| (1,1103) | 1:77:A:LEU:H     | 1:104:A:LEU:HD13 | 10       | 0.56          |
| (1,1099) | 1:77:A:LEU:HD11  | 1:160:A:TYR:HD1  | 2        | 0.56          |
| (1,1099) | 1:77:A:LEU:HD11  | 1:160:A:TYR:HD2  | 2        | 0.56          |
| (1,1099) | 1:77:A:LEU:HD12  | 1:160:A:TYR:HD1  | 2        | 0.56          |
| (1,1099) | 1:77:A:LEU:HD12  | 1:160:A:TYR:HD2  | 2        | 0.56          |
| (1,1099) | 1:77:A:LEU:HD13  | 1:160:A:TYR:HD1  | 2        | 0.56          |
| (1,1099) | 1:77:A:LEU:HD13  | 1:160:A:TYR:HD2  | 2        | 0.56          |
| (1,1099) | 1:77:A:LEU:HD21  | 1:160:A:TYR:HD1  | 2        | 0.56          |
| (1,1099) | 1:77:A:LEU:HD21  | 1:160:A:TYR:HD2  | 2        | 0.56          |
| (1,1099) | 1:77:A:LEU:HD22  | 1:160:A:TYR:HD1  | 2        | 0.56          |
| (1,1099) | 1:77:A:LEU:HD22  | 1:160:A:TYR:HD2  | 2        | 0.56          |
| (1,1099) | 1:77:A:LEU:HD23  | 1:160:A:TYR:HD1  | 2        | 0.56          |
| (1,1099) | 1:77:A:LEU:HD23  | 1:160:A:TYR:HD2  | 2        | 0.56          |
| (1,287)  | 1:36:A:ALA:HB1   | 1:36:A:ALA:H     | 2        | 0.56          |
| (1,287)  | 1:36:A:ALA:HB2   | 1:36:A:ALA:H     | 2        | 0.56          |
| (1,287)  | 1:36:A:ALA:HB3   | 1:36:A:ALA:H     | 2        | 0.56          |
| (1,282)  | 1:35:A:ALA:HB1   | 1:36:A:ALA:H     | 5        | 0.56          |
| (1,282)  | 1:35:A:ALA:HB2   | 1:36:A:ALA:H     | 5        | 0.56          |
| (1,282)  | 1:35:A:ALA:HB3   | 1:36:A:ALA:H     | 5        | 0.56          |
| (1,282)  | 1:35:A:ALA:HB1   | 1:36:A:ALA:H     | 7        | 0.56          |
| (1,282)  | 1:35:A:ALA:HB2   | 1:36:A:ALA:H     | 7        | 0.56          |
| (1,282)  | 1:35:A:ALA:HB3   | 1:36:A:ALA:H     | 7        | 0.56          |
| (1,139)  | 1:28:A:HIS:HD2   | 1:46:A:TYR:HE1   | 5        | 0.56          |
| (1,139)  | 1:28:A:HIS:HD2   | 1:46:A:TYR:HE2   | 5        | 0.56          |
| (1,6)    | 1:18:A:ALA:HB1   | 1:19:A:VAL:H     | 10       | 0.56          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,6)    | 1:18:A:ALA:HB2   | 1:19:A:VAL:H     | 10       | 0.56          |
| (1,6)    | 1:18:A:ALA:HB3   | 1:19:A:VAL:H     | 10       | 0.56          |
| (3,8)    | 1:111:A:ILE:HA   | 1:111:A:ILE:HG21 | 8        | 0.55          |
| (3,8)    | 1:111:A:ILE:HA   | 1:111:A:ILE:HG22 | 8        | 0.55          |
| (3,8)    | 1:111:A:ILE:HA   | 1:111:A:ILE:HG23 | 8        | 0.55          |
| (2,768)  | 1:173:A:VAL:HB   | 1:175:A:PHE:HE1  | 6        | 0.55          |
| (2,768)  | 1:173:A:VAL:HB   | 1:175:A:PHE:HE2  | 6        | 0.55          |
| (2,740)  | 1:162:A:ALA:HA   | 1:168:A:PHE:HE1  | 7        | 0.55          |
| (2,740)  | 1:162:A:ALA:HA   | 1:168:A:PHE:HE2  | 7        | 0.55          |
| (2,656)  | 1:125:A:LYS:HB2  | 1:126:A:THR:H    | 5        | 0.55          |
| (2,656)  | 1:125:A:LYS:HB3  | 1:126:A:THR:H    | 5        | 0.55          |
| (2,535)  | 1:85:A:TYR:HE1   | 1:153:A:ILE:H    | 5        | 0.55          |
| (2,535)  | 1:85:A:TYR:HE2   | 1:153:A:ILE:H    | 5        | 0.55          |
| (2,535)  | 1:85:A:TYR:HE1   | 1:153:A:ILE:H    | 9        | 0.55          |
| (2,535)  | 1:85:A:TYR:HE2   | 1:153:A:ILE:H    | 9        | 0.55          |
| (2,490)  | 1:81:A:ILE:HD11  | 1:101:A:VAL:H    | 1        | 0.55          |
| (2,490)  | 1:81:A:ILE:HD12  | 1:101:A:VAL:H    | 1        | 0.55          |
| (2,490)  | 1:81:A:ILE:HD13  | 1:101:A:VAL:H    | 1        | 0.55          |
| (2,473)  | 1:80:A:GLN:HB2   | 1:101:A:VAL:HA   | 2        | 0.55          |
| (2,473)  | 1:80:A:GLN:HB3   | 1:101:A:VAL:HA   | 2        | 0.55          |
| (2,367)  | 1:66:A:ASN:HD21  | 1:173:A:VAL:HG11 | 6        | 0.55          |
| (2,367)  | 1:66:A:ASN:HD21  | 1:173:A:VAL:HG12 | 6        | 0.55          |
| (2,367)  | 1:66:A:ASN:HD21  | 1:173:A:VAL:HG13 | 6        | 0.55          |
| (2,194)  | 1:38:A:ALA:HB1   | 1:39:A:GLN:HE21  | 5        | 0.55          |
| (2,194)  | 1:38:A:ALA:HB2   | 1:39:A:GLN:HE21  | 5        | 0.55          |
| (2,194)  | 1:38:A:ALA:HB3   | 1:39:A:GLN:HE21  | 5        | 0.55          |
| (2,5)    | 1:16:A:ALA:HB1   | 1:17:A:GLN:HE21  | 3        | 0.55          |
| (2,5)    | 1:16:A:ALA:HB2   | 1:17:A:GLN:HE21  | 3        | 0.55          |
| (2,5)    | 1:16:A:ALA:HB3   | 1:17:A:GLN:HE21  | 3        | 0.55          |
| (1,2324) | 1:171:A:LEU:HD21 | 1:171:A:LEU:H    | 4        | 0.55          |
| (1,2324) | 1:171:A:LEU:HD22 | 1:171:A:LEU:H    | 4        | 0.55          |
| (1,2324) | 1:171:A:LEU:HD23 | 1:171:A:LEU:H    | 4        | 0.55          |
| (1,1747) | 1:118:A:ILE:HD11 | 1:118:A:ILE:H    | 4        | 0.55          |
| (1,1747) | 1:118:A:ILE:HD12 | 1:118:A:ILE:H    | 4        | 0.55          |
| (1,1747) | 1:118:A:ILE:HD13 | 1:118:A:ILE:H    | 4        | 0.55          |
| (1,1274) | 1:82:A:THR:HG21  | 1:96:A:SER:HB3   | 2        | 0.55          |
| (1,1274) | 1:82:A:THR:HG22  | 1:96:A:SER:HB3   | 2        | 0.55          |
| (1,1274) | 1:82:A:THR:HG23  | 1:96:A:SER:HB3   | 2        | 0.55          |
| (1,991)  | 1:73:A:TYR:HE1   | 1:171:A:LEU:HD11 | 4        | 0.55          |
| (1,991)  | 1:73:A:TYR:HE1   | 1:171:A:LEU:HD12 | 4        | 0.55          |
| (1,991)  | 1:73:A:TYR:HE1   | 1:171:A:LEU:HD13 | 4        | 0.55          |
| (1,991)  | 1:73:A:TYR:HE2   | 1:171:A:LEU:HD11 | 4        | 0.55          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,991)  | 1:73:A:TYR:HE2   | 1:171:A:LEU:HD12 | 4        | 0.55          |
| (1,991)  | 1:73:A:TYR:HE2   | 1:171:A:LEU:HD13 | 4        | 0.55          |
| (1,923)  | 1:70:A:LEU:HD11  | 1:71:A:LYS:H     | 6        | 0.55          |
| (1,923)  | 1:70:A:LEU:HD12  | 1:71:A:LYS:H     | 6        | 0.55          |
| (1,923)  | 1:70:A:LEU:HD13  | 1:71:A:LYS:H     | 6        | 0.55          |
| (1,599)  | 1:53:A:ASP:H     | 1:55:A:VAL:HG11  | 9        | 0.55          |
| (1,599)  | 1:53:A:ASP:H     | 1:55:A:VAL:HG12  | 9        | 0.55          |
| (1,599)  | 1:53:A:ASP:H     | 1:55:A:VAL:HG13  | 9        | 0.55          |
| (1,139)  | 1:28:A:HIS:HD2   | 1:46:A:TYR:HE1   | 2        | 0.55          |
| (1,139)  | 1:28:A:HIS:HD2   | 1:46:A:TYR:HE2   | 2        | 0.55          |
| (1,139)  | 1:28:A:HIS:HD2   | 1:46:A:TYR:HE1   | 3        | 0.55          |
| (1,139)  | 1:28:A:HIS:HD2   | 1:46:A:TYR:HE2   | 3        | 0.55          |
| (1,139)  | 1:28:A:HIS:HD2   | 1:46:A:TYR:HE1   | 6        | 0.55          |
| (1,139)  | 1:28:A:HIS:HD2   | 1:46:A:TYR:HE2   | 6        | 0.55          |
| (2,740)  | 1:162:A:ALA:HA   | 1:168:A:PHE:HE1  | 3        | 0.54          |
| (2,740)  | 1:162:A:ALA:HA   | 1:168:A:PHE:HE2  | 3        | 0.54          |
| (2,740)  | 1:162:A:ALA:HA   | 1:168:A:PHE:HE1  | 4        | 0.54          |
| (2,740)  | 1:162:A:ALA:HA   | 1:168:A:PHE:HE2  | 4        | 0.54          |
| (2,740)  | 1:162:A:ALA:HA   | 1:168:A:PHE:HE1  | 5        | 0.54          |
| (2,740)  | 1:162:A:ALA:HA   | 1:168:A:PHE:HE2  | 5        | 0.54          |
| (2,517)  | 1:84:A:GLY:HA2   | 1:85:A:TYR:HD1   | 3        | 0.54          |
| (2,517)  | 1:84:A:GLY:HA2   | 1:85:A:TYR:HD2   | 3        | 0.54          |
| (2,517)  | 1:84:A:GLY:HA3   | 1:85:A:TYR:HD1   | 3        | 0.54          |
| (2,517)  | 1:84:A:GLY:HA3   | 1:85:A:TYR:HD2   | 3        | 0.54          |
| (2,490)  | 1:81:A:ILE:HD11  | 1:101:A:VAL:H    | 6        | 0.54          |
| (2,490)  | 1:81:A:ILE:HD12  | 1:101:A:VAL:H    | 6        | 0.54          |
| (2,490)  | 1:81:A:ILE:HD13  | 1:101:A:VAL:H    | 6        | 0.54          |
| (2,473)  | 1:80:A:GLN:HB2   | 1:101:A:VAL:HA   | 7        | 0.54          |
| (2,473)  | 1:80:A:GLN:HB3   | 1:101:A:VAL:HA   | 7        | 0.54          |
| (2,473)  | 1:80:A:GLN:HB2   | 1:101:A:VAL:HA   | 8        | 0.54          |
| (2,473)  | 1:80:A:GLN:HB3   | 1:101:A:VAL:HA   | 8        | 0.54          |
| (2,397)  | 1:73:A:TYR:HD1   | 1:74:A:PHE:HA    | 6        | 0.54          |
| (2,397)  | 1:73:A:TYR:HD2   | 1:74:A:PHE:HA    | 6        | 0.54          |
| (2,380)  | 1:69:A:GLN:HE22  | 1:73:A:TYR:HE1   | 2        | 0.54          |
| (2,380)  | 1:69:A:GLN:HE22  | 1:73:A:TYR:HE2   | 2        | 0.54          |
| (2,380)  | 1:69:A:GLN:HE22  | 1:73:A:TYR:HE1   | 10       | 0.54          |
| (2,380)  | 1:69:A:GLN:HE22  | 1:73:A:TYR:HE2   | 10       | 0.54          |
| (2,239)  | 1:46:A:TYR:HB3   | 1:155:A:ASN:HD21 | 5        | 0.54          |
| (2,239)  | 1:46:A:TYR:HB3   | 1:155:A:ASN:HD22 | 5        | 0.54          |
| (1,2069) | 1:148:A:THR:HG21 | 1:148:A:THR:H    | 7        | 0.54          |
| (1,2069) | 1:148:A:THR:HG22 | 1:148:A:THR:H    | 7        | 0.54          |
| (1,2069) | 1:148:A:THR:HG23 | 1:148:A:THR:H    | 7        | 0.54          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2028) | 1:143:A:ILE:HD11 | 1:143:A:ILE:H    | 8        | 0.54          |
| (1,2028) | 1:143:A:ILE:HD12 | 1:143:A:ILE:H    | 8        | 0.54          |
| (1,2028) | 1:143:A:ILE:HD13 | 1:143:A:ILE:H    | 8        | 0.54          |
| (1,2009) | 1:142:A:ILE:HD11 | 1:142:A:ILE:H    | 6        | 0.54          |
| (1,2009) | 1:142:A:ILE:HD12 | 1:142:A:ILE:H    | 6        | 0.54          |
| (1,2009) | 1:142:A:ILE:HD13 | 1:142:A:ILE:H    | 6        | 0.54          |
| (1,1895) | 1:134:A:TRP:HB3  | 1:142:A:ILE:HD11 | 1        | 0.54          |
| (1,1895) | 1:134:A:TRP:HB3  | 1:142:A:ILE:HD12 | 1        | 0.54          |
| (1,1895) | 1:134:A:TRP:HB3  | 1:142:A:ILE:HD13 | 1        | 0.54          |
| (1,1818) | 1:131:A:THR:HG21 | 1:131:A:THR:H    | 10       | 0.54          |
| (1,1818) | 1:131:A:THR:HG22 | 1:131:A:THR:H    | 10       | 0.54          |
| (1,1818) | 1:131:A:THR:HG23 | 1:131:A:THR:H    | 10       | 0.54          |
| (1,1544) | 1:102:A:ILE:HG21 | 1:103:A:SER:H    | 4        | 0.54          |
| (1,1544) | 1:102:A:ILE:HG22 | 1:103:A:SER:H    | 4        | 0.54          |
| (1,1544) | 1:102:A:ILE:HG23 | 1:103:A:SER:H    | 4        | 0.54          |
| (1,1104) | 1:77:A:LEU:H     | 1:104:A:LEU:HD21 | 8        | 0.54          |
| (1,1104) | 1:77:A:LEU:H     | 1:104:A:LEU:HD22 | 8        | 0.54          |
| (1,1104) | 1:77:A:LEU:H     | 1:104:A:LEU:HD23 | 8        | 0.54          |
| (1,1103) | 1:77:A:LEU:H     | 1:104:A:LEU:HD11 | 5        | 0.54          |
| (1,1103) | 1:77:A:LEU:H     | 1:104:A:LEU:HD12 | 5        | 0.54          |
| (1,1103) | 1:77:A:LEU:H     | 1:104:A:LEU:HD13 | 5        | 0.54          |
| (1,700)  | 1:61:A:LYS:HE2   | 1:108:A:SER:HB2  | 10       | 0.54          |
| (1,700)  | 1:61:A:LYS:HE2   | 1:108:A:SER:HB3  | 10       | 0.54          |
| (1,700)  | 1:61:A:LYS:HE3   | 1:108:A:SER:HB2  | 10       | 0.54          |
| (1,700)  | 1:61:A:LYS:HE3   | 1:108:A:SER:HB3  | 10       | 0.54          |
| (1,650)  | 1:58:A:VAL:HG11  | 1:58:A:VAL:H     | 6        | 0.54          |
| (1,650)  | 1:58:A:VAL:HG12  | 1:58:A:VAL:H     | 6        | 0.54          |
| (1,650)  | 1:58:A:VAL:HG13  | 1:58:A:VAL:H     | 6        | 0.54          |
| (1,650)  | 1:58:A:VAL:HG21  | 1:58:A:VAL:H     | 6        | 0.54          |
| (1,650)  | 1:58:A:VAL:HG22  | 1:58:A:VAL:H     | 6        | 0.54          |
| (1,650)  | 1:58:A:VAL:HG23  | 1:58:A:VAL:H     | 6        | 0.54          |
| (1,296)  | 1:38:A:ALA:HB1   | 1:39:A:GLN:H     | 3        | 0.54          |
| (1,296)  | 1:38:A:ALA:HB2   | 1:39:A:GLN:H     | 3        | 0.54          |
| (1,296)  | 1:38:A:ALA:HB3   | 1:39:A:GLN:H     | 3        | 0.54          |
| (3,8)    | 1:111:A:ILE:HA   | 1:111:A:ILE:HG21 | 1        | 0.53          |
| (3,8)    | 1:111:A:ILE:HA   | 1:111:A:ILE:HG22 | 1        | 0.53          |
| (3,8)    | 1:111:A:ILE:HA   | 1:111:A:ILE:HG23 | 1        | 0.53          |
| (2,740)  | 1:162:A:ALA:HA   | 1:168:A:PHE:HE1  | 8        | 0.53          |
| (2,740)  | 1:162:A:ALA:HA   | 1:168:A:PHE:HE2  | 8        | 0.53          |
| (2,702)  | 1:132:A:SER:HB2  | 1:145:A:TYR:HE1  | 6        | 0.53          |
| (2,702)  | 1:132:A:SER:HB2  | 1:145:A:TYR:HE2  | 6        | 0.53          |
| (2,661)  | 1:125:A:LYS:HG2  | 1:126:A:THR:H    | 3        | 0.53          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,661)  | 1:125:A:LYS:HG3  | 1:126:A:THR:H    | 3        | 0.53          |
| (2,635)  | 1:122:A:TYR:HD1  | 1:126:A:THR:H    | 1        | 0.53          |
| (2,635)  | 1:122:A:TYR:HD2  | 1:126:A:THR:H    | 1        | 0.53          |
| (2,635)  | 1:122:A:TYR:HD1  | 1:126:A:THR:H    | 3        | 0.53          |
| (2,635)  | 1:122:A:TYR:HD2  | 1:126:A:THR:H    | 3        | 0.53          |
| (2,535)  | 1:85:A:TYR:HE1   | 1:153:A:ILE:H    | 7        | 0.53          |
| (2,535)  | 1:85:A:TYR:HE2   | 1:153:A:ILE:H    | 7        | 0.53          |
| (2,535)  | 1:85:A:TYR:HE1   | 1:153:A:ILE:H    | 8        | 0.53          |
| (2,535)  | 1:85:A:TYR:HE2   | 1:153:A:ILE:H    | 8        | 0.53          |
| (2,534)  | 1:85:A:TYR:HE1   | 1:151:A:VAL:H    | 5        | 0.53          |
| (2,534)  | 1:85:A:TYR:HE2   | 1:151:A:VAL:H    | 5        | 0.53          |
| (2,490)  | 1:81:A:ILE:HD11  | 1:101:A:VAL:H    | 4        | 0.53          |
| (2,490)  | 1:81:A:ILE:HD12  | 1:101:A:VAL:H    | 4        | 0.53          |
| (2,490)  | 1:81:A:ILE:HD13  | 1:101:A:VAL:H    | 4        | 0.53          |
| (2,473)  | 1:80:A:GLN:HB2   | 1:101:A:VAL:HA   | 4        | 0.53          |
| (2,473)  | 1:80:A:GLN:HB3   | 1:101:A:VAL:HA   | 4        | 0.53          |
| (2,473)  | 1:80:A:GLN:HB2   | 1:101:A:VAL:HA   | 5        | 0.53          |
| (2,473)  | 1:80:A:GLN:HB3   | 1:101:A:VAL:HA   | 5        | 0.53          |
| (2,380)  | 1:69:A:GLN:HE22  | 1:73:A:TYR:HE1   | 9        | 0.53          |
| (2,380)  | 1:69:A:GLN:HE22  | 1:73:A:TYR:HE2   | 9        | 0.53          |
| (2,125)  | 1:28:A:HIS:HE1   | 1:46:A:TYR:HE1   | 2        | 0.53          |
| (2,125)  | 1:28:A:HIS:HE1   | 1:46:A:TYR:HE2   | 2        | 0.53          |
| (2,125)  | 1:28:A:HIS:HE1   | 1:46:A:TYR:HE1   | 3        | 0.53          |
| (2,125)  | 1:28:A:HIS:HE1   | 1:46:A:TYR:HE2   | 3        | 0.53          |
| (2,125)  | 1:28:A:HIS:HE1   | 1:46:A:TYR:HE1   | 8        | 0.53          |
| (2,125)  | 1:28:A:HIS:HE1   | 1:46:A:TYR:HE2   | 8        | 0.53          |
| (1,2028) | 1:143:A:ILE:HD11 | 1:143:A:ILE:H    | 4        | 0.53          |
| (1,2028) | 1:143:A:ILE:HD12 | 1:143:A:ILE:H    | 4        | 0.53          |
| (1,2028) | 1:143:A:ILE:HD13 | 1:143:A:ILE:H    | 4        | 0.53          |
| (1,2022) | 1:143:A:ILE:HA   | 1:143:A:ILE:HG21 | 3        | 0.53          |
| (1,2022) | 1:143:A:ILE:HA   | 1:143:A:ILE:HG22 | 3        | 0.53          |
| (1,2022) | 1:143:A:ILE:HA   | 1:143:A:ILE:HG23 | 3        | 0.53          |
| (1,2022) | 1:143:A:ILE:HA   | 1:143:A:ILE:HG21 | 6        | 0.53          |
| (1,2022) | 1:143:A:ILE:HA   | 1:143:A:ILE:HG22 | 6        | 0.53          |
| (1,2022) | 1:143:A:ILE:HA   | 1:143:A:ILE:HG23 | 6        | 0.53          |
| (1,2022) | 1:143:A:ILE:HA   | 1:143:A:ILE:HG21 | 7        | 0.53          |
| (1,2022) | 1:143:A:ILE:HA   | 1:143:A:ILE:HG22 | 7        | 0.53          |
| (1,2022) | 1:143:A:ILE:HA   | 1:143:A:ILE:HG23 | 7        | 0.53          |
| (1,2022) | 1:143:A:ILE:HA   | 1:143:A:ILE:HG21 | 9        | 0.53          |
| (1,2022) | 1:143:A:ILE:HA   | 1:143:A:ILE:HG22 | 9        | 0.53          |
| (1,2022) | 1:143:A:ILE:HA   | 1:143:A:ILE:HG23 | 9        | 0.53          |
| (1,2022) | 1:143:A:ILE:HA   | 1:143:A:ILE:HG21 | 10       | 0.53          |

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| Key      | Atom-1         | Atom-2           | Model ID | Violation (Å) |
|----------|----------------|------------------|----------|---------------|
| (1,2022) | 1:143:A:ILE:HA | 1:143:A:ILE:HG22 | 10       | 0.53          |
| (1,2022) | 1:143:A:ILE:HA | 1:143:A:ILE:HG23 | 10       | 0.53          |
| (1,1104) | 1:77:A:LEU:H   | 1:104:A:LEU:HD21 | 4        | 0.53          |
| (1,1104) | 1:77:A:LEU:H   | 1:104:A:LEU:HD22 | 4        | 0.53          |
| (1,1104) | 1:77:A:LEU:H   | 1:104:A:LEU:HD23 | 4        | 0.53          |
| (1,1103) | 1:77:A:LEU:H   | 1:104:A:LEU:HD11 | 1        | 0.53          |
| (1,1103) | 1:77:A:LEU:H   | 1:104:A:LEU:HD12 | 1        | 0.53          |
| (1,1103) | 1:77:A:LEU:H   | 1:104:A:LEU:HD13 | 1        | 0.53          |
| (1,1103) | 1:77:A:LEU:H   | 1:104:A:LEU:HD11 | 3        | 0.53          |
| (1,1103) | 1:77:A:LEU:H   | 1:104:A:LEU:HD12 | 3        | 0.53          |
| (1,1103) | 1:77:A:LEU:H   | 1:104:A:LEU:HD13 | 3        | 0.53          |
| (1,1103) | 1:77:A:LEU:H   | 1:104:A:LEU:HD11 | 6        | 0.53          |
| (1,1103) | 1:77:A:LEU:H   | 1:104:A:LEU:HD12 | 6        | 0.53          |
| (1,1103) | 1:77:A:LEU:H   | 1:104:A:LEU:HD13 | 6        | 0.53          |
| (1,1103) | 1:77:A:LEU:H   | 1:104:A:LEU:HD11 | 9        | 0.53          |
| (1,1103) | 1:77:A:LEU:H   | 1:104:A:LEU:HD12 | 9        | 0.53          |
| (1,1103) | 1:77:A:LEU:H   | 1:104:A:LEU:HD13 | 9        | 0.53          |
| (1,599)  | 1:53:A:ASP:H   | 1:55:A:VAL:HG11  | 5        | 0.53          |
| (1,599)  | 1:53:A:ASP:H   | 1:55:A:VAL:HG12  | 5        | 0.53          |
| (1,599)  | 1:53:A:ASP:H   | 1:55:A:VAL:HG13  | 5        | 0.53          |
| (1,545)  | 1:50:A:TRP:HA  | 1:151:A:VAL:HG21 | 2        | 0.53          |
| (1,545)  | 1:50:A:TRP:HA  | 1:151:A:VAL:HG22 | 2        | 0.53          |
| (1,545)  | 1:50:A:TRP:HA  | 1:151:A:VAL:HG23 | 2        | 0.53          |
| (1,545)  | 1:50:A:TRP:HA  | 1:151:A:VAL:HG21 | 8        | 0.53          |
| (1,545)  | 1:50:A:TRP:HA  | 1:151:A:VAL:HG22 | 8        | 0.53          |
| (1,545)  | 1:50:A:TRP:HA  | 1:151:A:VAL:HG23 | 8        | 0.53          |
| (1,296)  | 1:38:A:ALA:HB1 | 1:39:A:GLN:H     | 1        | 0.53          |
| (1,296)  | 1:38:A:ALA:HB2 | 1:39:A:GLN:H     | 1        | 0.53          |
| (1,296)  | 1:38:A:ALA:HB3 | 1:39:A:GLN:H     | 1        | 0.53          |
| (1,296)  | 1:38:A:ALA:HB1 | 1:39:A:GLN:H     | 2        | 0.53          |
| (1,296)  | 1:38:A:ALA:HB2 | 1:39:A:GLN:H     | 2        | 0.53          |
| (1,296)  | 1:38:A:ALA:HB3 | 1:39:A:GLN:H     | 2        | 0.53          |
| (1,296)  | 1:38:A:ALA:HB1 | 1:39:A:GLN:H     | 5        | 0.53          |
| (1,296)  | 1:38:A:ALA:HB2 | 1:39:A:GLN:H     | 5        | 0.53          |
| (1,296)  | 1:38:A:ALA:HB3 | 1:39:A:GLN:H     | 5        | 0.53          |
| (1,296)  | 1:38:A:ALA:HB1 | 1:39:A:GLN:H     | 6        | 0.53          |
| (1,296)  | 1:38:A:ALA:HB2 | 1:39:A:GLN:H     | 6        | 0.53          |
| (1,296)  | 1:38:A:ALA:HB3 | 1:39:A:GLN:H     | 6        | 0.53          |
| (1,288)  | 1:36:A:ALA:HB1 | 1:37:A:GLY:H     | 8        | 0.53          |
| (1,288)  | 1:36:A:ALA:HB2 | 1:37:A:GLY:H     | 8        | 0.53          |
| (1,288)  | 1:36:A:ALA:HB3 | 1:37:A:GLY:H     | 8        | 0.53          |
| (1,287)  | 1:36:A:ALA:HB1 | 1:36:A:ALA:H     | 9        | 0.53          |

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| Key     | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,287) | 1:36:A:ALA:HB2  | 1:36:A:ALA:H     | 9        | 0.53          |
| (1,287) | 1:36:A:ALA:HB3  | 1:36:A:ALA:H     | 9        | 0.53          |
| (3,8)   | 1:111:A:ILE:HA  | 1:111:A:ILE:HG21 | 2        | 0.52          |
| (3,8)   | 1:111:A:ILE:HA  | 1:111:A:ILE:HG22 | 2        | 0.52          |
| (3,8)   | 1:111:A:ILE:HA  | 1:111:A:ILE:HG23 | 2        | 0.52          |
| (3,8)   | 1:111:A:ILE:HA  | 1:111:A:ILE:HG21 | 3        | 0.52          |
| (3,8)   | 1:111:A:ILE:HA  | 1:111:A:ILE:HG22 | 3        | 0.52          |
| (3,8)   | 1:111:A:ILE:HA  | 1:111:A:ILE:HG23 | 3        | 0.52          |
| (2,768) | 1:173:A:VAL:HB  | 1:175:A:PHE:HE1  | 3        | 0.52          |
| (2,768) | 1:173:A:VAL:HB  | 1:175:A:PHE:HE2  | 3        | 0.52          |
| (2,765) | 1:169:A:ASP:H   | 1:171:A:LEU:HD11 | 1        | 0.52          |
| (2,765) | 1:169:A:ASP:H   | 1:171:A:LEU:HD12 | 1        | 0.52          |
| (2,765) | 1:169:A:ASP:H   | 1:171:A:LEU:HD13 | 1        | 0.52          |
| (2,635) | 1:122:A:TYR:HD1 | 1:126:A:THR:H    | 6        | 0.52          |
| (2,635) | 1:122:A:TYR:HD2 | 1:126:A:THR:H    | 6        | 0.52          |
| (2,592) | 1:114:A:ASP:HB3 | 1:116:A:GLU:HG2  | 4        | 0.52          |
| (2,592) | 1:114:A:ASP:HB3 | 1:116:A:GLU:HG3  | 4        | 0.52          |
| (2,523) | 1:85:A:TYR:HD1  | 1:134:A:TRP:H    | 4        | 0.52          |
| (2,523) | 1:85:A:TYR:HD2  | 1:134:A:TRP:H    | 4        | 0.52          |
| (2,518) | 1:84:A:GLY:HA2  | 1:95:A:PHE:HE1   | 9        | 0.52          |
| (2,518) | 1:84:A:GLY:HA2  | 1:95:A:PHE:HE2   | 9        | 0.52          |
| (2,518) | 1:84:A:GLY:HA3  | 1:95:A:PHE:HE1   | 9        | 0.52          |
| (2,518) | 1:84:A:GLY:HA3  | 1:95:A:PHE:HE2   | 9        | 0.52          |
| (2,443) | 1:76:A:TYR:HE1  | 1:78:A:GLN:HE22  | 10       | 0.52          |
| (2,443) | 1:76:A:TYR:HE2  | 1:78:A:GLN:HE22  | 10       | 0.52          |
| (2,383) | 1:70:A:LEU:HA   | 1:74:A:PHE:HD1   | 9        | 0.52          |
| (2,383) | 1:70:A:LEU:HA   | 1:74:A:PHE:HD2   | 9        | 0.52          |
| (2,380) | 1:69:A:GLN:HE22 | 1:73:A:TYR:HE1   | 1        | 0.52          |
| (2,380) | 1:69:A:GLN:HE22 | 1:73:A:TYR:HE2   | 1        | 0.52          |
| (2,380) | 1:69:A:GLN:HE22 | 1:73:A:TYR:HE1   | 7        | 0.52          |
| (2,380) | 1:69:A:GLN:HE22 | 1:73:A:TYR:HE2   | 7        | 0.52          |
| (2,350) | 1:63:A:THR:HA   | 1:175:A:PHE:HE1  | 6        | 0.52          |
| (2,350) | 1:63:A:THR:HA   | 1:175:A:PHE:HE2  | 6        | 0.52          |
| (2,239) | 1:46:A:TYR:HB3  | 1:155:A:ASN:HD21 | 9        | 0.52          |
| (2,239) | 1:46:A:TYR:HB3  | 1:155:A:ASN:HD22 | 9        | 0.52          |
| (2,125) | 1:28:A:HIS:HE1  | 1:46:A:TYR:HE1   | 4        | 0.52          |
| (2,125) | 1:28:A:HIS:HE1  | 1:46:A:TYR:HE2   | 4        | 0.52          |
| (2,125) | 1:28:A:HIS:HE1  | 1:46:A:TYR:HE1   | 5        | 0.52          |
| (2,125) | 1:28:A:HIS:HE1  | 1:46:A:TYR:HE2   | 5        | 0.52          |
| (2,125) | 1:28:A:HIS:HE1  | 1:46:A:TYR:HE1   | 9        | 0.52          |
| (2,125) | 1:28:A:HIS:HE1  | 1:46:A:TYR:HE2   | 9        | 0.52          |
| (2,125) | 1:28:A:HIS:HE1  | 1:46:A:TYR:HE1   | 10       | 0.52          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,125)  | 1:28:A:HIS:HE1   | 1:46:A:TYR:HE2   | 10       | 0.52          |
| (1,2463) | 1:182:A:VAL:HG21 | 1:182:A:VAL:H    | 1        | 0.52          |
| (1,2463) | 1:182:A:VAL:HG22 | 1:182:A:VAL:H    | 1        | 0.52          |
| (1,2463) | 1:182:A:VAL:HG23 | 1:182:A:VAL:H    | 1        | 0.52          |
| (1,2463) | 1:182:A:VAL:HG21 | 1:182:A:VAL:H    | 6        | 0.52          |
| (1,2463) | 1:182:A:VAL:HG22 | 1:182:A:VAL:H    | 6        | 0.52          |
| (1,2463) | 1:182:A:VAL:HG23 | 1:182:A:VAL:H    | 6        | 0.52          |
| (1,2463) | 1:182:A:VAL:HG21 | 1:182:A:VAL:H    | 8        | 0.52          |
| (1,2463) | 1:182:A:VAL:HG22 | 1:182:A:VAL:H    | 8        | 0.52          |
| (1,2463) | 1:182:A:VAL:HG23 | 1:182:A:VAL:H    | 8        | 0.52          |
| (1,2463) | 1:182:A:VAL:HG21 | 1:182:A:VAL:H    | 9        | 0.52          |
| (1,2463) | 1:182:A:VAL:HG22 | 1:182:A:VAL:H    | 9        | 0.52          |
| (1,2463) | 1:182:A:VAL:HG23 | 1:182:A:VAL:H    | 9        | 0.52          |
| (1,2460) | 1:182:A:VAL:HG11 | 1:182:A:VAL:HG21 | 3        | 0.52          |
| (1,2460) | 1:182:A:VAL:HG11 | 1:182:A:VAL:HG22 | 3        | 0.52          |
| (1,2460) | 1:182:A:VAL:HG11 | 1:182:A:VAL:HG23 | 3        | 0.52          |
| (1,2460) | 1:182:A:VAL:HG12 | 1:182:A:VAL:HG21 | 3        | 0.52          |
| (1,2460) | 1:182:A:VAL:HG12 | 1:182:A:VAL:HG22 | 3        | 0.52          |
| (1,2460) | 1:182:A:VAL:HG12 | 1:182:A:VAL:HG23 | 3        | 0.52          |
| (1,2460) | 1:182:A:VAL:HG13 | 1:182:A:VAL:HG21 | 3        | 0.52          |
| (1,2460) | 1:182:A:VAL:HG13 | 1:182:A:VAL:HG22 | 3        | 0.52          |
| (1,2460) | 1:182:A:VAL:HG13 | 1:182:A:VAL:HG23 | 3        | 0.52          |
| (1,2449) | 1:179:A:VAL:HG21 | 1:179:A:VAL:H    | 10       | 0.52          |
| (1,2449) | 1:179:A:VAL:HG22 | 1:179:A:VAL:H    | 10       | 0.52          |
| (1,2449) | 1:179:A:VAL:HG23 | 1:179:A:VAL:H    | 10       | 0.52          |
| (1,2324) | 1:171:A:LEU:HD21 | 1:171:A:LEU:H    | 2        | 0.52          |
| (1,2324) | 1:171:A:LEU:HD22 | 1:171:A:LEU:H    | 2        | 0.52          |
| (1,2324) | 1:171:A:LEU:HD23 | 1:171:A:LEU:H    | 2        | 0.52          |
| (1,2324) | 1:171:A:LEU:HD21 | 1:171:A:LEU:H    | 9        | 0.52          |
| (1,2324) | 1:171:A:LEU:HD22 | 1:171:A:LEU:H    | 9        | 0.52          |
| (1,2324) | 1:171:A:LEU:HD23 | 1:171:A:LEU:H    | 9        | 0.52          |
| (1,2022) | 1:143:A:ILE:HA   | 1:143:A:ILE:HG21 | 1        | 0.52          |
| (1,2022) | 1:143:A:ILE:HA   | 1:143:A:ILE:HG22 | 1        | 0.52          |
| (1,2022) | 1:143:A:ILE:HA   | 1:143:A:ILE:HG23 | 1        | 0.52          |
| (1,1546) | 1:102:A:ILE:HG21 | 1:108:A:SER:HA   | 3        | 0.52          |
| (1,1546) | 1:102:A:ILE:HG22 | 1:108:A:SER:HA   | 3        | 0.52          |
| (1,1546) | 1:102:A:ILE:HG23 | 1:108:A:SER:HA   | 3        | 0.52          |
| (1,1546) | 1:102:A:ILE:HG21 | 1:108:A:SER:HA   | 9        | 0.52          |
| (1,1546) | 1:102:A:ILE:HG22 | 1:108:A:SER:HA   | 9        | 0.52          |
| (1,1546) | 1:102:A:ILE:HG23 | 1:108:A:SER:HA   | 9        | 0.52          |
| (1,1537) | 1:102:A:ILE:HD11 | 1:107:A:PRO:HA   | 5        | 0.52          |
| (1,1537) | 1:102:A:ILE:HD12 | 1:107:A:PRO:HA   | 5        | 0.52          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1537) | 1:102:A:ILE:HD13 | 1:107:A:PRO:HA   | 5        | 0.52          |
| (1,1103) | 1:77:A:LEU:H     | 1:104:A:LEU:HD11 | 2        | 0.52          |
| (1,1103) | 1:77:A:LEU:H     | 1:104:A:LEU:HD12 | 2        | 0.52          |
| (1,1103) | 1:77:A:LEU:H     | 1:104:A:LEU:HD13 | 2        | 0.52          |
| (1,1088) | 1:77:A:LEU:HD11  | 1:78:A:GLN:H     | 3        | 0.52          |
| (1,1088) | 1:77:A:LEU:HD12  | 1:78:A:GLN:H     | 3        | 0.52          |
| (1,1088) | 1:77:A:LEU:HD13  | 1:78:A:GLN:H     | 3        | 0.52          |
| (1,1088) | 1:77:A:LEU:HD21  | 1:78:A:GLN:H     | 3        | 0.52          |
| (1,1088) | 1:77:A:LEU:HD22  | 1:78:A:GLN:H     | 3        | 0.52          |
| (1,1088) | 1:77:A:LEU:HD23  | 1:78:A:GLN:H     | 3        | 0.52          |
| (1,1088) | 1:77:A:LEU:HD11  | 1:78:A:GLN:H     | 4        | 0.52          |
| (1,1088) | 1:77:A:LEU:HD12  | 1:78:A:GLN:H     | 4        | 0.52          |
| (1,1088) | 1:77:A:LEU:HD13  | 1:78:A:GLN:H     | 4        | 0.52          |
| (1,1088) | 1:77:A:LEU:HD21  | 1:78:A:GLN:H     | 4        | 0.52          |
| (1,1088) | 1:77:A:LEU:HD22  | 1:78:A:GLN:H     | 4        | 0.52          |
| (1,1088) | 1:77:A:LEU:HD23  | 1:78:A:GLN:H     | 4        | 0.52          |
| (1,288)  | 1:36:A:ALA:HB1   | 1:37:A:GLY:H     | 1        | 0.52          |
| (1,288)  | 1:36:A:ALA:HB2   | 1:37:A:GLY:H     | 1        | 0.52          |
| (1,288)  | 1:36:A:ALA:HB3   | 1:37:A:GLY:H     | 1        | 0.52          |
| (1,139)  | 1:28:A:HIS:HD2   | 1:46:A:TYR:HE1   | 10       | 0.52          |
| (1,139)  | 1:28:A:HIS:HD2   | 1:46:A:TYR:HE2   | 10       | 0.52          |
| (3,8)    | 1:111:A:ILE:HA   | 1:111:A:ILE:HG21 | 10       | 0.51          |
| (3,8)    | 1:111:A:ILE:HA   | 1:111:A:ILE:HG22 | 10       | 0.51          |
| (3,8)    | 1:111:A:ILE:HA   | 1:111:A:ILE:HG23 | 10       | 0.51          |
| (2,768)  | 1:173:A:VAL:HB   | 1:175:A:PHE:HE1  | 5        | 0.51          |
| (2,768)  | 1:173:A:VAL:HB   | 1:175:A:PHE:HE2  | 5        | 0.51          |
| (2,740)  | 1:162:A:ALA:HA   | 1:168:A:PHE:HE1  | 9        | 0.51          |
| (2,740)  | 1:162:A:ALA:HA   | 1:168:A:PHE:HE2  | 9        | 0.51          |
| (2,716)  | 1:142:A:ILE:HB   | 1:145:A:TYR:HE1  | 5        | 0.51          |
| (2,716)  | 1:142:A:ILE:HB   | 1:145:A:TYR:HE2  | 5        | 0.51          |
| (2,716)  | 1:142:A:ILE:HB   | 1:145:A:TYR:HE1  | 6        | 0.51          |
| (2,716)  | 1:142:A:ILE:HB   | 1:145:A:TYR:HE2  | 6        | 0.51          |
| (2,702)  | 1:132:A:SER:HB2  | 1:145:A:TYR:HE1  | 9        | 0.51          |
| (2,702)  | 1:132:A:SER:HB2  | 1:145:A:TYR:HE2  | 9        | 0.51          |
| (2,700)  | 1:132:A:SER:HB3  | 1:145:A:TYR:HE1  | 1        | 0.51          |
| (2,700)  | 1:132:A:SER:HB3  | 1:145:A:TYR:HE2  | 1        | 0.51          |
| (2,700)  | 1:132:A:SER:HB3  | 1:145:A:TYR:HE1  | 2        | 0.51          |
| (2,700)  | 1:132:A:SER:HB3  | 1:145:A:TYR:HE2  | 2        | 0.51          |
| (2,631)  | 1:122:A:TYR:HD1  | 1:124:A:ASP:H    | 7        | 0.51          |
| (2,631)  | 1:122:A:TYR:HD2  | 1:124:A:ASP:H    | 7        | 0.51          |
| (2,631)  | 1:122:A:TYR:HD1  | 1:124:A:ASP:H    | 8        | 0.51          |
| (2,631)  | 1:122:A:TYR:HD2  | 1:124:A:ASP:H    | 8        | 0.51          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,614)  | 1:118:A:ILE:HG21 | 1:151:A:VAL:HA   | 4        | 0.51          |
| (2,614)  | 1:118:A:ILE:HG22 | 1:151:A:VAL:HA   | 4        | 0.51          |
| (2,614)  | 1:118:A:ILE:HG23 | 1:151:A:VAL:HA   | 4        | 0.51          |
| (2,593)  | 1:114:A:ASP:HB2  | 1:116:A:GLU:HG2  | 9        | 0.51          |
| (2,593)  | 1:114:A:ASP:HB2  | 1:116:A:GLU:HG3  | 9        | 0.51          |
| (2,535)  | 1:85:A:TYR:HE1   | 1:153:A:ILE:H    | 1        | 0.51          |
| (2,535)  | 1:85:A:TYR:HE2   | 1:153:A:ILE:H    | 1        | 0.51          |
| (2,535)  | 1:85:A:TYR:HE1   | 1:153:A:ILE:H    | 3        | 0.51          |
| (2,535)  | 1:85:A:TYR:HE2   | 1:153:A:ILE:H    | 3        | 0.51          |
| (2,523)  | 1:85:A:TYR:HD1   | 1:134:A:TRP:H    | 10       | 0.51          |
| (2,523)  | 1:85:A:TYR:HD2   | 1:134:A:TRP:H    | 10       | 0.51          |
| (2,490)  | 1:81:A:ILE:HD11  | 1:101:A:VAL:H    | 10       | 0.51          |
| (2,490)  | 1:81:A:ILE:HD12  | 1:101:A:VAL:H    | 10       | 0.51          |
| (2,490)  | 1:81:A:ILE:HD13  | 1:101:A:VAL:H    | 10       | 0.51          |
| (2,348)  | 1:62:A:VAL:HA    | 1:175:A:PHE:HD1  | 6        | 0.51          |
| (2,348)  | 1:62:A:VAL:HA    | 1:175:A:PHE:HD2  | 6        | 0.51          |
| (2,239)  | 1:46:A:TYR:HB3   | 1:155:A:ASN:HD21 | 2        | 0.51          |
| (2,239)  | 1:46:A:TYR:HB3   | 1:155:A:ASN:HD22 | 2        | 0.51          |
| (2,16)   | 1:17:A:GLN:HG2   | 1:18:A:ALA:H     | 7        | 0.51          |
| (2,16)   | 1:17:A:GLN:HG3   | 1:18:A:ALA:H     | 7        | 0.51          |
| (2,16)   | 1:17:A:GLN:HG2   | 1:18:A:ALA:H     | 9        | 0.51          |
| (2,16)   | 1:17:A:GLN:HG3   | 1:18:A:ALA:H     | 9        | 0.51          |
| (1,2460) | 1:182:A:VAL:HG11 | 1:182:A:VAL:HG21 | 1        | 0.51          |
| (1,2460) | 1:182:A:VAL:HG11 | 1:182:A:VAL:HG22 | 1        | 0.51          |
| (1,2460) | 1:182:A:VAL:HG11 | 1:182:A:VAL:HG23 | 1        | 0.51          |
| (1,2460) | 1:182:A:VAL:HG12 | 1:182:A:VAL:HG21 | 1        | 0.51          |
| (1,2460) | 1:182:A:VAL:HG12 | 1:182:A:VAL:HG22 | 1        | 0.51          |
| (1,2460) | 1:182:A:VAL:HG12 | 1:182:A:VAL:HG23 | 1        | 0.51          |
| (1,2460) | 1:182:A:VAL:HG13 | 1:182:A:VAL:HG21 | 1        | 0.51          |
| (1,2460) | 1:182:A:VAL:HG13 | 1:182:A:VAL:HG22 | 1        | 0.51          |
| (1,2460) | 1:182:A:VAL:HG13 | 1:182:A:VAL:HG23 | 1        | 0.51          |
| (1,2460) | 1:182:A:VAL:HG11 | 1:182:A:VAL:HG21 | 2        | 0.51          |
| (1,2460) | 1:182:A:VAL:HG11 | 1:182:A:VAL:HG22 | 2        | 0.51          |
| (1,2460) | 1:182:A:VAL:HG11 | 1:182:A:VAL:HG23 | 2        | 0.51          |
| (1,2460) | 1:182:A:VAL:HG12 | 1:182:A:VAL:HG21 | 2        | 0.51          |
| (1,2460) | 1:182:A:VAL:HG12 | 1:182:A:VAL:HG22 | 2        | 0.51          |
| (1,2460) | 1:182:A:VAL:HG12 | 1:182:A:VAL:HG23 | 2        | 0.51          |
| (1,2460) | 1:182:A:VAL:HG13 | 1:182:A:VAL:HG21 | 2        | 0.51          |
| (1,2460) | 1:182:A:VAL:HG13 | 1:182:A:VAL:HG22 | 2        | 0.51          |
| (1,2460) | 1:182:A:VAL:HG13 | 1:182:A:VAL:HG23 | 2        | 0.51          |
| (1,2460) | 1:182:A:VAL:HG11 | 1:182:A:VAL:HG21 | 4        | 0.51          |
| (1,2460) | 1:182:A:VAL:HG11 | 1:182:A:VAL:HG22 | 4        | 0.51          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2460) | 1:182:A:VAL:HG11 | 1:182:A:VAL:HG23 | 4        | 0.51          |
| (1,2460) | 1:182:A:VAL:HG12 | 1:182:A:VAL:HG21 | 4        | 0.51          |
| (1,2460) | 1:182:A:VAL:HG12 | 1:182:A:VAL:HG22 | 4        | 0.51          |
| (1,2460) | 1:182:A:VAL:HG12 | 1:182:A:VAL:HG23 | 4        | 0.51          |
| (1,2460) | 1:182:A:VAL:HG13 | 1:182:A:VAL:HG21 | 4        | 0.51          |
| (1,2460) | 1:182:A:VAL:HG13 | 1:182:A:VAL:HG22 | 4        | 0.51          |
| (1,2460) | 1:182:A:VAL:HG13 | 1:182:A:VAL:HG23 | 4        | 0.51          |
| (1,2460) | 1:182:A:VAL:HG11 | 1:182:A:VAL:HG21 | 5        | 0.51          |
| (1,2460) | 1:182:A:VAL:HG11 | 1:182:A:VAL:HG22 | 5        | 0.51          |
| (1,2460) | 1:182:A:VAL:HG11 | 1:182:A:VAL:HG23 | 5        | 0.51          |
| (1,2460) | 1:182:A:VAL:HG12 | 1:182:A:VAL:HG21 | 5        | 0.51          |
| (1,2460) | 1:182:A:VAL:HG12 | 1:182:A:VAL:HG22 | 5        | 0.51          |
| (1,2460) | 1:182:A:VAL:HG12 | 1:182:A:VAL:HG23 | 5        | 0.51          |
| (1,2460) | 1:182:A:VAL:HG13 | 1:182:A:VAL:HG21 | 5        | 0.51          |
| (1,2460) | 1:182:A:VAL:HG13 | 1:182:A:VAL:HG22 | 5        | 0.51          |
| (1,2460) | 1:182:A:VAL:HG13 | 1:182:A:VAL:HG23 | 5        | 0.51          |
| (1,2460) | 1:182:A:VAL:HG11 | 1:182:A:VAL:HG21 | 6        | 0.51          |
| (1,2460) | 1:182:A:VAL:HG11 | 1:182:A:VAL:HG22 | 6        | 0.51          |
| (1,2460) | 1:182:A:VAL:HG11 | 1:182:A:VAL:HG23 | 6        | 0.51          |
| (1,2460) | 1:182:A:VAL:HG12 | 1:182:A:VAL:HG21 | 6        | 0.51          |
| (1,2460) | 1:182:A:VAL:HG12 | 1:182:A:VAL:HG22 | 6        | 0.51          |
| (1,2460) | 1:182:A:VAL:HG12 | 1:182:A:VAL:HG23 | 6        | 0.51          |
| (1,2460) | 1:182:A:VAL:HG13 | 1:182:A:VAL:HG21 | 6        | 0.51          |
| (1,2460) | 1:182:A:VAL:HG13 | 1:182:A:VAL:HG22 | 6        | 0.51          |
| (1,2460) | 1:182:A:VAL:HG13 | 1:182:A:VAL:HG23 | 6        | 0.51          |
| (1,2460) | 1:182:A:VAL:HG11 | 1:182:A:VAL:HG21 | 7        | 0.51          |
| (1,2460) | 1:182:A:VAL:HG11 | 1:182:A:VAL:HG22 | 7        | 0.51          |
| (1,2460) | 1:182:A:VAL:HG11 | 1:182:A:VAL:HG23 | 7        | 0.51          |
| (1,2460) | 1:182:A:VAL:HG12 | 1:182:A:VAL:HG21 | 7        | 0.51          |
| (1,2460) | 1:182:A:VAL:HG12 | 1:182:A:VAL:HG22 | 7        | 0.51          |
| (1,2460) | 1:182:A:VAL:HG12 | 1:182:A:VAL:HG23 | 7        | 0.51          |
| (1,2460) | 1:182:A:VAL:HG13 | 1:182:A:VAL:HG21 | 7        | 0.51          |
| (1,2460) | 1:182:A:VAL:HG13 | 1:182:A:VAL:HG22 | 7        | 0.51          |
| (1,2460) | 1:182:A:VAL:HG13 | 1:182:A:VAL:HG23 | 7        | 0.51          |
| (1,2460) | 1:182:A:VAL:HG11 | 1:182:A:VAL:HG21 | 8        | 0.51          |
| (1,2460) | 1:182:A:VAL:HG11 | 1:182:A:VAL:HG22 | 8        | 0.51          |
| (1,2460) | 1:182:A:VAL:HG11 | 1:182:A:VAL:HG23 | 8        | 0.51          |
| (1,2460) | 1:182:A:VAL:HG12 | 1:182:A:VAL:HG21 | 8        | 0.51          |
| (1,2460) | 1:182:A:VAL:HG12 | 1:182:A:VAL:HG22 | 8        | 0.51          |
| (1,2460) | 1:182:A:VAL:HG12 | 1:182:A:VAL:HG23 | 8        | 0.51          |
| (1,2460) | 1:182:A:VAL:HG13 | 1:182:A:VAL:HG21 | 8        | 0.51          |
| (1,2460) | 1:182:A:VAL:HG13 | 1:182:A:VAL:HG22 | 8        | 0.51          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2460) | 1:182:A:VAL:HG13 | 1:182:A:VAL:HG23 | 8        | 0.51          |
| (1,2460) | 1:182:A:VAL:HG11 | 1:182:A:VAL:HG21 | 9        | 0.51          |
| (1,2460) | 1:182:A:VAL:HG11 | 1:182:A:VAL:HG22 | 9        | 0.51          |
| (1,2460) | 1:182:A:VAL:HG11 | 1:182:A:VAL:HG23 | 9        | 0.51          |
| (1,2460) | 1:182:A:VAL:HG12 | 1:182:A:VAL:HG21 | 9        | 0.51          |
| (1,2460) | 1:182:A:VAL:HG12 | 1:182:A:VAL:HG22 | 9        | 0.51          |
| (1,2460) | 1:182:A:VAL:HG12 | 1:182:A:VAL:HG23 | 9        | 0.51          |
| (1,2460) | 1:182:A:VAL:HG13 | 1:182:A:VAL:HG21 | 9        | 0.51          |
| (1,2460) | 1:182:A:VAL:HG13 | 1:182:A:VAL:HG22 | 9        | 0.51          |
| (1,2460) | 1:182:A:VAL:HG13 | 1:182:A:VAL:HG23 | 9        | 0.51          |
| (1,2460) | 1:182:A:VAL:HG11 | 1:182:A:VAL:HG21 | 10       | 0.51          |
| (1,2460) | 1:182:A:VAL:HG11 | 1:182:A:VAL:HG22 | 10       | 0.51          |
| (1,2460) | 1:182:A:VAL:HG11 | 1:182:A:VAL:HG23 | 10       | 0.51          |
| (1,2460) | 1:182:A:VAL:HG12 | 1:182:A:VAL:HG21 | 10       | 0.51          |
| (1,2460) | 1:182:A:VAL:HG12 | 1:182:A:VAL:HG22 | 10       | 0.51          |
| (1,2460) | 1:182:A:VAL:HG12 | 1:182:A:VAL:HG23 | 10       | 0.51          |
| (1,2460) | 1:182:A:VAL:HG13 | 1:182:A:VAL:HG21 | 10       | 0.51          |
| (1,2460) | 1:182:A:VAL:HG13 | 1:182:A:VAL:HG22 | 10       | 0.51          |
| (1,2460) | 1:182:A:VAL:HG13 | 1:182:A:VAL:HG23 | 10       | 0.51          |
| (1,2324) | 1:171:A:LEU:HD21 | 1:171:A:LEU:H    | 5        | 0.51          |
| (1,2324) | 1:171:A:LEU:HD22 | 1:171:A:LEU:H    | 5        | 0.51          |
| (1,2324) | 1:171:A:LEU:HD23 | 1:171:A:LEU:H    | 5        | 0.51          |
| (1,2032) | 1:143:A:ILE:HG21 | 1:144:A:VAL:H    | 10       | 0.51          |
| (1,2032) | 1:143:A:ILE:HG22 | 1:144:A:VAL:H    | 10       | 0.51          |
| (1,2032) | 1:143:A:ILE:HG23 | 1:144:A:VAL:H    | 10       | 0.51          |
| (1,2022) | 1:143:A:ILE:HA   | 1:143:A:ILE:HG21 | 2        | 0.51          |
| (1,2022) | 1:143:A:ILE:HA   | 1:143:A:ILE:HG22 | 2        | 0.51          |
| (1,2022) | 1:143:A:ILE:HA   | 1:143:A:ILE:HG23 | 2        | 0.51          |
| (1,1537) | 1:102:A:ILE:HD11 | 1:107:A:PRO:HA   | 6        | 0.51          |
| (1,1537) | 1:102:A:ILE:HD12 | 1:107:A:PRO:HA   | 6        | 0.51          |
| (1,1537) | 1:102:A:ILE:HD13 | 1:107:A:PRO:HA   | 6        | 0.51          |
| (1,1537) | 1:102:A:ILE:HD11 | 1:107:A:PRO:HA   | 8        | 0.51          |
| (1,1537) | 1:102:A:ILE:HD12 | 1:107:A:PRO:HA   | 8        | 0.51          |
| (1,1537) | 1:102:A:ILE:HD13 | 1:107:A:PRO:HA   | 8        | 0.51          |
| (1,1213) | 1:81:A:ILE:HD11  | 1:81:A:ILE:H     | 2        | 0.51          |
| (1,1213) | 1:81:A:ILE:HD12  | 1:81:A:ILE:H     | 2        | 0.51          |
| (1,1213) | 1:81:A:ILE:HD13  | 1:81:A:ILE:H     | 2        | 0.51          |
| (1,1213) | 1:81:A:ILE:HD11  | 1:81:A:ILE:H     | 4        | 0.51          |
| (1,1213) | 1:81:A:ILE:HD12  | 1:81:A:ILE:H     | 4        | 0.51          |
| (1,1213) | 1:81:A:ILE:HD13  | 1:81:A:ILE:H     | 4        | 0.51          |
| (1,1213) | 1:81:A:ILE:HD11  | 1:81:A:ILE:H     | 5        | 0.51          |
| (1,1213) | 1:81:A:ILE:HD12  | 1:81:A:ILE:H     | 5        | 0.51          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1213) | 1:81:A:ILE:HD13 | 1:81:A:ILE:H     | 5        | 0.51          |
| (1,1213) | 1:81:A:ILE:HD11 | 1:81:A:ILE:H     | 8        | 0.51          |
| (1,1213) | 1:81:A:ILE:HD12 | 1:81:A:ILE:H     | 8        | 0.51          |
| (1,1213) | 1:81:A:ILE:HD13 | 1:81:A:ILE:H     | 8        | 0.51          |
| (1,1213) | 1:81:A:ILE:HD11 | 1:81:A:ILE:H     | 9        | 0.51          |
| (1,1213) | 1:81:A:ILE:HD12 | 1:81:A:ILE:H     | 9        | 0.51          |
| (1,1213) | 1:81:A:ILE:HD13 | 1:81:A:ILE:H     | 9        | 0.51          |
| (1,1213) | 1:81:A:ILE:HD11 | 1:81:A:ILE:H     | 10       | 0.51          |
| (1,1213) | 1:81:A:ILE:HD12 | 1:81:A:ILE:H     | 10       | 0.51          |
| (1,1213) | 1:81:A:ILE:HD13 | 1:81:A:ILE:H     | 10       | 0.51          |
| (1,1104) | 1:77:A:LEU:H    | 1:104:A:LEU:HD21 | 7        | 0.51          |
| (1,1104) | 1:77:A:LEU:H    | 1:104:A:LEU:HD22 | 7        | 0.51          |
| (1,1104) | 1:77:A:LEU:H    | 1:104:A:LEU:HD23 | 7        | 0.51          |
| (1,1088) | 1:77:A:LEU:HD11 | 1:78:A:GLN:H     | 6        | 0.51          |
| (1,1088) | 1:77:A:LEU:HD12 | 1:78:A:GLN:H     | 6        | 0.51          |
| (1,1088) | 1:77:A:LEU:HD13 | 1:78:A:GLN:H     | 6        | 0.51          |
| (1,1088) | 1:77:A:LEU:HD21 | 1:78:A:GLN:H     | 6        | 0.51          |
| (1,1088) | 1:77:A:LEU:HD22 | 1:78:A:GLN:H     | 6        | 0.51          |
| (1,1088) | 1:77:A:LEU:HD23 | 1:78:A:GLN:H     | 6        | 0.51          |
| (1,851)  | 1:66:A:ASN:HD22 | 1:70:A:LEU:HD11  | 9        | 0.51          |
| (1,851)  | 1:66:A:ASN:HD22 | 1:70:A:LEU:HD12  | 9        | 0.51          |
| (1,851)  | 1:66:A:ASN:HD22 | 1:70:A:LEU:HD13  | 9        | 0.51          |
| (1,582)  | 1:51:A:ILE:HG21 | 1:55:A:VAL:H     | 2        | 0.51          |
| (1,582)  | 1:51:A:ILE:HG22 | 1:55:A:VAL:H     | 2        | 0.51          |
| (1,582)  | 1:51:A:ILE:HG23 | 1:55:A:VAL:H     | 2        | 0.51          |
| (1,545)  | 1:50:A:TRP:HA   | 1:151:A:VAL:HG21 | 1        | 0.51          |
| (1,545)  | 1:50:A:TRP:HA   | 1:151:A:VAL:HG22 | 1        | 0.51          |
| (1,545)  | 1:50:A:TRP:HA   | 1:151:A:VAL:HG23 | 1        | 0.51          |
| (1,545)  | 1:50:A:TRP:HA   | 1:151:A:VAL:HG21 | 3        | 0.51          |
| (1,545)  | 1:50:A:TRP:HA   | 1:151:A:VAL:HG22 | 3        | 0.51          |
| (1,545)  | 1:50:A:TRP:HA   | 1:151:A:VAL:HG23 | 3        | 0.51          |
| (1,545)  | 1:50:A:TRP:HA   | 1:151:A:VAL:HG21 | 4        | 0.51          |
| (1,545)  | 1:50:A:TRP:HA   | 1:151:A:VAL:HG22 | 4        | 0.51          |
| (1,545)  | 1:50:A:TRP:HA   | 1:151:A:VAL:HG23 | 4        | 0.51          |
| (1,545)  | 1:50:A:TRP:HA   | 1:151:A:VAL:HG21 | 9        | 0.51          |
| (1,545)  | 1:50:A:TRP:HA   | 1:151:A:VAL:HG22 | 9        | 0.51          |
| (1,545)  | 1:50:A:TRP:HA   | 1:151:A:VAL:HG23 | 9        | 0.51          |
| (1,205)  | 1:32:A:ILE:HA   | 1:32:A:ILE:HD11  | 8        | 0.51          |
| (1,205)  | 1:32:A:ILE:HA   | 1:32:A:ILE:HD12  | 8        | 0.51          |
| (1,205)  | 1:32:A:ILE:HA   | 1:32:A:ILE:HD13  | 8        | 0.51          |
| (3,8)    | 1:111:A:ILE:HA  | 1:111:A:ILE:HG21 | 9        | 0.5           |
| (3,8)    | 1:111:A:ILE:HA  | 1:111:A:ILE:HG22 | 9        | 0.5           |

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| Key     | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (3,8)   | 1:111:A:ILE:HA  | 1:111:A:ILE:HG23 | 9        | 0.5           |
| (2,768) | 1:173:A:VAL:HB  | 1:175:A:PHE:HE1  | 9        | 0.5           |
| (2,768) | 1:173:A:VAL:HB  | 1:175:A:PHE:HE2  | 9        | 0.5           |
| (2,768) | 1:173:A:VAL:HB  | 1:175:A:PHE:HE1  | 10       | 0.5           |
| (2,768) | 1:173:A:VAL:HB  | 1:175:A:PHE:HE2  | 10       | 0.5           |
| (2,740) | 1:162:A:ALA:HA  | 1:168:A:PHE:HE1  | 6        | 0.5           |
| (2,740) | 1:162:A:ALA:HA  | 1:168:A:PHE:HE2  | 6        | 0.5           |
| (2,735) | 1:158:A:ALA:H   | 1:160:A:TYR:HE1  | 4        | 0.5           |
| (2,735) | 1:158:A:ALA:H   | 1:160:A:TYR:HE2  | 4        | 0.5           |
| (2,702) | 1:132:A:SER:HB2 | 1:145:A:TYR:HE1  | 7        | 0.5           |
| (2,702) | 1:132:A:SER:HB2 | 1:145:A:TYR:HE2  | 7        | 0.5           |
| (2,659) | 1:125:A:LYS:HE2 | 1:125:A:LYS:H    | 9        | 0.5           |
| (2,659) | 1:125:A:LYS:HE3 | 1:125:A:LYS:H    | 9        | 0.5           |
| (2,656) | 1:125:A:LYS:HB2 | 1:126:A:THR:H    | 10       | 0.5           |
| (2,656) | 1:125:A:LYS:HB3 | 1:126:A:THR:H    | 10       | 0.5           |
| (2,635) | 1:122:A:TYR:HD1 | 1:126:A:THR:H    | 4        | 0.5           |
| (2,635) | 1:122:A:TYR:HD2 | 1:126:A:THR:H    | 4        | 0.5           |
| (2,635) | 1:122:A:TYR:HD1 | 1:126:A:THR:H    | 9        | 0.5           |
| (2,635) | 1:122:A:TYR:HD2 | 1:126:A:THR:H    | 9        | 0.5           |
| (2,632) | 1:122:A:TYR:HD1 | 1:125:A:LYS:H    | 2        | 0.5           |
| (2,632) | 1:122:A:TYR:HD2 | 1:125:A:LYS:H    | 2        | 0.5           |
| (2,631) | 1:122:A:TYR:HD1 | 1:124:A:ASP:H    | 5        | 0.5           |
| (2,631) | 1:122:A:TYR:HD2 | 1:124:A:ASP:H    | 5        | 0.5           |
| (2,631) | 1:122:A:TYR:HD1 | 1:124:A:ASP:H    | 10       | 0.5           |
| (2,631) | 1:122:A:TYR:HD2 | 1:124:A:ASP:H    | 10       | 0.5           |
| (2,592) | 1:114:A:ASP:HB3 | 1:116:A:GLU:HG2  | 7        | 0.5           |
| (2,592) | 1:114:A:ASP:HB3 | 1:116:A:GLU:HG3  | 7        | 0.5           |
| (2,590) | 1:110:A:VAL:H   | 1:111:A:ILE:HD11 | 5        | 0.5           |
| (2,590) | 1:110:A:VAL:H   | 1:111:A:ILE:HD12 | 5        | 0.5           |
| (2,590) | 1:110:A:VAL:H   | 1:111:A:ILE:HD13 | 5        | 0.5           |
| (2,523) | 1:85:A:TYR:HD1  | 1:134:A:TRP:H    | 1        | 0.5           |
| (2,523) | 1:85:A:TYR:HD2  | 1:134:A:TRP:H    | 1        | 0.5           |
| (2,523) | 1:85:A:TYR:HD1  | 1:134:A:TRP:H    | 3        | 0.5           |
| (2,523) | 1:85:A:TYR:HD2  | 1:134:A:TRP:H    | 3        | 0.5           |
| (2,365) | 1:66:A:ASN:HB3  | 1:173:A:VAL:HG21 | 1        | 0.5           |
| (2,365) | 1:66:A:ASN:HB3  | 1:173:A:VAL:HG22 | 1        | 0.5           |
| (2,365) | 1:66:A:ASN:HB3  | 1:173:A:VAL:HG23 | 1        | 0.5           |
| (2,355) | 1:64:A:LEU:H    | 1:175:A:PHE:HE1  | 6        | 0.5           |
| (2,355) | 1:64:A:LEU:H    | 1:175:A:PHE:HE2  | 6        | 0.5           |
| (2,125) | 1:28:A:HIS:HE1  | 1:46:A:TYR:HE1   | 6        | 0.5           |
| (2,125) | 1:28:A:HIS:HE1  | 1:46:A:TYR:HE2   | 6        | 0.5           |
| (2,16)  | 1:17:A:GLN:HG2  | 1:18:A:ALA:H     | 2        | 0.5           |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (2,16)   | 1:17:A:GLN:HG3   | 1:18:A:ALA:H    | 2        | 0.5           |
| (2,16)   | 1:17:A:GLN:HG2   | 1:18:A:ALA:H    | 4        | 0.5           |
| (2,16)   | 1:17:A:GLN:HG3   | 1:18:A:ALA:H    | 4        | 0.5           |
| (2,16)   | 1:17:A:GLN:HG2   | 1:18:A:ALA:H    | 5        | 0.5           |
| (2,16)   | 1:17:A:GLN:HG3   | 1:18:A:ALA:H    | 5        | 0.5           |
| (2,16)   | 1:17:A:GLN:HG2   | 1:18:A:ALA:H    | 10       | 0.5           |
| (2,16)   | 1:17:A:GLN:HG3   | 1:18:A:ALA:H    | 10       | 0.5           |
| (2,4)    | 1:15:A:THR:HG21  | 1:16:A:ALA:H    | 10       | 0.5           |
| (2,4)    | 1:15:A:THR:HG22  | 1:16:A:ALA:H    | 10       | 0.5           |
| (2,4)    | 1:15:A:THR:HG23  | 1:16:A:ALA:H    | 10       | 0.5           |
| (1,2449) | 1:179:A:VAL:HG21 | 1:179:A:VAL:H   | 2        | 0.5           |
| (1,2449) | 1:179:A:VAL:HG22 | 1:179:A:VAL:H   | 2        | 0.5           |
| (1,2449) | 1:179:A:VAL:HG23 | 1:179:A:VAL:H   | 2        | 0.5           |
| (1,2354) | 1:173:A:VAL:HG11 | 1:175:A:PHE:HE1 | 4        | 0.5           |
| (1,2354) | 1:173:A:VAL:HG11 | 1:175:A:PHE:HE2 | 4        | 0.5           |
| (1,2354) | 1:173:A:VAL:HG12 | 1:175:A:PHE:HE1 | 4        | 0.5           |
| (1,2354) | 1:173:A:VAL:HG12 | 1:175:A:PHE:HE2 | 4        | 0.5           |
| (1,2354) | 1:173:A:VAL:HG13 | 1:175:A:PHE:HE1 | 4        | 0.5           |
| (1,2354) | 1:173:A:VAL:HG13 | 1:175:A:PHE:HE2 | 4        | 0.5           |
| (1,2131) | 1:155:A:ASN:HD21 | 1:155:A:ASN:HA  | 5        | 0.5           |
| (1,2131) | 1:155:A:ASN:HD22 | 1:155:A:ASN:HA  | 5        | 0.5           |
| (1,2131) | 1:155:A:ASN:HD21 | 1:155:A:ASN:HA  | 6        | 0.5           |
| (1,2131) | 1:155:A:ASN:HD22 | 1:155:A:ASN:HA  | 6        | 0.5           |
| (1,2131) | 1:155:A:ASN:HD21 | 1:155:A:ASN:HA  | 10       | 0.5           |
| (1,2131) | 1:155:A:ASN:HD22 | 1:155:A:ASN:HA  | 10       | 0.5           |
| (1,1758) | 1:119:A:ALA:HB1  | 1:151:A:VAL:H   | 6        | 0.5           |
| (1,1758) | 1:119:A:ALA:HB2  | 1:151:A:VAL:H   | 6        | 0.5           |
| (1,1758) | 1:119:A:ALA:HB3  | 1:151:A:VAL:H   | 6        | 0.5           |
| (1,1213) | 1:81:A:ILE:HD11  | 1:81:A:ILE:H    | 3        | 0.5           |
| (1,1213) | 1:81:A:ILE:HD12  | 1:81:A:ILE:H    | 3        | 0.5           |
| (1,1213) | 1:81:A:ILE:HD13  | 1:81:A:ILE:H    | 3        | 0.5           |
| (1,1213) | 1:81:A:ILE:HD11  | 1:81:A:ILE:H    | 6        | 0.5           |
| (1,1213) | 1:81:A:ILE:HD12  | 1:81:A:ILE:H    | 6        | 0.5           |
| (1,1213) | 1:81:A:ILE:HD13  | 1:81:A:ILE:H    | 6        | 0.5           |
| (1,1213) | 1:81:A:ILE:HD11  | 1:81:A:ILE:H    | 7        | 0.5           |
| (1,1213) | 1:81:A:ILE:HD12  | 1:81:A:ILE:H    | 7        | 0.5           |
| (1,1213) | 1:81:A:ILE:HD13  | 1:81:A:ILE:H    | 7        | 0.5           |
| (1,1090) | 1:77:A:LEU:HD11  | 1:79:A:ILE:H    | 4        | 0.5           |
| (1,1090) | 1:77:A:LEU:HD12  | 1:79:A:ILE:H    | 4        | 0.5           |
| (1,1090) | 1:77:A:LEU:HD13  | 1:79:A:ILE:H    | 4        | 0.5           |
| (1,1090) | 1:77:A:LEU:HD21  | 1:79:A:ILE:H    | 4        | 0.5           |
| (1,1090) | 1:77:A:LEU:HD22  | 1:79:A:ILE:H    | 4        | 0.5           |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1090) | 1:77:A:LEU:HD23 | 1:79:A:ILE:H     | 4        | 0.5           |
| (1,679)  | 1:60:A:LEU:HD11 | 1:177:A:PHE:HD1  | 6        | 0.5           |
| (1,679)  | 1:60:A:LEU:HD11 | 1:177:A:PHE:HD2  | 6        | 0.5           |
| (1,679)  | 1:60:A:LEU:HD12 | 1:177:A:PHE:HD1  | 6        | 0.5           |
| (1,679)  | 1:60:A:LEU:HD12 | 1:177:A:PHE:HD2  | 6        | 0.5           |
| (1,679)  | 1:60:A:LEU:HD13 | 1:177:A:PHE:HD1  | 6        | 0.5           |
| (1,679)  | 1:60:A:LEU:HD13 | 1:177:A:PHE:HD2  | 6        | 0.5           |
| (1,581)  | 1:51:A:ILE:HG21 | 1:53:A:ASP:H     | 5        | 0.5           |
| (1,581)  | 1:51:A:ILE:HG22 | 1:53:A:ASP:H     | 5        | 0.5           |
| (1,581)  | 1:51:A:ILE:HG23 | 1:53:A:ASP:H     | 5        | 0.5           |
| (1,580)  | 1:51:A:ILE:HG21 | 1:53:A:ASP:H     | 5        | 0.5           |
| (1,580)  | 1:51:A:ILE:HG22 | 1:53:A:ASP:H     | 5        | 0.5           |
| (1,580)  | 1:51:A:ILE:HG23 | 1:53:A:ASP:H     | 5        | 0.5           |
| (1,545)  | 1:50:A:TRP:HA   | 1:151:A:VAL:HG21 | 5        | 0.5           |
| (1,545)  | 1:50:A:TRP:HA   | 1:151:A:VAL:HG22 | 5        | 0.5           |
| (1,545)  | 1:50:A:TRP:HA   | 1:151:A:VAL:HG23 | 5        | 0.5           |
| (1,545)  | 1:50:A:TRP:HA   | 1:151:A:VAL:HG21 | 7        | 0.5           |
| (1,545)  | 1:50:A:TRP:HA   | 1:151:A:VAL:HG22 | 7        | 0.5           |
| (1,545)  | 1:50:A:TRP:HA   | 1:151:A:VAL:HG23 | 7        | 0.5           |
| (1,389)  | 1:44:A:ILE:HG21 | 1:44:A:ILE:H     | 6        | 0.5           |
| (1,389)  | 1:44:A:ILE:HG22 | 1:44:A:ILE:H     | 6        | 0.5           |
| (1,389)  | 1:44:A:ILE:HG23 | 1:44:A:ILE:H     | 6        | 0.5           |
| (1,296)  | 1:38:A:ALA:HB1  | 1:39:A:GLN:H     | 4        | 0.5           |
| (1,296)  | 1:38:A:ALA:HB2  | 1:39:A:GLN:H     | 4        | 0.5           |
| (1,296)  | 1:38:A:ALA:HB3  | 1:39:A:GLN:H     | 4        | 0.5           |
| (1,287)  | 1:36:A:ALA:HB1  | 1:36:A:ALA:H     | 3        | 0.5           |
| (1,287)  | 1:36:A:ALA:HB2  | 1:36:A:ALA:H     | 3        | 0.5           |
| (1,287)  | 1:36:A:ALA:HB3  | 1:36:A:ALA:H     | 3        | 0.5           |
| (2,673)  | 1:127:A:GLY:H   | 1:128:A:TYR:HD1  | 10       | 0.49          |
| (2,673)  | 1:127:A:GLY:H   | 1:128:A:TYR:HD2  | 10       | 0.49          |
| (2,593)  | 1:114:A:ASP:HB2 | 1:116:A:GLU:HG2  | 6        | 0.49          |
| (2,593)  | 1:114:A:ASP:HB2 | 1:116:A:GLU:HG3  | 6        | 0.49          |
| (2,523)  | 1:85:A:TYR:HD1  | 1:134:A:TRP:H    | 8        | 0.49          |
| (2,523)  | 1:85:A:TYR:HD2  | 1:134:A:TRP:H    | 8        | 0.49          |
| (2,425)  | 1:74:A:PHE:HZ   | 1:160:A:TYR:HE1  | 7        | 0.49          |
| (2,425)  | 1:74:A:PHE:HZ   | 1:160:A:TYR:HE2  | 7        | 0.49          |
| (2,389)  | 1:70:A:LEU:HD21 | 1:172:A:PRO:HD2  | 7        | 0.49          |
| (2,389)  | 1:70:A:LEU:HD22 | 1:172:A:PRO:HD2  | 7        | 0.49          |
| (2,389)  | 1:70:A:LEU:HD23 | 1:172:A:PRO:HD2  | 7        | 0.49          |
| (2,365)  | 1:66:A:ASN:HB3  | 1:173:A:VAL:HG21 | 9        | 0.49          |
| (2,365)  | 1:66:A:ASN:HB3  | 1:173:A:VAL:HG22 | 9        | 0.49          |
| (2,365)  | 1:66:A:ASN:HB3  | 1:173:A:VAL:HG23 | 9        | 0.49          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,125)  | 1:28:A:HIS:HE1   | 1:46:A:TYR:HE1   | 1        | 0.49          |
| (2,125)  | 1:28:A:HIS:HE1   | 1:46:A:TYR:HE2   | 1        | 0.49          |
| (2,16)   | 1:17:A:GLN:HG2   | 1:18:A:ALA:H     | 1        | 0.49          |
| (2,16)   | 1:17:A:GLN:HG3   | 1:18:A:ALA:H     | 1        | 0.49          |
| (2,16)   | 1:17:A:GLN:HG2   | 1:18:A:ALA:H     | 8        | 0.49          |
| (2,16)   | 1:17:A:GLN:HG3   | 1:18:A:ALA:H     | 8        | 0.49          |
| (1,2462) | 1:182:A:VAL:HG11 | 1:183:A:GLY:H    | 2        | 0.49          |
| (1,2462) | 1:182:A:VAL:HG12 | 1:183:A:GLY:H    | 2        | 0.49          |
| (1,2462) | 1:182:A:VAL:HG13 | 1:183:A:GLY:H    | 2        | 0.49          |
| (1,2462) | 1:182:A:VAL:HG11 | 1:183:A:GLY:H    | 4        | 0.49          |
| (1,2462) | 1:182:A:VAL:HG12 | 1:183:A:GLY:H    | 4        | 0.49          |
| (1,2462) | 1:182:A:VAL:HG13 | 1:183:A:GLY:H    | 4        | 0.49          |
| (1,2462) | 1:182:A:VAL:HG11 | 1:183:A:GLY:H    | 5        | 0.49          |
| (1,2462) | 1:182:A:VAL:HG12 | 1:183:A:GLY:H    | 5        | 0.49          |
| (1,2462) | 1:182:A:VAL:HG13 | 1:183:A:GLY:H    | 5        | 0.49          |
| (1,2462) | 1:182:A:VAL:HG11 | 1:183:A:GLY:H    | 7        | 0.49          |
| (1,2462) | 1:182:A:VAL:HG12 | 1:183:A:GLY:H    | 7        | 0.49          |
| (1,2462) | 1:182:A:VAL:HG13 | 1:183:A:GLY:H    | 7        | 0.49          |
| (1,2462) | 1:182:A:VAL:HG11 | 1:183:A:GLY:H    | 10       | 0.49          |
| (1,2462) | 1:182:A:VAL:HG12 | 1:183:A:GLY:H    | 10       | 0.49          |
| (1,2462) | 1:182:A:VAL:HG13 | 1:183:A:GLY:H    | 10       | 0.49          |
| (1,2131) | 1:155:A:ASN:HD21 | 1:155:A:ASN:HA   | 3        | 0.49          |
| (1,2131) | 1:155:A:ASN:HD22 | 1:155:A:ASN:HA   | 3        | 0.49          |
| (1,2131) | 1:155:A:ASN:HD21 | 1:155:A:ASN:HA   | 4        | 0.49          |
| (1,2131) | 1:155:A:ASN:HD22 | 1:155:A:ASN:HA   | 4        | 0.49          |
| (1,2106) | 1:153:A:ILE:HG21 | 1:155:A:ASN:HD21 | 6        | 0.49          |
| (1,2106) | 1:153:A:ILE:HG21 | 1:155:A:ASN:HD22 | 6        | 0.49          |
| (1,2106) | 1:153:A:ILE:HG22 | 1:155:A:ASN:HD21 | 6        | 0.49          |
| (1,2106) | 1:153:A:ILE:HG22 | 1:155:A:ASN:HD22 | 6        | 0.49          |
| (1,2106) | 1:153:A:ILE:HG23 | 1:155:A:ASN:HD21 | 6        | 0.49          |
| (1,2106) | 1:153:A:ILE:HG23 | 1:155:A:ASN:HD22 | 6        | 0.49          |
| (1,2015) | 1:142:A:ILE:HG21 | 1:144:A:VAL:H    | 5        | 0.49          |
| (1,2015) | 1:142:A:ILE:HG22 | 1:144:A:VAL:H    | 5        | 0.49          |
| (1,2015) | 1:142:A:ILE:HG23 | 1:144:A:VAL:H    | 5        | 0.49          |
| (1,2015) | 1:142:A:ILE:HG21 | 1:144:A:VAL:H    | 8        | 0.49          |
| (1,2015) | 1:142:A:ILE:HG22 | 1:144:A:VAL:H    | 8        | 0.49          |
| (1,2015) | 1:142:A:ILE:HG23 | 1:144:A:VAL:H    | 8        | 0.49          |
| (1,1840) | 1:132:A:SER:HB3  | 1:142:A:ILE:HG21 | 5        | 0.49          |
| (1,1840) | 1:132:A:SER:HB3  | 1:142:A:ILE:HG22 | 5        | 0.49          |
| (1,1840) | 1:132:A:SER:HB3  | 1:142:A:ILE:HG23 | 5        | 0.49          |
| (1,1777) | 1:121:A:LEU:HD21 | 1:121:A:LEU:H    | 8        | 0.49          |
| (1,1777) | 1:121:A:LEU:HD22 | 1:121:A:LEU:H    | 8        | 0.49          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1777) | 1:121:A:LEU:HD23 | 1:121:A:LEU:H    | 8        | 0.49          |
| (1,1548) | 1:102:A:ILE:HG21 | 1:109:A:ALA:HB1  | 6        | 0.49          |
| (1,1548) | 1:102:A:ILE:HG21 | 1:109:A:ALA:HB2  | 6        | 0.49          |
| (1,1548) | 1:102:A:ILE:HG21 | 1:109:A:ALA:HB3  | 6        | 0.49          |
| (1,1548) | 1:102:A:ILE:HG22 | 1:109:A:ALA:HB1  | 6        | 0.49          |
| (1,1548) | 1:102:A:ILE:HG22 | 1:109:A:ALA:HB2  | 6        | 0.49          |
| (1,1548) | 1:102:A:ILE:HG22 | 1:109:A:ALA:HB3  | 6        | 0.49          |
| (1,1548) | 1:102:A:ILE:HG23 | 1:109:A:ALA:HB1  | 6        | 0.49          |
| (1,1548) | 1:102:A:ILE:HG23 | 1:109:A:ALA:HB2  | 6        | 0.49          |
| (1,1548) | 1:102:A:ILE:HG23 | 1:109:A:ALA:HB3  | 6        | 0.49          |
| (1,1546) | 1:102:A:ILE:HG21 | 1:108:A:SER:HA   | 7        | 0.49          |
| (1,1546) | 1:102:A:ILE:HG22 | 1:108:A:SER:HA   | 7        | 0.49          |
| (1,1546) | 1:102:A:ILE:HG23 | 1:108:A:SER:HA   | 7        | 0.49          |
| (1,1520) | 1:100:A:ALA:HB1  | 1:111:A:ILE:HG21 | 8        | 0.49          |
| (1,1520) | 1:100:A:ALA:HB1  | 1:111:A:ILE:HG22 | 8        | 0.49          |
| (1,1520) | 1:100:A:ALA:HB1  | 1:111:A:ILE:HG23 | 8        | 0.49          |
| (1,1520) | 1:100:A:ALA:HB2  | 1:111:A:ILE:HG21 | 8        | 0.49          |
| (1,1520) | 1:100:A:ALA:HB2  | 1:111:A:ILE:HG22 | 8        | 0.49          |
| (1,1520) | 1:100:A:ALA:HB2  | 1:111:A:ILE:HG23 | 8        | 0.49          |
| (1,1520) | 1:100:A:ALA:HB3  | 1:111:A:ILE:HG21 | 8        | 0.49          |
| (1,1520) | 1:100:A:ALA:HB3  | 1:111:A:ILE:HG22 | 8        | 0.49          |
| (1,1520) | 1:100:A:ALA:HB3  | 1:111:A:ILE:HG23 | 8        | 0.49          |
| (1,1228) | 1:81:A:ILE:HG21  | 1:82:A:THR:HA    | 6        | 0.49          |
| (1,1228) | 1:81:A:ILE:HG22  | 1:82:A:THR:HA    | 6        | 0.49          |
| (1,1228) | 1:81:A:ILE:HG23  | 1:82:A:THR:HA    | 6        | 0.49          |
| (1,1213) | 1:81:A:ILE:HD11  | 1:81:A:ILE:H     | 1        | 0.49          |
| (1,1213) | 1:81:A:ILE:HD12  | 1:81:A:ILE:H     | 1        | 0.49          |
| (1,1213) | 1:81:A:ILE:HD13  | 1:81:A:ILE:H     | 1        | 0.49          |
| (1,1090) | 1:77:A:LEU:HD11  | 1:79:A:ILE:H     | 8        | 0.49          |
| (1,1090) | 1:77:A:LEU:HD12  | 1:79:A:ILE:H     | 8        | 0.49          |
| (1,1090) | 1:77:A:LEU:HD13  | 1:79:A:ILE:H     | 8        | 0.49          |
| (1,1090) | 1:77:A:LEU:HD21  | 1:79:A:ILE:H     | 8        | 0.49          |
| (1,1090) | 1:77:A:LEU:HD22  | 1:79:A:ILE:H     | 8        | 0.49          |
| (1,1090) | 1:77:A:LEU:HD23  | 1:79:A:ILE:H     | 8        | 0.49          |
| (1,852)  | 1:66:A:ASN:HD22  | 1:70:A:LEU:HD21  | 3        | 0.49          |
| (1,852)  | 1:66:A:ASN:HD22  | 1:70:A:LEU:HD22  | 3        | 0.49          |
| (1,852)  | 1:66:A:ASN:HD22  | 1:70:A:LEU:HD23  | 3        | 0.49          |
| (1,581)  | 1:51:A:ILE:HG21  | 1:53:A:ASP:H     | 1        | 0.49          |
| (1,581)  | 1:51:A:ILE:HG22  | 1:53:A:ASP:H     | 1        | 0.49          |
| (1,581)  | 1:51:A:ILE:HG23  | 1:53:A:ASP:H     | 1        | 0.49          |
| (1,580)  | 1:51:A:ILE:HG21  | 1:53:A:ASP:H     | 1        | 0.49          |
| (1,580)  | 1:51:A:ILE:HG22  | 1:53:A:ASP:H     | 1        | 0.49          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,580)  | 1:51:A:ILE:HG23  | 1:53:A:ASP:H     | 1        | 0.49          |
| (1,495)  | 1:48:A:ILE:HG21  | 1:50:A:TRP:HE1   | 3        | 0.49          |
| (1,495)  | 1:48:A:ILE:HG22  | 1:50:A:TRP:HE1   | 3        | 0.49          |
| (1,495)  | 1:48:A:ILE:HG23  | 1:50:A:TRP:HE1   | 3        | 0.49          |
| (1,495)  | 1:48:A:ILE:HG21  | 1:50:A:TRP:HE1   | 5        | 0.49          |
| (1,495)  | 1:48:A:ILE:HG22  | 1:50:A:TRP:HE1   | 5        | 0.49          |
| (1,495)  | 1:48:A:ILE:HG23  | 1:50:A:TRP:HE1   | 5        | 0.49          |
| (1,294)  | 1:38:A:ALA:HA    | 1:38:A:ALA:HB1   | 9        | 0.49          |
| (1,294)  | 1:38:A:ALA:HA    | 1:38:A:ALA:HB2   | 9        | 0.49          |
| (1,294)  | 1:38:A:ALA:HA    | 1:38:A:ALA:HB3   | 9        | 0.49          |
| (2,631)  | 1:122:A:TYR:HD1  | 1:124:A:ASP:H    | 2        | 0.48          |
| (2,631)  | 1:122:A:TYR:HD2  | 1:124:A:ASP:H    | 2        | 0.48          |
| (2,592)  | 1:114:A:ASP:HB3  | 1:116:A:GLU:HG2  | 10       | 0.48          |
| (2,592)  | 1:114:A:ASP:HB3  | 1:116:A:GLU:HG3  | 10       | 0.48          |
| (1,2448) | 1:179:A:VAL:HG11 | 1:179:A:VAL:H    | 9        | 0.48          |
| (1,2448) | 1:179:A:VAL:HG12 | 1:179:A:VAL:H    | 9        | 0.48          |
| (1,2448) | 1:179:A:VAL:HG13 | 1:179:A:VAL:H    | 9        | 0.48          |
| (1,2131) | 1:155:A:ASN:HD21 | 1:155:A:ASN:HA   | 8        | 0.48          |
| (1,2131) | 1:155:A:ASN:HD22 | 1:155:A:ASN:HA   | 8        | 0.48          |
| (1,2015) | 1:142:A:ILE:HG21 | 1:144:A:VAL:H    | 4        | 0.48          |
| (1,2015) | 1:142:A:ILE:HG22 | 1:144:A:VAL:H    | 4        | 0.48          |
| (1,2015) | 1:142:A:ILE:HG23 | 1:144:A:VAL:H    | 4        | 0.48          |
| (1,1758) | 1:119:A:ALA:HB1  | 1:151:A:VAL:H    | 8        | 0.48          |
| (1,1758) | 1:119:A:ALA:HB2  | 1:151:A:VAL:H    | 8        | 0.48          |
| (1,1758) | 1:119:A:ALA:HB3  | 1:151:A:VAL:H    | 8        | 0.48          |
| (1,1662) | 1:113:A:LEU:HD11 | 1:113:A:LEU:H    | 1        | 0.48          |
| (1,1662) | 1:113:A:LEU:HD12 | 1:113:A:LEU:H    | 1        | 0.48          |
| (1,1662) | 1:113:A:LEU:HD13 | 1:113:A:LEU:H    | 1        | 0.48          |
| (1,1662) | 1:113:A:LEU:HD11 | 1:113:A:LEU:H    | 7        | 0.48          |
| (1,1662) | 1:113:A:LEU:HD12 | 1:113:A:LEU:H    | 7        | 0.48          |
| (1,1662) | 1:113:A:LEU:HD13 | 1:113:A:LEU:H    | 7        | 0.48          |
| (1,1647) | 1:112:A:VAL:HG11 | 1:112:A:VAL:H    | 2        | 0.48          |
| (1,1647) | 1:112:A:VAL:HG12 | 1:112:A:VAL:H    | 2        | 0.48          |
| (1,1647) | 1:112:A:VAL:HG13 | 1:112:A:VAL:H    | 2        | 0.48          |
| (1,1510) | 1:98:A:THR:HG21  | 1:100:A:ALA:H    | 2        | 0.48          |
| (1,1510) | 1:98:A:THR:HG22  | 1:100:A:ALA:H    | 2        | 0.48          |
| (1,1510) | 1:98:A:THR:HG23  | 1:100:A:ALA:H    | 2        | 0.48          |
| (1,1510) | 1:98:A:THR:HG21  | 1:100:A:ALA:H    | 10       | 0.48          |
| (1,1510) | 1:98:A:THR:HG22  | 1:100:A:ALA:H    | 10       | 0.48          |
| (1,1510) | 1:98:A:THR:HG23  | 1:100:A:ALA:H    | 10       | 0.48          |
| (1,436)  | 1:46:A:TYR:HB2   | 1:153:A:ILE:HG21 | 5        | 0.48          |
| (1,436)  | 1:46:A:TYR:HB2   | 1:153:A:ILE:HG22 | 5        | 0.48          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,436)  | 1:46:A:TYR:HB2   | 1:153:A:ILE:HG23 | 5        | 0.48          |
| (1,289)  | 1:37:A:GLY:HA3   | 1:37:A:GLY:H     | 2        | 0.48          |
| (1,205)  | 1:32:A:ILE:HA    | 1:32:A:ILE:HD11  | 2        | 0.48          |
| (1,205)  | 1:32:A:ILE:HA    | 1:32:A:ILE:HD12  | 2        | 0.48          |
| (1,205)  | 1:32:A:ILE:HA    | 1:32:A:ILE:HD13  | 2        | 0.48          |
| (1,126)  | 1:27:A:SER:HB2   | 1:177:A:PHE:HE1  | 10       | 0.48          |
| (1,126)  | 1:27:A:SER:HB2   | 1:177:A:PHE:HE2  | 10       | 0.48          |
| (1,126)  | 1:27:A:SER:HB3   | 1:177:A:PHE:HE1  | 10       | 0.48          |
| (1,126)  | 1:27:A:SER:HB3   | 1:177:A:PHE:HE2  | 10       | 0.48          |
| (2,740)  | 1:162:A:ALA:HA   | 1:168:A:PHE:HE1  | 2        | 0.47          |
| (2,740)  | 1:162:A:ALA:HA   | 1:168:A:PHE:HE2  | 2        | 0.47          |
| (2,740)  | 1:162:A:ALA:HA   | 1:168:A:PHE:HE1  | 10       | 0.47          |
| (2,740)  | 1:162:A:ALA:HA   | 1:168:A:PHE:HE2  | 10       | 0.47          |
| (2,656)  | 1:125:A:LYS:HB2  | 1:126:A:THR:H    | 3        | 0.47          |
| (2,656)  | 1:125:A:LYS:HB3  | 1:126:A:THR:H    | 3        | 0.47          |
| (2,523)  | 1:85:A:TYR:HD1   | 1:134:A:TRP:H    | 5        | 0.47          |
| (2,523)  | 1:85:A:TYR:HD2   | 1:134:A:TRP:H    | 5        | 0.47          |
| (2,523)  | 1:85:A:TYR:HD1   | 1:134:A:TRP:H    | 7        | 0.47          |
| (2,523)  | 1:85:A:TYR:HD2   | 1:134:A:TRP:H    | 7        | 0.47          |
| (2,425)  | 1:74:A:PHE:HZ    | 1:160:A:TYR:HE1  | 1        | 0.47          |
| (2,425)  | 1:74:A:PHE:HZ    | 1:160:A:TYR:HE2  | 1        | 0.47          |
| (2,389)  | 1:70:A:LEU:HD21  | 1:172:A:PRO:HD2  | 6        | 0.47          |
| (2,389)  | 1:70:A:LEU:HD22  | 1:172:A:PRO:HD2  | 6        | 0.47          |
| (2,389)  | 1:70:A:LEU:HD23  | 1:172:A:PRO:HD2  | 6        | 0.47          |
| (2,240)  | 1:46:A:TYR:HB2   | 1:155:A:ASN:HD21 | 1        | 0.47          |
| (2,240)  | 1:46:A:TYR:HB2   | 1:155:A:ASN:HD22 | 1        | 0.47          |
| (2,94)   | 1:23:A:ILE:HD11  | 1:53:A:ASP:H     | 9        | 0.47          |
| (2,94)   | 1:23:A:ILE:HD12  | 1:53:A:ASP:H     | 9        | 0.47          |
| (2,94)   | 1:23:A:ILE:HD13  | 1:53:A:ASP:H     | 9        | 0.47          |
| (1,2463) | 1:182:A:VAL:HG21 | 1:182:A:VAL:H    | 7        | 0.47          |
| (1,2463) | 1:182:A:VAL:HG22 | 1:182:A:VAL:H    | 7        | 0.47          |
| (1,2463) | 1:182:A:VAL:HG23 | 1:182:A:VAL:H    | 7        | 0.47          |
| (1,2462) | 1:182:A:VAL:HG11 | 1:183:A:GLY:H    | 3        | 0.47          |
| (1,2462) | 1:182:A:VAL:HG12 | 1:183:A:GLY:H    | 3        | 0.47          |
| (1,2462) | 1:182:A:VAL:HG13 | 1:183:A:GLY:H    | 3        | 0.47          |
| (1,2448) | 1:179:A:VAL:HG11 | 1:179:A:VAL:H    | 1        | 0.47          |
| (1,2448) | 1:179:A:VAL:HG12 | 1:179:A:VAL:H    | 1        | 0.47          |
| (1,2448) | 1:179:A:VAL:HG13 | 1:179:A:VAL:H    | 1        | 0.47          |
| (1,2448) | 1:179:A:VAL:HG11 | 1:179:A:VAL:H    | 7        | 0.47          |
| (1,2448) | 1:179:A:VAL:HG12 | 1:179:A:VAL:H    | 7        | 0.47          |
| (1,2448) | 1:179:A:VAL:HG13 | 1:179:A:VAL:H    | 7        | 0.47          |
| (1,2131) | 1:155:A:ASN:HD21 | 1:155:A:ASN:HA   | 1        | 0.47          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2131) | 1:155:A:ASN:HD22 | 1:155:A:ASN:HA   | 1        | 0.47          |
| (1,2081) | 1:151:A:VAL:HG11 | 1:153:A:ILE:H    | 6        | 0.47          |
| (1,2081) | 1:151:A:VAL:HG12 | 1:153:A:ILE:H    | 6        | 0.47          |
| (1,2081) | 1:151:A:VAL:HG13 | 1:153:A:ILE:H    | 6        | 0.47          |
| (1,2032) | 1:143:A:ILE:HG21 | 1:144:A:VAL:H    | 3        | 0.47          |
| (1,2032) | 1:143:A:ILE:HG22 | 1:144:A:VAL:H    | 3        | 0.47          |
| (1,2032) | 1:143:A:ILE:HG23 | 1:144:A:VAL:H    | 3        | 0.47          |
| (1,1859) | 1:133:A:ILE:HD11 | 1:144:A:VAL:HB   | 10       | 0.47          |
| (1,1859) | 1:133:A:ILE:HD12 | 1:144:A:VAL:HB   | 10       | 0.47          |
| (1,1859) | 1:133:A:ILE:HD13 | 1:144:A:VAL:HB   | 10       | 0.47          |
| (1,1804) | 1:129:A:THR:HB   | 1:129:A:THR:HG21 | 8        | 0.47          |
| (1,1804) | 1:129:A:THR:HB   | 1:129:A:THR:HG22 | 8        | 0.47          |
| (1,1804) | 1:129:A:THR:HB   | 1:129:A:THR:HG23 | 8        | 0.47          |
| (1,1758) | 1:119:A:ALA:HB1  | 1:151:A:VAL:H    | 9        | 0.47          |
| (1,1758) | 1:119:A:ALA:HB2  | 1:151:A:VAL:H    | 9        | 0.47          |
| (1,1758) | 1:119:A:ALA:HB3  | 1:151:A:VAL:H    | 9        | 0.47          |
| (1,1647) | 1:112:A:VAL:HG11 | 1:112:A:VAL:H    | 1        | 0.47          |
| (1,1647) | 1:112:A:VAL:HG12 | 1:112:A:VAL:H    | 1        | 0.47          |
| (1,1647) | 1:112:A:VAL:HG13 | 1:112:A:VAL:H    | 1        | 0.47          |
| (1,1647) | 1:112:A:VAL:HG11 | 1:112:A:VAL:H    | 10       | 0.47          |
| (1,1647) | 1:112:A:VAL:HG12 | 1:112:A:VAL:H    | 10       | 0.47          |
| (1,1647) | 1:112:A:VAL:HG13 | 1:112:A:VAL:H    | 10       | 0.47          |
| (1,1630) | 1:110:A:VAL:HG21 | 1:110:A:VAL:H    | 3        | 0.47          |
| (1,1630) | 1:110:A:VAL:HG22 | 1:110:A:VAL:H    | 3        | 0.47          |
| (1,1630) | 1:110:A:VAL:HG23 | 1:110:A:VAL:H    | 3        | 0.47          |
| (1,1630) | 1:110:A:VAL:HG21 | 1:110:A:VAL:H    | 9        | 0.47          |
| (1,1630) | 1:110:A:VAL:HG22 | 1:110:A:VAL:H    | 9        | 0.47          |
| (1,1630) | 1:110:A:VAL:HG23 | 1:110:A:VAL:H    | 9        | 0.47          |
| (1,1510) | 1:98:A:THR:HG21  | 1:100:A:ALA:H    | 1        | 0.47          |
| (1,1510) | 1:98:A:THR:HG22  | 1:100:A:ALA:H    | 1        | 0.47          |
| (1,1510) | 1:98:A:THR:HG23  | 1:100:A:ALA:H    | 1        | 0.47          |
| (1,1510) | 1:98:A:THR:HG21  | 1:100:A:ALA:H    | 4        | 0.47          |
| (1,1510) | 1:98:A:THR:HG22  | 1:100:A:ALA:H    | 4        | 0.47          |
| (1,1510) | 1:98:A:THR:HG23  | 1:100:A:ALA:H    | 4        | 0.47          |
| (1,1510) | 1:98:A:THR:HG21  | 1:100:A:ALA:H    | 8        | 0.47          |
| (1,1510) | 1:98:A:THR:HG22  | 1:100:A:ALA:H    | 8        | 0.47          |
| (1,1510) | 1:98:A:THR:HG23  | 1:100:A:ALA:H    | 8        | 0.47          |
| (1,1510) | 1:98:A:THR:HG21  | 1:100:A:ALA:H    | 9        | 0.47          |
| (1,1510) | 1:98:A:THR:HG22  | 1:100:A:ALA:H    | 9        | 0.47          |
| (1,1510) | 1:98:A:THR:HG23  | 1:100:A:ALA:H    | 9        | 0.47          |
| (1,1475) | 1:95:A:PHE:HB2   | 1:96:A:SER:H     | 2        | 0.47          |
| (1,1475) | 1:95:A:PHE:HB3   | 1:96:A:SER:H     | 2        | 0.47          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1460) | 1:92:A:LEU:HG   | 1:93:A:GLY:H    | 8        | 0.47          |
| (1,1097) | 1:77:A:LEU:HD11 | 1:160:A:TYR:HB3 | 9        | 0.47          |
| (1,1097) | 1:77:A:LEU:HD12 | 1:160:A:TYR:HB3 | 9        | 0.47          |
| (1,1097) | 1:77:A:LEU:HD13 | 1:160:A:TYR:HB3 | 9        | 0.47          |
| (1,1097) | 1:77:A:LEU:HD21 | 1:160:A:TYR:HB3 | 9        | 0.47          |
| (1,1097) | 1:77:A:LEU:HD22 | 1:160:A:TYR:HB3 | 9        | 0.47          |
| (1,1097) | 1:77:A:LEU:HD23 | 1:160:A:TYR:HB3 | 9        | 0.47          |
| (1,1088) | 1:77:A:LEU:HD11 | 1:78:A:GLN:H    | 5        | 0.47          |
| (1,1088) | 1:77:A:LEU:HD12 | 1:78:A:GLN:H    | 5        | 0.47          |
| (1,1088) | 1:77:A:LEU:HD13 | 1:78:A:GLN:H    | 5        | 0.47          |
| (1,1088) | 1:77:A:LEU:HD21 | 1:78:A:GLN:H    | 5        | 0.47          |
| (1,1088) | 1:77:A:LEU:HD22 | 1:78:A:GLN:H    | 5        | 0.47          |
| (1,1088) | 1:77:A:LEU:HD23 | 1:78:A:GLN:H    | 5        | 0.47          |
| (1,852)  | 1:66:A:ASN:HD22 | 1:70:A:LEU:HD21 | 9        | 0.47          |
| (1,852)  | 1:66:A:ASN:HD22 | 1:70:A:LEU:HD22 | 9        | 0.47          |
| (1,852)  | 1:66:A:ASN:HD22 | 1:70:A:LEU:HD23 | 9        | 0.47          |
| (1,582)  | 1:51:A:ILE:HG21 | 1:55:A:VAL:H    | 9        | 0.47          |
| (1,582)  | 1:51:A:ILE:HG22 | 1:55:A:VAL:H    | 9        | 0.47          |
| (1,582)  | 1:51:A:ILE:HG23 | 1:55:A:VAL:H    | 9        | 0.47          |
| (1,581)  | 1:51:A:ILE:HG21 | 1:53:A:ASP:H    | 2        | 0.47          |
| (1,581)  | 1:51:A:ILE:HG22 | 1:53:A:ASP:H    | 2        | 0.47          |
| (1,581)  | 1:51:A:ILE:HG23 | 1:53:A:ASP:H    | 2        | 0.47          |
| (1,581)  | 1:51:A:ILE:HG21 | 1:53:A:ASP:H    | 3        | 0.47          |
| (1,581)  | 1:51:A:ILE:HG22 | 1:53:A:ASP:H    | 3        | 0.47          |
| (1,581)  | 1:51:A:ILE:HG23 | 1:53:A:ASP:H    | 3        | 0.47          |
| (1,581)  | 1:51:A:ILE:HG21 | 1:53:A:ASP:H    | 8        | 0.47          |
| (1,581)  | 1:51:A:ILE:HG22 | 1:53:A:ASP:H    | 8        | 0.47          |
| (1,581)  | 1:51:A:ILE:HG23 | 1:53:A:ASP:H    | 8        | 0.47          |
| (1,581)  | 1:51:A:ILE:HG21 | 1:53:A:ASP:H    | 9        | 0.47          |
| (1,581)  | 1:51:A:ILE:HG22 | 1:53:A:ASP:H    | 9        | 0.47          |
| (1,581)  | 1:51:A:ILE:HG23 | 1:53:A:ASP:H    | 9        | 0.47          |
| (1,581)  | 1:51:A:ILE:HG21 | 1:53:A:ASP:H    | 10       | 0.47          |
| (1,581)  | 1:51:A:ILE:HG22 | 1:53:A:ASP:H    | 10       | 0.47          |
| (1,581)  | 1:51:A:ILE:HG23 | 1:53:A:ASP:H    | 10       | 0.47          |
| (1,580)  | 1:51:A:ILE:HG21 | 1:53:A:ASP:H    | 2        | 0.47          |
| (1,580)  | 1:51:A:ILE:HG22 | 1:53:A:ASP:H    | 2        | 0.47          |
| (1,580)  | 1:51:A:ILE:HG23 | 1:53:A:ASP:H    | 2        | 0.47          |
| (1,580)  | 1:51:A:ILE:HG21 | 1:53:A:ASP:H    | 3        | 0.47          |
| (1,580)  | 1:51:A:ILE:HG22 | 1:53:A:ASP:H    | 3        | 0.47          |
| (1,580)  | 1:51:A:ILE:HG23 | 1:53:A:ASP:H    | 3        | 0.47          |
| (1,580)  | 1:51:A:ILE:HG21 | 1:53:A:ASP:H    | 8        | 0.47          |
| (1,580)  | 1:51:A:ILE:HG22 | 1:53:A:ASP:H    | 8        | 0.47          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,580) | 1:51:A:ILE:HG23 | 1:53:A:ASP:H    | 8        | 0.47          |
| (1,580) | 1:51:A:ILE:HG21 | 1:53:A:ASP:H    | 9        | 0.47          |
| (1,580) | 1:51:A:ILE:HG22 | 1:53:A:ASP:H    | 9        | 0.47          |
| (1,580) | 1:51:A:ILE:HG23 | 1:53:A:ASP:H    | 9        | 0.47          |
| (1,580) | 1:51:A:ILE:HG21 | 1:53:A:ASP:H    | 10       | 0.47          |
| (1,580) | 1:51:A:ILE:HG22 | 1:53:A:ASP:H    | 10       | 0.47          |
| (1,580) | 1:51:A:ILE:HG23 | 1:53:A:ASP:H    | 10       | 0.47          |
| (1,294) | 1:38:A:ALA:HA   | 1:38:A:ALA:HB1  | 1        | 0.47          |
| (1,294) | 1:38:A:ALA:HA   | 1:38:A:ALA:HB2  | 1        | 0.47          |
| (1,294) | 1:38:A:ALA:HA   | 1:38:A:ALA:HB3  | 1        | 0.47          |
| (1,294) | 1:38:A:ALA:HA   | 1:38:A:ALA:HB1  | 2        | 0.47          |
| (1,294) | 1:38:A:ALA:HA   | 1:38:A:ALA:HB2  | 2        | 0.47          |
| (1,294) | 1:38:A:ALA:HA   | 1:38:A:ALA:HB3  | 2        | 0.47          |
| (1,294) | 1:38:A:ALA:HA   | 1:38:A:ALA:HB1  | 3        | 0.47          |
| (1,294) | 1:38:A:ALA:HA   | 1:38:A:ALA:HB2  | 3        | 0.47          |
| (1,294) | 1:38:A:ALA:HA   | 1:38:A:ALA:HB3  | 3        | 0.47          |
| (1,294) | 1:38:A:ALA:HA   | 1:38:A:ALA:HB1  | 6        | 0.47          |
| (1,294) | 1:38:A:ALA:HA   | 1:38:A:ALA:HB2  | 6        | 0.47          |
| (1,294) | 1:38:A:ALA:HA   | 1:38:A:ALA:HB3  | 6        | 0.47          |
| (1,294) | 1:38:A:ALA:HA   | 1:38:A:ALA:HB1  | 7        | 0.47          |
| (1,294) | 1:38:A:ALA:HA   | 1:38:A:ALA:HB2  | 7        | 0.47          |
| (1,294) | 1:38:A:ALA:HA   | 1:38:A:ALA:HB3  | 7        | 0.47          |
| (1,294) | 1:38:A:ALA:HA   | 1:38:A:ALA:HB1  | 8        | 0.47          |
| (1,294) | 1:38:A:ALA:HA   | 1:38:A:ALA:HB2  | 8        | 0.47          |
| (1,294) | 1:38:A:ALA:HA   | 1:38:A:ALA:HB3  | 8        | 0.47          |
| (1,294) | 1:38:A:ALA:HA   | 1:38:A:ALA:HB1  | 10       | 0.47          |
| (1,294) | 1:38:A:ALA:HA   | 1:38:A:ALA:HB2  | 10       | 0.47          |
| (1,294) | 1:38:A:ALA:HA   | 1:38:A:ALA:HB3  | 10       | 0.47          |
| (1,287) | 1:36:A:ALA:HB1  | 1:36:A:ALA:H    | 7        | 0.47          |
| (1,287) | 1:36:A:ALA:HB2  | 1:36:A:ALA:H    | 7        | 0.47          |
| (1,287) | 1:36:A:ALA:HB3  | 1:36:A:ALA:H    | 7        | 0.47          |
| (1,223) | 1:32:A:ILE:HD11 | 1:160:A:TYR:HE1 | 9        | 0.47          |
| (1,223) | 1:32:A:ILE:HD11 | 1:160:A:TYR:HE2 | 9        | 0.47          |
| (1,223) | 1:32:A:ILE:HD12 | 1:160:A:TYR:HE1 | 9        | 0.47          |
| (1,223) | 1:32:A:ILE:HD12 | 1:160:A:TYR:HE2 | 9        | 0.47          |
| (1,223) | 1:32:A:ILE:HD13 | 1:160:A:TYR:HE1 | 9        | 0.47          |
| (1,223) | 1:32:A:ILE:HD13 | 1:160:A:TYR:HE2 | 9        | 0.47          |
| (1,205) | 1:32:A:ILE:HA   | 1:32:A:ILE:HD11 | 6        | 0.47          |
| (1,205) | 1:32:A:ILE:HA   | 1:32:A:ILE:HD12 | 6        | 0.47          |
| (1,205) | 1:32:A:ILE:HA   | 1:32:A:ILE:HD13 | 6        | 0.47          |
| (1,3)   | 1:16:A:ALA:HB1  | 1:16:A:ALA:H    | 2        | 0.47          |
| (1,3)   | 1:16:A:ALA:HB2  | 1:16:A:ALA:H    | 2        | 0.47          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3)    | 1:16:A:ALA:HB3   | 1:16:A:ALA:H     | 2        | 0.47          |
| (1,3)    | 1:16:A:ALA:HB1   | 1:16:A:ALA:H     | 4        | 0.47          |
| (1,3)    | 1:16:A:ALA:HB2   | 1:16:A:ALA:H     | 4        | 0.47          |
| (1,3)    | 1:16:A:ALA:HB3   | 1:16:A:ALA:H     | 4        | 0.47          |
| (2,16)   | 1:17:A:GLN:HG2   | 1:18:A:ALA:H     | 3        | 0.46          |
| (2,16)   | 1:17:A:GLN:HG3   | 1:18:A:ALA:H     | 3        | 0.46          |
| (1,2463) | 1:182:A:VAL:HG21 | 1:182:A:VAL:H    | 5        | 0.46          |
| (1,2463) | 1:182:A:VAL:HG22 | 1:182:A:VAL:H    | 5        | 0.46          |
| (1,2463) | 1:182:A:VAL:HG23 | 1:182:A:VAL:H    | 5        | 0.46          |
| (1,2320) | 1:171:A:LEU:HD11 | 1:171:A:LEU:HD21 | 8        | 0.46          |
| (1,2320) | 1:171:A:LEU:HD11 | 1:171:A:LEU:HD22 | 8        | 0.46          |
| (1,2320) | 1:171:A:LEU:HD11 | 1:171:A:LEU:HD23 | 8        | 0.46          |
| (1,2320) | 1:171:A:LEU:HD12 | 1:171:A:LEU:HD21 | 8        | 0.46          |
| (1,2320) | 1:171:A:LEU:HD12 | 1:171:A:LEU:HD22 | 8        | 0.46          |
| (1,2320) | 1:171:A:LEU:HD12 | 1:171:A:LEU:HD23 | 8        | 0.46          |
| (1,2320) | 1:171:A:LEU:HD13 | 1:171:A:LEU:HD21 | 8        | 0.46          |
| (1,2320) | 1:171:A:LEU:HD13 | 1:171:A:LEU:HD22 | 8        | 0.46          |
| (1,2320) | 1:171:A:LEU:HD13 | 1:171:A:LEU:HD23 | 8        | 0.46          |
| (1,2176) | 1:157:A:LYS:HE2  | 1:159:A:PHE:HE1  | 10       | 0.46          |
| (1,2176) | 1:157:A:LYS:HE2  | 1:159:A:PHE:HE2  | 10       | 0.46          |
| (1,2176) | 1:157:A:LYS:HE3  | 1:159:A:PHE:HE1  | 10       | 0.46          |
| (1,2176) | 1:157:A:LYS:HE3  | 1:159:A:PHE:HE2  | 10       | 0.46          |
| (1,2083) | 1:151:A:VAL:HG21 | 1:152:A:ALA:H    | 5        | 0.46          |
| (1,2083) | 1:151:A:VAL:HG22 | 1:152:A:ALA:H    | 5        | 0.46          |
| (1,2083) | 1:151:A:VAL:HG23 | 1:152:A:ALA:H    | 5        | 0.46          |
| (1,2083) | 1:151:A:VAL:HG21 | 1:152:A:ALA:H    | 7        | 0.46          |
| (1,2083) | 1:151:A:VAL:HG22 | 1:152:A:ALA:H    | 7        | 0.46          |
| (1,2083) | 1:151:A:VAL:HG23 | 1:152:A:ALA:H    | 7        | 0.46          |
| (1,1804) | 1:129:A:THR:HB   | 1:129:A:THR:HG21 | 1        | 0.46          |
| (1,1804) | 1:129:A:THR:HB   | 1:129:A:THR:HG22 | 1        | 0.46          |
| (1,1804) | 1:129:A:THR:HB   | 1:129:A:THR:HG23 | 1        | 0.46          |
| (1,1804) | 1:129:A:THR:HB   | 1:129:A:THR:HG21 | 2        | 0.46          |
| (1,1804) | 1:129:A:THR:HB   | 1:129:A:THR:HG22 | 2        | 0.46          |
| (1,1804) | 1:129:A:THR:HB   | 1:129:A:THR:HG23 | 2        | 0.46          |
| (1,1804) | 1:129:A:THR:HB   | 1:129:A:THR:HG21 | 3        | 0.46          |
| (1,1804) | 1:129:A:THR:HB   | 1:129:A:THR:HG22 | 3        | 0.46          |
| (1,1804) | 1:129:A:THR:HB   | 1:129:A:THR:HG23 | 3        | 0.46          |
| (1,1804) | 1:129:A:THR:HB   | 1:129:A:THR:HG21 | 4        | 0.46          |
| (1,1804) | 1:129:A:THR:HB   | 1:129:A:THR:HG22 | 4        | 0.46          |
| (1,1804) | 1:129:A:THR:HB   | 1:129:A:THR:HG23 | 4        | 0.46          |
| (1,1804) | 1:129:A:THR:HB   | 1:129:A:THR:HG21 | 5        | 0.46          |
| (1,1804) | 1:129:A:THR:HB   | 1:129:A:THR:HG22 | 5        | 0.46          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1804) | 1:129:A:THR:HB   | 1:129:A:THR:HG23 | 5        | 0.46          |
| (1,1804) | 1:129:A:THR:HB   | 1:129:A:THR:HG21 | 6        | 0.46          |
| (1,1804) | 1:129:A:THR:HB   | 1:129:A:THR:HG22 | 6        | 0.46          |
| (1,1804) | 1:129:A:THR:HB   | 1:129:A:THR:HG23 | 6        | 0.46          |
| (1,1804) | 1:129:A:THR:HB   | 1:129:A:THR:HG21 | 7        | 0.46          |
| (1,1804) | 1:129:A:THR:HB   | 1:129:A:THR:HG22 | 7        | 0.46          |
| (1,1804) | 1:129:A:THR:HB   | 1:129:A:THR:HG23 | 7        | 0.46          |
| (1,1804) | 1:129:A:THR:HB   | 1:129:A:THR:HG21 | 9        | 0.46          |
| (1,1804) | 1:129:A:THR:HB   | 1:129:A:THR:HG22 | 9        | 0.46          |
| (1,1804) | 1:129:A:THR:HB   | 1:129:A:THR:HG23 | 9        | 0.46          |
| (1,1804) | 1:129:A:THR:HB   | 1:129:A:THR:HG21 | 10       | 0.46          |
| (1,1804) | 1:129:A:THR:HB   | 1:129:A:THR:HG22 | 10       | 0.46          |
| (1,1804) | 1:129:A:THR:HB   | 1:129:A:THR:HG23 | 10       | 0.46          |
| (1,1647) | 1:112:A:VAL:HG11 | 1:112:A:VAL:H    | 5        | 0.46          |
| (1,1647) | 1:112:A:VAL:HG12 | 1:112:A:VAL:H    | 5        | 0.46          |
| (1,1647) | 1:112:A:VAL:HG13 | 1:112:A:VAL:H    | 5        | 0.46          |
| (1,1647) | 1:112:A:VAL:HG11 | 1:112:A:VAL:H    | 7        | 0.46          |
| (1,1647) | 1:112:A:VAL:HG12 | 1:112:A:VAL:H    | 7        | 0.46          |
| (1,1647) | 1:112:A:VAL:HG13 | 1:112:A:VAL:H    | 7        | 0.46          |
| (1,1630) | 1:110:A:VAL:HG21 | 1:110:A:VAL:H    | 2        | 0.46          |
| (1,1630) | 1:110:A:VAL:HG22 | 1:110:A:VAL:H    | 2        | 0.46          |
| (1,1630) | 1:110:A:VAL:HG23 | 1:110:A:VAL:H    | 2        | 0.46          |
| (1,1630) | 1:110:A:VAL:HG21 | 1:110:A:VAL:H    | 4        | 0.46          |
| (1,1630) | 1:110:A:VAL:HG22 | 1:110:A:VAL:H    | 4        | 0.46          |
| (1,1630) | 1:110:A:VAL:HG23 | 1:110:A:VAL:H    | 4        | 0.46          |
| (1,1630) | 1:110:A:VAL:HG21 | 1:110:A:VAL:H    | 5        | 0.46          |
| (1,1630) | 1:110:A:VAL:HG22 | 1:110:A:VAL:H    | 5        | 0.46          |
| (1,1630) | 1:110:A:VAL:HG23 | 1:110:A:VAL:H    | 5        | 0.46          |
| (1,1630) | 1:110:A:VAL:HG21 | 1:110:A:VAL:H    | 7        | 0.46          |
| (1,1630) | 1:110:A:VAL:HG22 | 1:110:A:VAL:H    | 7        | 0.46          |
| (1,1630) | 1:110:A:VAL:HG23 | 1:110:A:VAL:H    | 7        | 0.46          |
| (1,1630) | 1:110:A:VAL:HG21 | 1:110:A:VAL:H    | 10       | 0.46          |
| (1,1630) | 1:110:A:VAL:HG22 | 1:110:A:VAL:H    | 10       | 0.46          |
| (1,1630) | 1:110:A:VAL:HG23 | 1:110:A:VAL:H    | 10       | 0.46          |
| (1,1546) | 1:102:A:ILE:HG21 | 1:108:A:SER:HA   | 10       | 0.46          |
| (1,1546) | 1:102:A:ILE:HG22 | 1:108:A:SER:HA   | 10       | 0.46          |
| (1,1546) | 1:102:A:ILE:HG23 | 1:108:A:SER:HA   | 10       | 0.46          |
| (1,1545) | 1:102:A:ILE:HG21 | 1:107:A:PRO:HA   | 4        | 0.46          |
| (1,1545) | 1:102:A:ILE:HG22 | 1:107:A:PRO:HA   | 4        | 0.46          |
| (1,1545) | 1:102:A:ILE:HG23 | 1:107:A:PRO:HA   | 4        | 0.46          |
| (1,1343) | 1:85:A:TYR:HE1   | 1:152:A:ALA:HA   | 5        | 0.46          |
| (1,1343) | 1:85:A:TYR:HE2   | 1:152:A:ALA:HA   | 5        | 0.46          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1228) | 1:81:A:ILE:HG21 | 1:82:A:THR:HA   | 3        | 0.46          |
| (1,1228) | 1:81:A:ILE:HG22 | 1:82:A:THR:HA   | 3        | 0.46          |
| (1,1228) | 1:81:A:ILE:HG23 | 1:82:A:THR:HA   | 3        | 0.46          |
| (1,852)  | 1:66:A:ASN:HD22 | 1:70:A:LEU:HD21 | 4        | 0.46          |
| (1,852)  | 1:66:A:ASN:HD22 | 1:70:A:LEU:HD22 | 4        | 0.46          |
| (1,852)  | 1:66:A:ASN:HD22 | 1:70:A:LEU:HD23 | 4        | 0.46          |
| (1,599)  | 1:53:A:ASP:H    | 1:55:A:VAL:HG11 | 1        | 0.46          |
| (1,599)  | 1:53:A:ASP:H    | 1:55:A:VAL:HG12 | 1        | 0.46          |
| (1,599)  | 1:53:A:ASP:H    | 1:55:A:VAL:HG13 | 1        | 0.46          |
| (1,581)  | 1:51:A:ILE:HG21 | 1:53:A:ASP:H    | 7        | 0.46          |
| (1,581)  | 1:51:A:ILE:HG22 | 1:53:A:ASP:H    | 7        | 0.46          |
| (1,581)  | 1:51:A:ILE:HG23 | 1:53:A:ASP:H    | 7        | 0.46          |
| (1,580)  | 1:51:A:ILE:HG21 | 1:53:A:ASP:H    | 7        | 0.46          |
| (1,580)  | 1:51:A:ILE:HG22 | 1:53:A:ASP:H    | 7        | 0.46          |
| (1,580)  | 1:51:A:ILE:HG23 | 1:53:A:ASP:H    | 7        | 0.46          |
| (1,294)  | 1:38:A:ALA:HA   | 1:38:A:ALA:HB1  | 4        | 0.46          |
| (1,294)  | 1:38:A:ALA:HA   | 1:38:A:ALA:HB2  | 4        | 0.46          |
| (1,294)  | 1:38:A:ALA:HA   | 1:38:A:ALA:HB3  | 4        | 0.46          |
| (1,294)  | 1:38:A:ALA:HA   | 1:38:A:ALA:HB1  | 5        | 0.46          |
| (1,294)  | 1:38:A:ALA:HA   | 1:38:A:ALA:HB2  | 5        | 0.46          |
| (1,294)  | 1:38:A:ALA:HA   | 1:38:A:ALA:HB3  | 5        | 0.46          |
| (1,242)  | 1:32:A:ILE:HG21 | 1:160:A:TYR:HE1 | 2        | 0.46          |
| (1,242)  | 1:32:A:ILE:HG21 | 1:160:A:TYR:HE2 | 2        | 0.46          |
| (1,242)  | 1:32:A:ILE:HG22 | 1:160:A:TYR:HE1 | 2        | 0.46          |
| (1,242)  | 1:32:A:ILE:HG22 | 1:160:A:TYR:HE2 | 2        | 0.46          |
| (1,242)  | 1:32:A:ILE:HG23 | 1:160:A:TYR:HE1 | 2        | 0.46          |
| (1,242)  | 1:32:A:ILE:HG23 | 1:160:A:TYR:HE2 | 2        | 0.46          |
| (1,1)    | 1:15:A:THR:HB   | 1:15:A:THR:HG21 | 1        | 0.46          |
| (1,1)    | 1:15:A:THR:HB   | 1:15:A:THR:HG22 | 1        | 0.46          |
| (1,1)    | 1:15:A:THR:HB   | 1:15:A:THR:HG23 | 1        | 0.46          |
| (1,1)    | 1:15:A:THR:HB   | 1:15:A:THR:HG21 | 2        | 0.46          |
| (1,1)    | 1:15:A:THR:HB   | 1:15:A:THR:HG22 | 2        | 0.46          |
| (1,1)    | 1:15:A:THR:HB   | 1:15:A:THR:HG23 | 2        | 0.46          |
| (1,1)    | 1:15:A:THR:HB   | 1:15:A:THR:HG21 | 3        | 0.46          |
| (1,1)    | 1:15:A:THR:HB   | 1:15:A:THR:HG22 | 3        | 0.46          |
| (1,1)    | 1:15:A:THR:HB   | 1:15:A:THR:HG23 | 3        | 0.46          |
| (1,1)    | 1:15:A:THR:HB   | 1:15:A:THR:HG21 | 4        | 0.46          |
| (1,1)    | 1:15:A:THR:HB   | 1:15:A:THR:HG22 | 4        | 0.46          |
| (1,1)    | 1:15:A:THR:HB   | 1:15:A:THR:HG23 | 4        | 0.46          |
| (1,1)    | 1:15:A:THR:HB   | 1:15:A:THR:HG21 | 5        | 0.46          |
| (1,1)    | 1:15:A:THR:HB   | 1:15:A:THR:HG22 | 5        | 0.46          |
| (1,1)    | 1:15:A:THR:HB   | 1:15:A:THR:HG23 | 5        | 0.46          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1)    | 1:15:A:THR:HB    | 1:15:A:THR:HG21 | 6        | 0.46          |
| (1,1)    | 1:15:A:THR:HB    | 1:15:A:THR:HG22 | 6        | 0.46          |
| (1,1)    | 1:15:A:THR:HB    | 1:15:A:THR:HG23 | 6        | 0.46          |
| (1,1)    | 1:15:A:THR:HB    | 1:15:A:THR:HG21 | 7        | 0.46          |
| (1,1)    | 1:15:A:THR:HB    | 1:15:A:THR:HG22 | 7        | 0.46          |
| (1,1)    | 1:15:A:THR:HB    | 1:15:A:THR:HG23 | 7        | 0.46          |
| (1,1)    | 1:15:A:THR:HB    | 1:15:A:THR:HG21 | 8        | 0.46          |
| (1,1)    | 1:15:A:THR:HB    | 1:15:A:THR:HG22 | 8        | 0.46          |
| (1,1)    | 1:15:A:THR:HB    | 1:15:A:THR:HG23 | 8        | 0.46          |
| (1,1)    | 1:15:A:THR:HB    | 1:15:A:THR:HG21 | 9        | 0.46          |
| (1,1)    | 1:15:A:THR:HB    | 1:15:A:THR:HG22 | 9        | 0.46          |
| (1,1)    | 1:15:A:THR:HB    | 1:15:A:THR:HG23 | 9        | 0.46          |
| (1,1)    | 1:15:A:THR:HB    | 1:15:A:THR:HG21 | 10       | 0.46          |
| (1,1)    | 1:15:A:THR:HB    | 1:15:A:THR:HG22 | 10       | 0.46          |
| (1,1)    | 1:15:A:THR:HB    | 1:15:A:THR:HG23 | 10       | 0.46          |
| (2,733)  | 1:157:A:LYS:HE2  | 1:159:A:PHE:HD1 | 2        | 0.45          |
| (2,733)  | 1:157:A:LYS:HE2  | 1:159:A:PHE:HD2 | 2        | 0.45          |
| (2,733)  | 1:157:A:LYS:HE3  | 1:159:A:PHE:HD1 | 2        | 0.45          |
| (2,733)  | 1:157:A:LYS:HE3  | 1:159:A:PHE:HD2 | 2        | 0.45          |
| (2,490)  | 1:81:A:ILE:HD11  | 1:101:A:VAL:H   | 8        | 0.45          |
| (2,490)  | 1:81:A:ILE:HD12  | 1:101:A:VAL:H   | 8        | 0.45          |
| (2,490)  | 1:81:A:ILE:HD13  | 1:101:A:VAL:H   | 8        | 0.45          |
| (2,4)    | 1:15:A:THR:HG21  | 1:16:A:ALA:H    | 1        | 0.45          |
| (2,4)    | 1:15:A:THR:HG22  | 1:16:A:ALA:H    | 1        | 0.45          |
| (2,4)    | 1:15:A:THR:HG23  | 1:16:A:ALA:H    | 1        | 0.45          |
| (1,2449) | 1:179:A:VAL:HG21 | 1:179:A:VAL:H   | 3        | 0.45          |
| (1,2449) | 1:179:A:VAL:HG22 | 1:179:A:VAL:H   | 3        | 0.45          |
| (1,2449) | 1:179:A:VAL:HG23 | 1:179:A:VAL:H   | 3        | 0.45          |
| (1,2449) | 1:179:A:VAL:HG21 | 1:179:A:VAL:H   | 8        | 0.45          |
| (1,2449) | 1:179:A:VAL:HG22 | 1:179:A:VAL:H   | 8        | 0.45          |
| (1,2449) | 1:179:A:VAL:HG23 | 1:179:A:VAL:H   | 8        | 0.45          |
| (1,2246) | 1:162:A:ALA:HB1  | 1:168:A:PHE:HZ  | 3        | 0.45          |
| (1,2246) | 1:162:A:ALA:HB2  | 1:168:A:PHE:HZ  | 3        | 0.45          |
| (1,2246) | 1:162:A:ALA:HB3  | 1:168:A:PHE:HZ  | 3        | 0.45          |
| (1,2246) | 1:162:A:ALA:HB1  | 1:168:A:PHE:HZ  | 10       | 0.45          |
| (1,2246) | 1:162:A:ALA:HB2  | 1:168:A:PHE:HZ  | 10       | 0.45          |
| (1,2246) | 1:162:A:ALA:HB3  | 1:168:A:PHE:HZ  | 10       | 0.45          |
| (1,2083) | 1:151:A:VAL:HG21 | 1:152:A:ALA:H   | 1        | 0.45          |
| (1,2083) | 1:151:A:VAL:HG22 | 1:152:A:ALA:H   | 1        | 0.45          |
| (1,2083) | 1:151:A:VAL:HG23 | 1:152:A:ALA:H   | 1        | 0.45          |
| (1,2083) | 1:151:A:VAL:HG21 | 1:152:A:ALA:H   | 4        | 0.45          |
| (1,2083) | 1:151:A:VAL:HG22 | 1:152:A:ALA:H   | 4        | 0.45          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2083) | 1:151:A:VAL:HG23 | 1:152:A:ALA:H    | 4        | 0.45          |
| (1,2083) | 1:151:A:VAL:HG21 | 1:152:A:ALA:H    | 9        | 0.45          |
| (1,2083) | 1:151:A:VAL:HG22 | 1:152:A:ALA:H    | 9        | 0.45          |
| (1,2083) | 1:151:A:VAL:HG23 | 1:152:A:ALA:H    | 9        | 0.45          |
| (1,2038) | 1:144:A:VAL:HG21 | 1:144:A:VAL:H    | 10       | 0.45          |
| (1,2038) | 1:144:A:VAL:HG22 | 1:144:A:VAL:H    | 10       | 0.45          |
| (1,2038) | 1:144:A:VAL:HG23 | 1:144:A:VAL:H    | 10       | 0.45          |
| (1,2015) | 1:142:A:ILE:HG21 | 1:144:A:VAL:H    | 3        | 0.45          |
| (1,2015) | 1:142:A:ILE:HG22 | 1:144:A:VAL:H    | 3        | 0.45          |
| (1,2015) | 1:142:A:ILE:HG23 | 1:144:A:VAL:H    | 3        | 0.45          |
| (1,1844) | 1:132:A:SER:HB2  | 1:142:A:ILE:HG21 | 1        | 0.45          |
| (1,1844) | 1:132:A:SER:HB2  | 1:142:A:ILE:HG22 | 1        | 0.45          |
| (1,1844) | 1:132:A:SER:HB2  | 1:142:A:ILE:HG23 | 1        | 0.45          |
| (1,1840) | 1:132:A:SER:HB3  | 1:142:A:ILE:HG21 | 4        | 0.45          |
| (1,1840) | 1:132:A:SER:HB3  | 1:142:A:ILE:HG22 | 4        | 0.45          |
| (1,1840) | 1:132:A:SER:HB3  | 1:142:A:ILE:HG23 | 4        | 0.45          |
| (1,1840) | 1:132:A:SER:HB3  | 1:142:A:ILE:HG21 | 10       | 0.45          |
| (1,1840) | 1:132:A:SER:HB3  | 1:142:A:ILE:HG22 | 10       | 0.45          |
| (1,1840) | 1:132:A:SER:HB3  | 1:142:A:ILE:HG23 | 10       | 0.45          |
| (1,1766) | 1:120:A:VAL:HG11 | 1:120:A:VAL:H    | 4        | 0.45          |
| (1,1766) | 1:120:A:VAL:HG12 | 1:120:A:VAL:H    | 4        | 0.45          |
| (1,1766) | 1:120:A:VAL:HG13 | 1:120:A:VAL:H    | 4        | 0.45          |
| (1,1647) | 1:112:A:VAL:HG11 | 1:112:A:VAL:H    | 8        | 0.45          |
| (1,1647) | 1:112:A:VAL:HG12 | 1:112:A:VAL:H    | 8        | 0.45          |
| (1,1647) | 1:112:A:VAL:HG13 | 1:112:A:VAL:H    | 8        | 0.45          |
| (1,1630) | 1:110:A:VAL:HG21 | 1:110:A:VAL:H    | 6        | 0.45          |
| (1,1630) | 1:110:A:VAL:HG22 | 1:110:A:VAL:H    | 6        | 0.45          |
| (1,1630) | 1:110:A:VAL:HG23 | 1:110:A:VAL:H    | 6        | 0.45          |
| (1,1338) | 1:85:A:TYR:HD1   | 1:86:A:GLU:H     | 5        | 0.45          |
| (1,1338) | 1:85:A:TYR:HD2   | 1:86:A:GLU:H     | 5        | 0.45          |
| (1,1270) | 1:82:A:THR:HG21  | 1:83:A:SER:HA    | 8        | 0.45          |
| (1,1270) | 1:82:A:THR:HG22  | 1:83:A:SER:HA    | 8        | 0.45          |
| (1,1270) | 1:82:A:THR:HG23  | 1:83:A:SER:HA    | 8        | 0.45          |
| (1,1236) | 1:81:A:ILE:HG21  | 1:154:A:LEU:HB3  | 2        | 0.45          |
| (1,1236) | 1:81:A:ILE:HG22  | 1:154:A:LEU:HB3  | 2        | 0.45          |
| (1,1236) | 1:81:A:ILE:HG23  | 1:154:A:LEU:HB3  | 2        | 0.45          |
| (1,1228) | 1:81:A:ILE:HG21  | 1:82:A:THR:HA    | 4        | 0.45          |
| (1,1228) | 1:81:A:ILE:HG22  | 1:82:A:THR:HA    | 4        | 0.45          |
| (1,1228) | 1:81:A:ILE:HG23  | 1:82:A:THR:HA    | 4        | 0.45          |
| (1,1228) | 1:81:A:ILE:HG21  | 1:82:A:THR:HA    | 5        | 0.45          |
| (1,1228) | 1:81:A:ILE:HG22  | 1:82:A:THR:HA    | 5        | 0.45          |
| (1,1228) | 1:81:A:ILE:HG23  | 1:82:A:THR:HA    | 5        | 0.45          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1228) | 1:81:A:ILE:HG21 | 1:82:A:THR:HA    | 7        | 0.45          |
| (1,1228) | 1:81:A:ILE:HG22 | 1:82:A:THR:HA    | 7        | 0.45          |
| (1,1228) | 1:81:A:ILE:HG23 | 1:82:A:THR:HA    | 7        | 0.45          |
| (1,947)  | 1:71:A:LYS:HG3  | 1:71:A:LYS:H     | 5        | 0.45          |
| (1,852)  | 1:66:A:ASN:HD22 | 1:70:A:LEU:HD21  | 1        | 0.45          |
| (1,852)  | 1:66:A:ASN:HD22 | 1:70:A:LEU:HD22  | 1        | 0.45          |
| (1,852)  | 1:66:A:ASN:HD22 | 1:70:A:LEU:HD23  | 1        | 0.45          |
| (1,840)  | 1:66:A:ASN:HB2  | 1:174:A:ILE:HD11 | 1        | 0.45          |
| (1,840)  | 1:66:A:ASN:HB2  | 1:174:A:ILE:HD12 | 1        | 0.45          |
| (1,840)  | 1:66:A:ASN:HB2  | 1:174:A:ILE:HD13 | 1        | 0.45          |
| (1,840)  | 1:66:A:ASN:HB2  | 1:174:A:ILE:HD11 | 2        | 0.45          |
| (1,840)  | 1:66:A:ASN:HB2  | 1:174:A:ILE:HD12 | 2        | 0.45          |
| (1,840)  | 1:66:A:ASN:HB2  | 1:174:A:ILE:HD13 | 2        | 0.45          |
| (1,840)  | 1:66:A:ASN:HB2  | 1:174:A:ILE:HD11 | 3        | 0.45          |
| (1,840)  | 1:66:A:ASN:HB2  | 1:174:A:ILE:HD12 | 3        | 0.45          |
| (1,840)  | 1:66:A:ASN:HB2  | 1:174:A:ILE:HD13 | 3        | 0.45          |
| (1,840)  | 1:66:A:ASN:HB2  | 1:174:A:ILE:HD11 | 4        | 0.45          |
| (1,840)  | 1:66:A:ASN:HB2  | 1:174:A:ILE:HD12 | 4        | 0.45          |
| (1,840)  | 1:66:A:ASN:HB2  | 1:174:A:ILE:HD13 | 4        | 0.45          |
| (1,840)  | 1:66:A:ASN:HB2  | 1:174:A:ILE:HD11 | 5        | 0.45          |
| (1,840)  | 1:66:A:ASN:HB2  | 1:174:A:ILE:HD12 | 5        | 0.45          |
| (1,840)  | 1:66:A:ASN:HB2  | 1:174:A:ILE:HD13 | 5        | 0.45          |
| (1,840)  | 1:66:A:ASN:HB2  | 1:174:A:ILE:HD11 | 6        | 0.45          |
| (1,840)  | 1:66:A:ASN:HB2  | 1:174:A:ILE:HD12 | 6        | 0.45          |
| (1,840)  | 1:66:A:ASN:HB2  | 1:174:A:ILE:HD13 | 6        | 0.45          |
| (1,840)  | 1:66:A:ASN:HB2  | 1:174:A:ILE:HD11 | 7        | 0.45          |
| (1,840)  | 1:66:A:ASN:HB2  | 1:174:A:ILE:HD12 | 7        | 0.45          |
| (1,840)  | 1:66:A:ASN:HB2  | 1:174:A:ILE:HD13 | 7        | 0.45          |
| (1,840)  | 1:66:A:ASN:HB2  | 1:174:A:ILE:HD11 | 8        | 0.45          |
| (1,840)  | 1:66:A:ASN:HB2  | 1:174:A:ILE:HD12 | 8        | 0.45          |
| (1,840)  | 1:66:A:ASN:HB2  | 1:174:A:ILE:HD13 | 8        | 0.45          |
| (1,840)  | 1:66:A:ASN:HB2  | 1:174:A:ILE:HD11 | 10       | 0.45          |
| (1,840)  | 1:66:A:ASN:HB2  | 1:174:A:ILE:HD12 | 10       | 0.45          |
| (1,840)  | 1:66:A:ASN:HB2  | 1:174:A:ILE:HD13 | 10       | 0.45          |
| (1,679)  | 1:60:A:LEU:HD11 | 1:177:A:PHE:HD1  | 3        | 0.45          |
| (1,679)  | 1:60:A:LEU:HD11 | 1:177:A:PHE:HD2  | 3        | 0.45          |
| (1,679)  | 1:60:A:LEU:HD12 | 1:177:A:PHE:HD1  | 3        | 0.45          |
| (1,679)  | 1:60:A:LEU:HD12 | 1:177:A:PHE:HD2  | 3        | 0.45          |
| (1,679)  | 1:60:A:LEU:HD13 | 1:177:A:PHE:HD1  | 3        | 0.45          |
| (1,679)  | 1:60:A:LEU:HD13 | 1:177:A:PHE:HD2  | 3        | 0.45          |
| (1,581)  | 1:51:A:ILE:HG21 | 1:53:A:ASP:H     | 4        | 0.45          |
| (1,581)  | 1:51:A:ILE:HG22 | 1:53:A:ASP:H     | 4        | 0.45          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,581)  | 1:51:A:ILE:HG23  | 1:53:A:ASP:H     | 4        | 0.45          |
| (1,580)  | 1:51:A:ILE:HG21  | 1:53:A:ASP:H     | 4        | 0.45          |
| (1,580)  | 1:51:A:ILE:HG22  | 1:53:A:ASP:H     | 4        | 0.45          |
| (1,580)  | 1:51:A:ILE:HG23  | 1:53:A:ASP:H     | 4        | 0.45          |
| (1,495)  | 1:48:A:ILE:HG21  | 1:50:A:TRP:HE1   | 7        | 0.45          |
| (1,495)  | 1:48:A:ILE:HG22  | 1:50:A:TRP:HE1   | 7        | 0.45          |
| (1,495)  | 1:48:A:ILE:HG23  | 1:50:A:TRP:HE1   | 7        | 0.45          |
| (1,209)  | 1:32:A:ILE:HA    | 1:32:A:ILE:HG21  | 5        | 0.45          |
| (1,209)  | 1:32:A:ILE:HA    | 1:32:A:ILE:HG22  | 5        | 0.45          |
| (1,209)  | 1:32:A:ILE:HA    | 1:32:A:ILE:HG23  | 5        | 0.45          |
| (1,162)  | 1:29:A:LEU:HD11  | 1:29:A:LEU:HD21  | 5        | 0.45          |
| (1,162)  | 1:29:A:LEU:HD11  | 1:29:A:LEU:HD22  | 5        | 0.45          |
| (1,162)  | 1:29:A:LEU:HD11  | 1:29:A:LEU:HD23  | 5        | 0.45          |
| (1,162)  | 1:29:A:LEU:HD12  | 1:29:A:LEU:HD21  | 5        | 0.45          |
| (1,162)  | 1:29:A:LEU:HD12  | 1:29:A:LEU:HD22  | 5        | 0.45          |
| (1,162)  | 1:29:A:LEU:HD12  | 1:29:A:LEU:HD23  | 5        | 0.45          |
| (1,162)  | 1:29:A:LEU:HD13  | 1:29:A:LEU:HD21  | 5        | 0.45          |
| (1,162)  | 1:29:A:LEU:HD13  | 1:29:A:LEU:HD22  | 5        | 0.45          |
| (1,162)  | 1:29:A:LEU:HD13  | 1:29:A:LEU:HD23  | 5        | 0.45          |
| (1,139)  | 1:28:A:HIS:HD2   | 1:46:A:TYR:HE1   | 4        | 0.45          |
| (1,139)  | 1:28:A:HIS:HD2   | 1:46:A:TYR:HE2   | 4        | 0.45          |
| (2,768)  | 1:173:A:VAL:HB   | 1:175:A:PHE:HE1  | 4        | 0.44          |
| (2,768)  | 1:173:A:VAL:HB   | 1:175:A:PHE:HE2  | 4        | 0.44          |
| (2,689)  | 1:131:A:THR:HA   | 1:145:A:TYR:HD1  | 1        | 0.44          |
| (2,689)  | 1:131:A:THR:HA   | 1:145:A:TYR:HD2  | 1        | 0.44          |
| (2,689)  | 1:131:A:THR:HA   | 1:145:A:TYR:HD1  | 4        | 0.44          |
| (2,689)  | 1:131:A:THR:HA   | 1:145:A:TYR:HD2  | 4        | 0.44          |
| (2,607)  | 1:115:A:LYS:H    | 1:116:A:GLU:HG2  | 1        | 0.44          |
| (2,607)  | 1:115:A:LYS:H    | 1:116:A:GLU:HG3  | 1        | 0.44          |
| (2,607)  | 1:115:A:LYS:H    | 1:116:A:GLU:HG2  | 8        | 0.44          |
| (2,607)  | 1:115:A:LYS:H    | 1:116:A:GLU:HG3  | 8        | 0.44          |
| (2,592)  | 1:114:A:ASP:HB3  | 1:116:A:GLU:HG2  | 2        | 0.44          |
| (2,592)  | 1:114:A:ASP:HB3  | 1:116:A:GLU:HG3  | 2        | 0.44          |
| (2,454)  | 1:78:A:GLN:HE21  | 1:101:A:VAL:HG11 | 3        | 0.44          |
| (2,454)  | 1:78:A:GLN:HE21  | 1:101:A:VAL:HG12 | 3        | 0.44          |
| (2,454)  | 1:78:A:GLN:HE21  | 1:101:A:VAL:HG13 | 3        | 0.44          |
| (2,295)  | 1:52:A:LYS:HE2   | 1:54:A:GLN:HE22  | 4        | 0.44          |
| (2,295)  | 1:52:A:LYS:HE3   | 1:54:A:GLN:HE22  | 4        | 0.44          |
| (1,2449) | 1:179:A:VAL:HG21 | 1:179:A:VAL:H    | 4        | 0.44          |
| (1,2449) | 1:179:A:VAL:HG22 | 1:179:A:VAL:H    | 4        | 0.44          |
| (1,2449) | 1:179:A:VAL:HG23 | 1:179:A:VAL:H    | 4        | 0.44          |
| (1,2449) | 1:179:A:VAL:HG21 | 1:179:A:VAL:H    | 5        | 0.44          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2449) | 1:179:A:VAL:HG22 | 1:179:A:VAL:H    | 5        | 0.44          |
| (1,2449) | 1:179:A:VAL:HG23 | 1:179:A:VAL:H    | 5        | 0.44          |
| (1,2449) | 1:179:A:VAL:HG21 | 1:179:A:VAL:H    | 6        | 0.44          |
| (1,2449) | 1:179:A:VAL:HG22 | 1:179:A:VAL:H    | 6        | 0.44          |
| (1,2449) | 1:179:A:VAL:HG23 | 1:179:A:VAL:H    | 6        | 0.44          |
| (1,2246) | 1:162:A:ALA:HB1  | 1:168:A:PHE:HZ   | 5        | 0.44          |
| (1,2246) | 1:162:A:ALA:HB2  | 1:168:A:PHE:HZ   | 5        | 0.44          |
| (1,2246) | 1:162:A:ALA:HB3  | 1:168:A:PHE:HZ   | 5        | 0.44          |
| (1,2106) | 1:153:A:ILE:HG21 | 1:155:A:ASN:HD21 | 3        | 0.44          |
| (1,2106) | 1:153:A:ILE:HG21 | 1:155:A:ASN:HD22 | 3        | 0.44          |
| (1,2106) | 1:153:A:ILE:HG22 | 1:155:A:ASN:HD21 | 3        | 0.44          |
| (1,2106) | 1:153:A:ILE:HG22 | 1:155:A:ASN:HD22 | 3        | 0.44          |
| (1,2106) | 1:153:A:ILE:HG23 | 1:155:A:ASN:HD21 | 3        | 0.44          |
| (1,2106) | 1:153:A:ILE:HG23 | 1:155:A:ASN:HD22 | 3        | 0.44          |
| (1,2083) | 1:151:A:VAL:HG21 | 1:152:A:ALA:H    | 2        | 0.44          |
| (1,2083) | 1:151:A:VAL:HG22 | 1:152:A:ALA:H    | 2        | 0.44          |
| (1,2083) | 1:151:A:VAL:HG23 | 1:152:A:ALA:H    | 2        | 0.44          |
| (1,2083) | 1:151:A:VAL:HG21 | 1:152:A:ALA:H    | 3        | 0.44          |
| (1,2083) | 1:151:A:VAL:HG22 | 1:152:A:ALA:H    | 3        | 0.44          |
| (1,2083) | 1:151:A:VAL:HG23 | 1:152:A:ALA:H    | 3        | 0.44          |
| (1,2083) | 1:151:A:VAL:HG21 | 1:152:A:ALA:H    | 8        | 0.44          |
| (1,2083) | 1:151:A:VAL:HG22 | 1:152:A:ALA:H    | 8        | 0.44          |
| (1,2083) | 1:151:A:VAL:HG23 | 1:152:A:ALA:H    | 8        | 0.44          |
| (1,2038) | 1:144:A:VAL:HG21 | 1:144:A:VAL:H    | 7        | 0.44          |
| (1,2038) | 1:144:A:VAL:HG22 | 1:144:A:VAL:H    | 7        | 0.44          |
| (1,2038) | 1:144:A:VAL:HG23 | 1:144:A:VAL:H    | 7        | 0.44          |
| (1,1840) | 1:132:A:SER:HB3  | 1:142:A:ILE:HG21 | 8        | 0.44          |
| (1,1840) | 1:132:A:SER:HB3  | 1:142:A:ILE:HG22 | 8        | 0.44          |
| (1,1840) | 1:132:A:SER:HB3  | 1:142:A:ILE:HG23 | 8        | 0.44          |
| (1,1766) | 1:120:A:VAL:HG11 | 1:120:A:VAL:H    | 7        | 0.44          |
| (1,1766) | 1:120:A:VAL:HG12 | 1:120:A:VAL:H    | 7        | 0.44          |
| (1,1766) | 1:120:A:VAL:HG13 | 1:120:A:VAL:H    | 7        | 0.44          |
| (1,1766) | 1:120:A:VAL:HG11 | 1:120:A:VAL:H    | 10       | 0.44          |
| (1,1766) | 1:120:A:VAL:HG12 | 1:120:A:VAL:H    | 10       | 0.44          |
| (1,1766) | 1:120:A:VAL:HG13 | 1:120:A:VAL:H    | 10       | 0.44          |
| (1,1546) | 1:102:A:ILE:HG21 | 1:108:A:SER:HA   | 8        | 0.44          |
| (1,1546) | 1:102:A:ILE:HG22 | 1:108:A:SER:HA   | 8        | 0.44          |
| (1,1546) | 1:102:A:ILE:HG23 | 1:108:A:SER:HA   | 8        | 0.44          |
| (1,1343) | 1:85:A:TYR:HE1   | 1:152:A:ALA:HA   | 4        | 0.44          |
| (1,1343) | 1:85:A:TYR:HE2   | 1:152:A:ALA:HA   | 4        | 0.44          |
| (1,1228) | 1:81:A:ILE:HG21  | 1:82:A:THR:HA    | 8        | 0.44          |
| (1,1228) | 1:81:A:ILE:HG22  | 1:82:A:THR:HA    | 8        | 0.44          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1228) | 1:81:A:ILE:HG23 | 1:82:A:THR:HA   | 8        | 0.44          |
| (1,1228) | 1:81:A:ILE:HG21 | 1:82:A:THR:HA   | 10       | 0.44          |
| (1,1228) | 1:81:A:ILE:HG22 | 1:82:A:THR:HA   | 10       | 0.44          |
| (1,1228) | 1:81:A:ILE:HG23 | 1:82:A:THR:HA   | 10       | 0.44          |
| (1,679)  | 1:60:A:LEU:HD11 | 1:177:A:PHE:HD1 | 5        | 0.44          |
| (1,679)  | 1:60:A:LEU:HD11 | 1:177:A:PHE:HD2 | 5        | 0.44          |
| (1,679)  | 1:60:A:LEU:HD12 | 1:177:A:PHE:HD1 | 5        | 0.44          |
| (1,679)  | 1:60:A:LEU:HD12 | 1:177:A:PHE:HD2 | 5        | 0.44          |
| (1,679)  | 1:60:A:LEU:HD13 | 1:177:A:PHE:HD1 | 5        | 0.44          |
| (1,679)  | 1:60:A:LEU:HD13 | 1:177:A:PHE:HD2 | 5        | 0.44          |
| (1,582)  | 1:51:A:ILE:HG21 | 1:55:A:VAL:H    | 3        | 0.44          |
| (1,582)  | 1:51:A:ILE:HG22 | 1:55:A:VAL:H    | 3        | 0.44          |
| (1,582)  | 1:51:A:ILE:HG23 | 1:55:A:VAL:H    | 3        | 0.44          |
| (1,353)  | 1:42:A:ASP:HB2  | 1:158:A:ALA:HB1 | 1        | 0.44          |
| (1,353)  | 1:42:A:ASP:HB2  | 1:158:A:ALA:HB2 | 1        | 0.44          |
| (1,353)  | 1:42:A:ASP:HB2  | 1:158:A:ALA:HB3 | 1        | 0.44          |
| (1,353)  | 1:42:A:ASP:HB3  | 1:158:A:ALA:HB1 | 1        | 0.44          |
| (1,353)  | 1:42:A:ASP:HB3  | 1:158:A:ALA:HB2 | 1        | 0.44          |
| (1,353)  | 1:42:A:ASP:HB3  | 1:158:A:ALA:HB3 | 1        | 0.44          |
| (1,242)  | 1:32:A:ILE:HG21 | 1:160:A:TYR:HE1 | 5        | 0.44          |
| (1,242)  | 1:32:A:ILE:HG21 | 1:160:A:TYR:HE2 | 5        | 0.44          |
| (1,242)  | 1:32:A:ILE:HG22 | 1:160:A:TYR:HE1 | 5        | 0.44          |
| (1,242)  | 1:32:A:ILE:HG22 | 1:160:A:TYR:HE2 | 5        | 0.44          |
| (1,242)  | 1:32:A:ILE:HG23 | 1:160:A:TYR:HE1 | 5        | 0.44          |
| (1,242)  | 1:32:A:ILE:HG23 | 1:160:A:TYR:HE2 | 5        | 0.44          |
| (1,242)  | 1:32:A:ILE:HG21 | 1:160:A:TYR:HE1 | 9        | 0.44          |
| (1,242)  | 1:32:A:ILE:HG21 | 1:160:A:TYR:HE2 | 9        | 0.44          |
| (1,242)  | 1:32:A:ILE:HG22 | 1:160:A:TYR:HE1 | 9        | 0.44          |
| (1,242)  | 1:32:A:ILE:HG22 | 1:160:A:TYR:HE2 | 9        | 0.44          |
| (1,242)  | 1:32:A:ILE:HG23 | 1:160:A:TYR:HE1 | 9        | 0.44          |
| (1,242)  | 1:32:A:ILE:HG23 | 1:160:A:TYR:HE2 | 9        | 0.44          |
| (1,162)  | 1:29:A:LEU:HD11 | 1:29:A:LEU:HD21 | 1        | 0.44          |
| (1,162)  | 1:29:A:LEU:HD11 | 1:29:A:LEU:HD22 | 1        | 0.44          |
| (1,162)  | 1:29:A:LEU:HD11 | 1:29:A:LEU:HD23 | 1        | 0.44          |
| (1,162)  | 1:29:A:LEU:HD12 | 1:29:A:LEU:HD21 | 1        | 0.44          |
| (1,162)  | 1:29:A:LEU:HD12 | 1:29:A:LEU:HD22 | 1        | 0.44          |
| (1,162)  | 1:29:A:LEU:HD12 | 1:29:A:LEU:HD23 | 1        | 0.44          |
| (1,162)  | 1:29:A:LEU:HD13 | 1:29:A:LEU:HD21 | 1        | 0.44          |
| (1,162)  | 1:29:A:LEU:HD13 | 1:29:A:LEU:HD22 | 1        | 0.44          |
| (1,162)  | 1:29:A:LEU:HD13 | 1:29:A:LEU:HD23 | 1        | 0.44          |
| (1,162)  | 1:29:A:LEU:HD11 | 1:29:A:LEU:HD21 | 2        | 0.44          |
| (1,162)  | 1:29:A:LEU:HD11 | 1:29:A:LEU:HD22 | 2        | 0.44          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,162)  | 1:29:A:LEU:HD11  | 1:29:A:LEU:HD23  | 2        | 0.44          |
| (1,162)  | 1:29:A:LEU:HD12  | 1:29:A:LEU:HD21  | 2        | 0.44          |
| (1,162)  | 1:29:A:LEU:HD12  | 1:29:A:LEU:HD22  | 2        | 0.44          |
| (1,162)  | 1:29:A:LEU:HD12  | 1:29:A:LEU:HD23  | 2        | 0.44          |
| (1,162)  | 1:29:A:LEU:HD13  | 1:29:A:LEU:HD21  | 2        | 0.44          |
| (1,162)  | 1:29:A:LEU:HD13  | 1:29:A:LEU:HD22  | 2        | 0.44          |
| (1,162)  | 1:29:A:LEU:HD13  | 1:29:A:LEU:HD23  | 2        | 0.44          |
| (1,162)  | 1:29:A:LEU:HD11  | 1:29:A:LEU:HD21  | 7        | 0.44          |
| (1,162)  | 1:29:A:LEU:HD11  | 1:29:A:LEU:HD22  | 7        | 0.44          |
| (1,162)  | 1:29:A:LEU:HD11  | 1:29:A:LEU:HD23  | 7        | 0.44          |
| (1,162)  | 1:29:A:LEU:HD12  | 1:29:A:LEU:HD21  | 7        | 0.44          |
| (1,162)  | 1:29:A:LEU:HD12  | 1:29:A:LEU:HD22  | 7        | 0.44          |
| (1,162)  | 1:29:A:LEU:HD12  | 1:29:A:LEU:HD23  | 7        | 0.44          |
| (1,162)  | 1:29:A:LEU:HD13  | 1:29:A:LEU:HD21  | 7        | 0.44          |
| (1,162)  | 1:29:A:LEU:HD13  | 1:29:A:LEU:HD22  | 7        | 0.44          |
| (1,162)  | 1:29:A:LEU:HD13  | 1:29:A:LEU:HD23  | 7        | 0.44          |
| (1,86)   | 1:25:A:VAL:HG21  | 1:49:A:VAL:HG21  | 10       | 0.44          |
| (1,86)   | 1:25:A:VAL:HG21  | 1:49:A:VAL:HG22  | 10       | 0.44          |
| (1,86)   | 1:25:A:VAL:HG21  | 1:49:A:VAL:HG23  | 10       | 0.44          |
| (1,86)   | 1:25:A:VAL:HG22  | 1:49:A:VAL:HG21  | 10       | 0.44          |
| (1,86)   | 1:25:A:VAL:HG22  | 1:49:A:VAL:HG22  | 10       | 0.44          |
| (1,86)   | 1:25:A:VAL:HG22  | 1:49:A:VAL:HG23  | 10       | 0.44          |
| (1,86)   | 1:25:A:VAL:HG23  | 1:49:A:VAL:HG21  | 10       | 0.44          |
| (1,86)   | 1:25:A:VAL:HG23  | 1:49:A:VAL:HG22  | 10       | 0.44          |
| (1,86)   | 1:25:A:VAL:HG23  | 1:49:A:VAL:HG23  | 10       | 0.44          |
| (1,6)    | 1:18:A:ALA:HB1   | 1:19:A:VAL:H     | 7        | 0.44          |
| (1,6)    | 1:18:A:ALA:HB2   | 1:19:A:VAL:H     | 7        | 0.44          |
| (1,6)    | 1:18:A:ALA:HB3   | 1:19:A:VAL:H     | 7        | 0.44          |
| (2,756)  | 1:167:A:LEU:H    | 1:167:A:LEU:HD21 | 7        | 0.43          |
| (2,756)  | 1:167:A:LEU:H    | 1:167:A:LEU:HD22 | 7        | 0.43          |
| (2,756)  | 1:167:A:LEU:H    | 1:167:A:LEU:HD23 | 7        | 0.43          |
| (2,754)  | 1:167:A:LEU:HD21 | 1:167:A:LEU:H    | 7        | 0.43          |
| (2,754)  | 1:167:A:LEU:HD22 | 1:167:A:LEU:H    | 7        | 0.43          |
| (2,754)  | 1:167:A:LEU:HD23 | 1:167:A:LEU:H    | 7        | 0.43          |
| (2,425)  | 1:74:A:PHE:HZ    | 1:160:A:TYR:HE1  | 9        | 0.43          |
| (2,425)  | 1:74:A:PHE:HZ    | 1:160:A:TYR:HE2  | 9        | 0.43          |
| (1,2320) | 1:171:A:LEU:HD11 | 1:171:A:LEU:HD21 | 4        | 0.43          |
| (1,2320) | 1:171:A:LEU:HD11 | 1:171:A:LEU:HD22 | 4        | 0.43          |
| (1,2320) | 1:171:A:LEU:HD11 | 1:171:A:LEU:HD23 | 4        | 0.43          |
| (1,2320) | 1:171:A:LEU:HD12 | 1:171:A:LEU:HD21 | 4        | 0.43          |
| (1,2320) | 1:171:A:LEU:HD12 | 1:171:A:LEU:HD22 | 4        | 0.43          |
| (1,2320) | 1:171:A:LEU:HD12 | 1:171:A:LEU:HD23 | 4        | 0.43          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2320) | 1:171:A:LEU:HD13 | 1:171:A:LEU:HD21 | 4        | 0.43          |
| (1,2320) | 1:171:A:LEU:HD13 | 1:171:A:LEU:HD22 | 4        | 0.43          |
| (1,2320) | 1:171:A:LEU:HD13 | 1:171:A:LEU:HD23 | 4        | 0.43          |
| (1,2320) | 1:171:A:LEU:HD11 | 1:171:A:LEU:HD21 | 5        | 0.43          |
| (1,2320) | 1:171:A:LEU:HD11 | 1:171:A:LEU:HD22 | 5        | 0.43          |
| (1,2320) | 1:171:A:LEU:HD11 | 1:171:A:LEU:HD23 | 5        | 0.43          |
| (1,2320) | 1:171:A:LEU:HD12 | 1:171:A:LEU:HD21 | 5        | 0.43          |
| (1,2320) | 1:171:A:LEU:HD12 | 1:171:A:LEU:HD22 | 5        | 0.43          |
| (1,2320) | 1:171:A:LEU:HD12 | 1:171:A:LEU:HD23 | 5        | 0.43          |
| (1,2320) | 1:171:A:LEU:HD13 | 1:171:A:LEU:HD21 | 5        | 0.43          |
| (1,2320) | 1:171:A:LEU:HD13 | 1:171:A:LEU:HD22 | 5        | 0.43          |
| (1,2320) | 1:171:A:LEU:HD13 | 1:171:A:LEU:HD23 | 5        | 0.43          |
| (1,1954) | 1:136:A:PRO:HG2  | 1:155:A:ASN:HD21 | 3        | 0.43          |
| (1,1954) | 1:136:A:PRO:HG2  | 1:155:A:ASN:HD22 | 3        | 0.43          |
| (1,1954) | 1:136:A:PRO:HG2  | 1:155:A:ASN:HD21 | 8        | 0.43          |
| (1,1954) | 1:136:A:PRO:HG2  | 1:155:A:ASN:HD22 | 8        | 0.43          |
| (1,1630) | 1:110:A:VAL:HG21 | 1:110:A:VAL:H    | 1        | 0.43          |
| (1,1630) | 1:110:A:VAL:HG22 | 1:110:A:VAL:H    | 1        | 0.43          |
| (1,1630) | 1:110:A:VAL:HG23 | 1:110:A:VAL:H    | 1        | 0.43          |
| (1,1510) | 1:98:A:THR:HG21  | 1:100:A:ALA:H    | 5        | 0.43          |
| (1,1510) | 1:98:A:THR:HG22  | 1:100:A:ALA:H    | 5        | 0.43          |
| (1,1510) | 1:98:A:THR:HG23  | 1:100:A:ALA:H    | 5        | 0.43          |
| (1,1342) | 1:85:A:TYR:HE1   | 1:143:A:ILE:HG21 | 6        | 0.43          |
| (1,1342) | 1:85:A:TYR:HE1   | 1:143:A:ILE:HG22 | 6        | 0.43          |
| (1,1342) | 1:85:A:TYR:HE1   | 1:143:A:ILE:HG23 | 6        | 0.43          |
| (1,1342) | 1:85:A:TYR:HE2   | 1:143:A:ILE:HG21 | 6        | 0.43          |
| (1,1342) | 1:85:A:TYR:HE2   | 1:143:A:ILE:HG22 | 6        | 0.43          |
| (1,1342) | 1:85:A:TYR:HE2   | 1:143:A:ILE:HG23 | 6        | 0.43          |
| (1,1337) | 1:85:A:TYR:HD1   | 1:85:A:TYR:H     | 2        | 0.43          |
| (1,1337) | 1:85:A:TYR:HD2   | 1:85:A:TYR:H     | 2        | 0.43          |
| (1,1228) | 1:81:A:ILE:HG21  | 1:82:A:THR:HA    | 9        | 0.43          |
| (1,1228) | 1:81:A:ILE:HG22  | 1:82:A:THR:HA    | 9        | 0.43          |
| (1,1228) | 1:81:A:ILE:HG23  | 1:82:A:THR:HA    | 9        | 0.43          |
| (1,1169) | 1:79:A:ILE:HG21  | 1:79:A:ILE:HD11  | 9        | 0.43          |
| (1,1169) | 1:79:A:ILE:HG21  | 1:79:A:ILE:HD12  | 9        | 0.43          |
| (1,1169) | 1:79:A:ILE:HG21  | 1:79:A:ILE:HD13  | 9        | 0.43          |
| (1,1169) | 1:79:A:ILE:HG22  | 1:79:A:ILE:HD11  | 9        | 0.43          |
| (1,1169) | 1:79:A:ILE:HG22  | 1:79:A:ILE:HD12  | 9        | 0.43          |
| (1,1169) | 1:79:A:ILE:HG22  | 1:79:A:ILE:HD13  | 9        | 0.43          |
| (1,1169) | 1:79:A:ILE:HG23  | 1:79:A:ILE:HD11  | 9        | 0.43          |
| (1,1169) | 1:79:A:ILE:HG23  | 1:79:A:ILE:HD12  | 9        | 0.43          |
| (1,1169) | 1:79:A:ILE:HG23  | 1:79:A:ILE:HD13  | 9        | 0.43          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,436) | 1:46:A:TYR:HB2   | 1:153:A:ILE:HG21 | 7        | 0.43          |
| (1,436) | 1:46:A:TYR:HB2   | 1:153:A:ILE:HG22 | 7        | 0.43          |
| (1,436) | 1:46:A:TYR:HB2   | 1:153:A:ILE:HG23 | 7        | 0.43          |
| (1,389) | 1:44:A:ILE:HG21  | 1:44:A:ILE:H     | 7        | 0.43          |
| (1,389) | 1:44:A:ILE:HG22  | 1:44:A:ILE:H     | 7        | 0.43          |
| (1,389) | 1:44:A:ILE:HG23  | 1:44:A:ILE:H     | 7        | 0.43          |
| (1,353) | 1:42:A:ASP:HB2   | 1:158:A:ALA:HB1  | 9        | 0.43          |
| (1,353) | 1:42:A:ASP:HB2   | 1:158:A:ALA:HB2  | 9        | 0.43          |
| (1,353) | 1:42:A:ASP:HB2   | 1:158:A:ALA:HB3  | 9        | 0.43          |
| (1,353) | 1:42:A:ASP:HB3   | 1:158:A:ALA:HB1  | 9        | 0.43          |
| (1,353) | 1:42:A:ASP:HB3   | 1:158:A:ALA:HB2  | 9        | 0.43          |
| (1,353) | 1:42:A:ASP:HB3   | 1:158:A:ALA:HB3  | 9        | 0.43          |
| (1,205) | 1:32:A:ILE:HA    | 1:32:A:ILE:HD11  | 5        | 0.43          |
| (1,205) | 1:32:A:ILE:HA    | 1:32:A:ILE:HD12  | 5        | 0.43          |
| (1,205) | 1:32:A:ILE:HA    | 1:32:A:ILE:HD13  | 5        | 0.43          |
| (1,205) | 1:32:A:ILE:HA    | 1:32:A:ILE:HD11  | 9        | 0.43          |
| (1,205) | 1:32:A:ILE:HA    | 1:32:A:ILE:HD12  | 9        | 0.43          |
| (1,205) | 1:32:A:ILE:HA    | 1:32:A:ILE:HD13  | 9        | 0.43          |
| (1,162) | 1:29:A:LEU:HD11  | 1:29:A:LEU:HD21  | 9        | 0.43          |
| (1,162) | 1:29:A:LEU:HD11  | 1:29:A:LEU:HD22  | 9        | 0.43          |
| (1,162) | 1:29:A:LEU:HD11  | 1:29:A:LEU:HD23  | 9        | 0.43          |
| (1,162) | 1:29:A:LEU:HD12  | 1:29:A:LEU:HD21  | 9        | 0.43          |
| (1,162) | 1:29:A:LEU:HD12  | 1:29:A:LEU:HD22  | 9        | 0.43          |
| (1,162) | 1:29:A:LEU:HD12  | 1:29:A:LEU:HD23  | 9        | 0.43          |
| (1,162) | 1:29:A:LEU:HD13  | 1:29:A:LEU:HD21  | 9        | 0.43          |
| (1,162) | 1:29:A:LEU:HD13  | 1:29:A:LEU:HD22  | 9        | 0.43          |
| (1,162) | 1:29:A:LEU:HD13  | 1:29:A:LEU:HD23  | 9        | 0.43          |
| (1,11)  | 1:20:A:SER:HB2   | 1:21:A:GLU:H     | 10       | 0.43          |
| (1,11)  | 1:20:A:SER:HB3   | 1:21:A:GLU:H     | 10       | 0.43          |
| (2,719) | 1:142:A:ILE:HG21 | 1:145:A:TYR:HA   | 5        | 0.42          |
| (2,719) | 1:142:A:ILE:HG22 | 1:145:A:TYR:HA   | 5        | 0.42          |
| (2,719) | 1:142:A:ILE:HG23 | 1:145:A:TYR:HA   | 5        | 0.42          |
| (2,614) | 1:118:A:ILE:HG21 | 1:151:A:VAL:HA   | 2        | 0.42          |
| (2,614) | 1:118:A:ILE:HG22 | 1:151:A:VAL:HA   | 2        | 0.42          |
| (2,614) | 1:118:A:ILE:HG23 | 1:151:A:VAL:HA   | 2        | 0.42          |
| (2,607) | 1:115:A:LYS:H    | 1:116:A:GLU:HG2  | 10       | 0.42          |
| (2,607) | 1:115:A:LYS:H    | 1:116:A:GLU:HG3  | 10       | 0.42          |
| (2,517) | 1:84:A:GLY:HA2   | 1:85:A:TYR:HD1   | 10       | 0.42          |
| (2,517) | 1:84:A:GLY:HA2   | 1:85:A:TYR:HD2   | 10       | 0.42          |
| (2,517) | 1:84:A:GLY:HA3   | 1:85:A:TYR:HD1   | 10       | 0.42          |
| (2,517) | 1:84:A:GLY:HA3   | 1:85:A:TYR:HD2   | 10       | 0.42          |
| (2,380) | 1:69:A:GLN:HE22  | 1:73:A:TYR:HE1   | 8        | 0.42          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,380)  | 1:69:A:GLN:HE22  | 1:73:A:TYR:HE2   | 8        | 0.42          |
| (1,2245) | 1:162:A:ALA:HB1  | 1:168:A:PHE:HE1  | 1        | 0.42          |
| (1,2245) | 1:162:A:ALA:HB1  | 1:168:A:PHE:HE2  | 1        | 0.42          |
| (1,2245) | 1:162:A:ALA:HB2  | 1:168:A:PHE:HE1  | 1        | 0.42          |
| (1,2245) | 1:162:A:ALA:HB2  | 1:168:A:PHE:HE2  | 1        | 0.42          |
| (1,2245) | 1:162:A:ALA:HB3  | 1:168:A:PHE:HE1  | 1        | 0.42          |
| (1,2245) | 1:162:A:ALA:HB3  | 1:168:A:PHE:HE2  | 1        | 0.42          |
| (1,2110) | 1:154:A:LEU:HA   | 1:154:A:LEU:HD21 | 6        | 0.42          |
| (1,2110) | 1:154:A:LEU:HA   | 1:154:A:LEU:HD22 | 6        | 0.42          |
| (1,2110) | 1:154:A:LEU:HA   | 1:154:A:LEU:HD23 | 6        | 0.42          |
| (1,2110) | 1:154:A:LEU:HA   | 1:154:A:LEU:HD21 | 9        | 0.42          |
| (1,2110) | 1:154:A:LEU:HA   | 1:154:A:LEU:HD22 | 9        | 0.42          |
| (1,2110) | 1:154:A:LEU:HA   | 1:154:A:LEU:HD23 | 9        | 0.42          |
| (1,2093) | 1:153:A:ILE:HA   | 1:153:A:ILE:HG21 | 1        | 0.42          |
| (1,2093) | 1:153:A:ILE:HA   | 1:153:A:ILE:HG22 | 1        | 0.42          |
| (1,2093) | 1:153:A:ILE:HA   | 1:153:A:ILE:HG23 | 1        | 0.42          |
| (1,2080) | 1:151:A:VAL:HG11 | 1:152:A:ALA:H    | 10       | 0.42          |
| (1,2080) | 1:151:A:VAL:HG12 | 1:152:A:ALA:H    | 10       | 0.42          |
| (1,2080) | 1:151:A:VAL:HG13 | 1:152:A:ALA:H    | 10       | 0.42          |
| (1,1954) | 1:136:A:PRO:HG2  | 1:155:A:ASN:HD21 | 6        | 0.42          |
| (1,1954) | 1:136:A:PRO:HG2  | 1:155:A:ASN:HD22 | 6        | 0.42          |
| (1,1953) | 1:136:A:PRO:HG3  | 1:155:A:ASN:HD21 | 9        | 0.42          |
| (1,1953) | 1:136:A:PRO:HG3  | 1:155:A:ASN:HD22 | 9        | 0.42          |
| (1,1270) | 1:82:A:THR:HG21  | 1:83:A:SER:HA    | 4        | 0.42          |
| (1,1270) | 1:82:A:THR:HG22  | 1:83:A:SER:HA    | 4        | 0.42          |
| (1,1270) | 1:82:A:THR:HG23  | 1:83:A:SER:HA    | 4        | 0.42          |
| (1,1088) | 1:77:A:LEU:HD11  | 1:78:A:GLN:H     | 10       | 0.42          |
| (1,1088) | 1:77:A:LEU:HD12  | 1:78:A:GLN:H     | 10       | 0.42          |
| (1,1088) | 1:77:A:LEU:HD13  | 1:78:A:GLN:H     | 10       | 0.42          |
| (1,1088) | 1:77:A:LEU:HD21  | 1:78:A:GLN:H     | 10       | 0.42          |
| (1,1088) | 1:77:A:LEU:HD22  | 1:78:A:GLN:H     | 10       | 0.42          |
| (1,1088) | 1:77:A:LEU:HD23  | 1:78:A:GLN:H     | 10       | 0.42          |
| (1,162)  | 1:29:A:LEU:HD11  | 1:29:A:LEU:HD21  | 3        | 0.42          |
| (1,162)  | 1:29:A:LEU:HD11  | 1:29:A:LEU:HD22  | 3        | 0.42          |
| (1,162)  | 1:29:A:LEU:HD11  | 1:29:A:LEU:HD23  | 3        | 0.42          |
| (1,162)  | 1:29:A:LEU:HD12  | 1:29:A:LEU:HD21  | 3        | 0.42          |
| (1,162)  | 1:29:A:LEU:HD12  | 1:29:A:LEU:HD22  | 3        | 0.42          |
| (1,162)  | 1:29:A:LEU:HD12  | 1:29:A:LEU:HD23  | 3        | 0.42          |
| (1,162)  | 1:29:A:LEU:HD13  | 1:29:A:LEU:HD21  | 3        | 0.42          |
| (1,162)  | 1:29:A:LEU:HD13  | 1:29:A:LEU:HD22  | 3        | 0.42          |
| (1,162)  | 1:29:A:LEU:HD13  | 1:29:A:LEU:HD23  | 3        | 0.42          |
| (1,162)  | 1:29:A:LEU:HD11  | 1:29:A:LEU:HD21  | 4        | 0.42          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,162)  | 1:29:A:LEU:HD11 | 1:29:A:LEU:HD22  | 4        | 0.42          |
| (1,162)  | 1:29:A:LEU:HD11 | 1:29:A:LEU:HD23  | 4        | 0.42          |
| (1,162)  | 1:29:A:LEU:HD12 | 1:29:A:LEU:HD21  | 4        | 0.42          |
| (1,162)  | 1:29:A:LEU:HD12 | 1:29:A:LEU:HD22  | 4        | 0.42          |
| (1,162)  | 1:29:A:LEU:HD12 | 1:29:A:LEU:HD23  | 4        | 0.42          |
| (1,162)  | 1:29:A:LEU:HD13 | 1:29:A:LEU:HD21  | 4        | 0.42          |
| (1,162)  | 1:29:A:LEU:HD13 | 1:29:A:LEU:HD22  | 4        | 0.42          |
| (1,162)  | 1:29:A:LEU:HD13 | 1:29:A:LEU:HD23  | 4        | 0.42          |
| (1,162)  | 1:29:A:LEU:HD11 | 1:29:A:LEU:HD21  | 10       | 0.42          |
| (1,162)  | 1:29:A:LEU:HD11 | 1:29:A:LEU:HD22  | 10       | 0.42          |
| (1,162)  | 1:29:A:LEU:HD11 | 1:29:A:LEU:HD23  | 10       | 0.42          |
| (1,162)  | 1:29:A:LEU:HD12 | 1:29:A:LEU:HD21  | 10       | 0.42          |
| (1,162)  | 1:29:A:LEU:HD12 | 1:29:A:LEU:HD22  | 10       | 0.42          |
| (1,162)  | 1:29:A:LEU:HD12 | 1:29:A:LEU:HD23  | 10       | 0.42          |
| (1,162)  | 1:29:A:LEU:HD13 | 1:29:A:LEU:HD21  | 10       | 0.42          |
| (1,162)  | 1:29:A:LEU:HD13 | 1:29:A:LEU:HD22  | 10       | 0.42          |
| (1,162)  | 1:29:A:LEU:HD13 | 1:29:A:LEU:HD23  | 10       | 0.42          |
| (1,23)   | 1:23:A:ILE:HA   | 1:23:A:ILE:HD11  | 1        | 0.42          |
| (1,23)   | 1:23:A:ILE:HA   | 1:23:A:ILE:HD12  | 1        | 0.42          |
| (1,23)   | 1:23:A:ILE:HA   | 1:23:A:ILE:HD13  | 1        | 0.42          |
| (1,23)   | 1:23:A:ILE:HA   | 1:23:A:ILE:HD11  | 2        | 0.42          |
| (1,23)   | 1:23:A:ILE:HA   | 1:23:A:ILE:HD12  | 2        | 0.42          |
| (1,23)   | 1:23:A:ILE:HA   | 1:23:A:ILE:HD13  | 2        | 0.42          |
| (1,3)    | 1:16:A:ALA:HB1  | 1:16:A:ALA:H     | 10       | 0.42          |
| (1,3)    | 1:16:A:ALA:HB2  | 1:16:A:ALA:H     | 10       | 0.42          |
| (1,3)    | 1:16:A:ALA:HB3  | 1:16:A:ALA:H     | 10       | 0.42          |
| (2,607)  | 1:115:A:LYS:H   | 1:116:A:GLU:HG2  | 2        | 0.41          |
| (2,607)  | 1:115:A:LYS:H   | 1:116:A:GLU:HG3  | 2        | 0.41          |
| (2,601)  | 1:115:A:LYS:HE2 | 1:116:A:GLU:H    | 6        | 0.41          |
| (2,601)  | 1:115:A:LYS:HE3 | 1:116:A:GLU:H    | 6        | 0.41          |
| (2,240)  | 1:46:A:TYR:HB2  | 1:155:A:ASN:HD21 | 5        | 0.41          |
| (2,240)  | 1:46:A:TYR:HB2  | 1:155:A:ASN:HD22 | 5        | 0.41          |
| (2,194)  | 1:38:A:ALA:HB1  | 1:39:A:GLN:HE21  | 4        | 0.41          |
| (2,194)  | 1:38:A:ALA:HB2  | 1:39:A:GLN:HE21  | 4        | 0.41          |
| (2,194)  | 1:38:A:ALA:HB3  | 1:39:A:GLN:HE21  | 4        | 0.41          |
| (2,4)    | 1:15:A:THR:HG21 | 1:16:A:ALA:H     | 3        | 0.41          |
| (2,4)    | 1:15:A:THR:HG22 | 1:16:A:ALA:H     | 3        | 0.41          |
| (2,4)    | 1:15:A:THR:HG23 | 1:16:A:ALA:H     | 3        | 0.41          |
| (1,2246) | 1:162:A:ALA:HB1 | 1:168:A:PHE:HZ   | 6        | 0.41          |
| (1,2246) | 1:162:A:ALA:HB2 | 1:168:A:PHE:HZ   | 6        | 0.41          |
| (1,2246) | 1:162:A:ALA:HB3 | 1:168:A:PHE:HZ   | 6        | 0.41          |
| (1,2110) | 1:154:A:LEU:HA  | 1:154:A:LEU:HD21 | 1        | 0.41          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2110) | 1:154:A:LEU:HA   | 1:154:A:LEU:HD22 | 1        | 0.41          |
| (1,2110) | 1:154:A:LEU:HA   | 1:154:A:LEU:HD23 | 1        | 0.41          |
| (1,2110) | 1:154:A:LEU:HA   | 1:154:A:LEU:HD21 | 3        | 0.41          |
| (1,2110) | 1:154:A:LEU:HA   | 1:154:A:LEU:HD22 | 3        | 0.41          |
| (1,2110) | 1:154:A:LEU:HA   | 1:154:A:LEU:HD23 | 3        | 0.41          |
| (1,2110) | 1:154:A:LEU:HA   | 1:154:A:LEU:HD21 | 7        | 0.41          |
| (1,2110) | 1:154:A:LEU:HA   | 1:154:A:LEU:HD22 | 7        | 0.41          |
| (1,2110) | 1:154:A:LEU:HA   | 1:154:A:LEU:HD23 | 7        | 0.41          |
| (1,2110) | 1:154:A:LEU:HA   | 1:154:A:LEU:HD21 | 10       | 0.41          |
| (1,2110) | 1:154:A:LEU:HA   | 1:154:A:LEU:HD22 | 10       | 0.41          |
| (1,2110) | 1:154:A:LEU:HA   | 1:154:A:LEU:HD23 | 10       | 0.41          |
| (1,2098) | 1:153:A:ILE:HB   | 1:153:A:ILE:HG21 | 10       | 0.41          |
| (1,2098) | 1:153:A:ILE:HB   | 1:153:A:ILE:HG22 | 10       | 0.41          |
| (1,2098) | 1:153:A:ILE:HB   | 1:153:A:ILE:HG23 | 10       | 0.41          |
| (1,2093) | 1:153:A:ILE:HA   | 1:153:A:ILE:HG21 | 4        | 0.41          |
| (1,2093) | 1:153:A:ILE:HA   | 1:153:A:ILE:HG22 | 4        | 0.41          |
| (1,2093) | 1:153:A:ILE:HA   | 1:153:A:ILE:HG23 | 4        | 0.41          |
| (1,2081) | 1:151:A:VAL:HG11 | 1:153:A:ILE:H    | 10       | 0.41          |
| (1,2081) | 1:151:A:VAL:HG12 | 1:153:A:ILE:H    | 10       | 0.41          |
| (1,2081) | 1:151:A:VAL:HG13 | 1:153:A:ILE:H    | 10       | 0.41          |
| (1,2080) | 1:151:A:VAL:HG11 | 1:152:A:ALA:H    | 6        | 0.41          |
| (1,2080) | 1:151:A:VAL:HG12 | 1:152:A:ALA:H    | 6        | 0.41          |
| (1,2080) | 1:151:A:VAL:HG13 | 1:152:A:ALA:H    | 6        | 0.41          |
| (1,1801) | 1:128:A:TYR:HD1  | 1:131:A:THR:HG21 | 8        | 0.41          |
| (1,1801) | 1:128:A:TYR:HD1  | 1:131:A:THR:HG22 | 8        | 0.41          |
| (1,1801) | 1:128:A:TYR:HD1  | 1:131:A:THR:HG23 | 8        | 0.41          |
| (1,1801) | 1:128:A:TYR:HD2  | 1:131:A:THR:HG21 | 8        | 0.41          |
| (1,1801) | 1:128:A:TYR:HD2  | 1:131:A:THR:HG22 | 8        | 0.41          |
| (1,1801) | 1:128:A:TYR:HD2  | 1:131:A:THR:HG23 | 8        | 0.41          |
| (1,1475) | 1:95:A:PHE:HB2   | 1:96:A:SER:H     | 5        | 0.41          |
| (1,1475) | 1:95:A:PHE:HB3   | 1:96:A:SER:H     | 5        | 0.41          |
| (1,1275) | 1:82:A:THR:HG21  | 1:96:A:SER:HB2   | 9        | 0.41          |
| (1,1275) | 1:82:A:THR:HG22  | 1:96:A:SER:HB2   | 9        | 0.41          |
| (1,1275) | 1:82:A:THR:HG23  | 1:96:A:SER:HB2   | 9        | 0.41          |
| (1,1270) | 1:82:A:THR:HG21  | 1:83:A:SER:HA    | 1        | 0.41          |
| (1,1270) | 1:82:A:THR:HG22  | 1:83:A:SER:HA    | 1        | 0.41          |
| (1,1270) | 1:82:A:THR:HG23  | 1:83:A:SER:HA    | 1        | 0.41          |
| (1,1270) | 1:82:A:THR:HG21  | 1:83:A:SER:HA    | 3        | 0.41          |
| (1,1270) | 1:82:A:THR:HG22  | 1:83:A:SER:HA    | 3        | 0.41          |
| (1,1270) | 1:82:A:THR:HG23  | 1:83:A:SER:HA    | 3        | 0.41          |
| (1,1270) | 1:82:A:THR:HG21  | 1:83:A:SER:HA    | 6        | 0.41          |
| (1,1270) | 1:82:A:THR:HG22  | 1:83:A:SER:HA    | 6        | 0.41          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1270) | 1:82:A:THR:HG23 | 1:83:A:SER:HA    | 6        | 0.41          |
| (1,1270) | 1:82:A:THR:HG21 | 1:83:A:SER:HA    | 10       | 0.41          |
| (1,1270) | 1:82:A:THR:HG22 | 1:83:A:SER:HA    | 10       | 0.41          |
| (1,1270) | 1:82:A:THR:HG23 | 1:83:A:SER:HA    | 10       | 0.41          |
| (1,837)  | 1:66:A:ASN:HB2  | 1:66:A:ASN:HD22  | 2        | 0.41          |
| (1,520)  | 1:49:A:VAL:HB   | 1:152:A:ALA:HB1  | 6        | 0.41          |
| (1,520)  | 1:49:A:VAL:HB   | 1:152:A:ALA:HB2  | 6        | 0.41          |
| (1,520)  | 1:49:A:VAL:HB   | 1:152:A:ALA:HB3  | 6        | 0.41          |
| (1,209)  | 1:32:A:ILE:HA   | 1:32:A:ILE:HG21  | 9        | 0.41          |
| (1,209)  | 1:32:A:ILE:HA   | 1:32:A:ILE:HG22  | 9        | 0.41          |
| (1,209)  | 1:32:A:ILE:HA   | 1:32:A:ILE:HG23  | 9        | 0.41          |
| (1,205)  | 1:32:A:ILE:HA   | 1:32:A:ILE:HD11  | 1        | 0.41          |
| (1,205)  | 1:32:A:ILE:HA   | 1:32:A:ILE:HD12  | 1        | 0.41          |
| (1,205)  | 1:32:A:ILE:HA   | 1:32:A:ILE:HD13  | 1        | 0.41          |
| (1,162)  | 1:29:A:LEU:HD11 | 1:29:A:LEU:HD21  | 6        | 0.41          |
| (1,162)  | 1:29:A:LEU:HD11 | 1:29:A:LEU:HD22  | 6        | 0.41          |
| (1,162)  | 1:29:A:LEU:HD11 | 1:29:A:LEU:HD23  | 6        | 0.41          |
| (1,162)  | 1:29:A:LEU:HD12 | 1:29:A:LEU:HD21  | 6        | 0.41          |
| (1,162)  | 1:29:A:LEU:HD12 | 1:29:A:LEU:HD22  | 6        | 0.41          |
| (1,162)  | 1:29:A:LEU:HD12 | 1:29:A:LEU:HD23  | 6        | 0.41          |
| (1,162)  | 1:29:A:LEU:HD13 | 1:29:A:LEU:HD21  | 6        | 0.41          |
| (1,162)  | 1:29:A:LEU:HD13 | 1:29:A:LEU:HD22  | 6        | 0.41          |
| (1,162)  | 1:29:A:LEU:HD13 | 1:29:A:LEU:HD23  | 6        | 0.41          |
| (1,162)  | 1:29:A:LEU:HD11 | 1:29:A:LEU:HD21  | 8        | 0.41          |
| (1,162)  | 1:29:A:LEU:HD11 | 1:29:A:LEU:HD22  | 8        | 0.41          |
| (1,162)  | 1:29:A:LEU:HD11 | 1:29:A:LEU:HD23  | 8        | 0.41          |
| (1,162)  | 1:29:A:LEU:HD12 | 1:29:A:LEU:HD21  | 8        | 0.41          |
| (1,162)  | 1:29:A:LEU:HD12 | 1:29:A:LEU:HD22  | 8        | 0.41          |
| (1,162)  | 1:29:A:LEU:HD12 | 1:29:A:LEU:HD23  | 8        | 0.41          |
| (1,162)  | 1:29:A:LEU:HD13 | 1:29:A:LEU:HD21  | 8        | 0.41          |
| (1,162)  | 1:29:A:LEU:HD13 | 1:29:A:LEU:HD22  | 8        | 0.41          |
| (1,162)  | 1:29:A:LEU:HD13 | 1:29:A:LEU:HD23  | 8        | 0.41          |
| (1,23)   | 1:23:A:ILE:HA   | 1:23:A:ILE:HD11  | 9        | 0.41          |
| (1,23)   | 1:23:A:ILE:HA   | 1:23:A:ILE:HD12  | 9        | 0.41          |
| (1,23)   | 1:23:A:ILE:HA   | 1:23:A:ILE:HD13  | 9        | 0.41          |
| (2,756)  | 1:167:A:LEU:H   | 1:167:A:LEU:HD21 | 6        | 0.4           |
| (2,756)  | 1:167:A:LEU:H   | 1:167:A:LEU:HD22 | 6        | 0.4           |
| (2,756)  | 1:167:A:LEU:H   | 1:167:A:LEU:HD23 | 6        | 0.4           |
| (2,756)  | 1:167:A:LEU:H   | 1:167:A:LEU:HD21 | 8        | 0.4           |
| (2,756)  | 1:167:A:LEU:H   | 1:167:A:LEU:HD22 | 8        | 0.4           |
| (2,756)  | 1:167:A:LEU:H   | 1:167:A:LEU:HD23 | 8        | 0.4           |
| (2,756)  | 1:167:A:LEU:H   | 1:167:A:LEU:HD21 | 9        | 0.4           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,756)  | 1:167:A:LEU:H    | 1:167:A:LEU:HD22 | 9        | 0.4           |
| (2,756)  | 1:167:A:LEU:H    | 1:167:A:LEU:HD23 | 9        | 0.4           |
| (2,754)  | 1:167:A:LEU:HD21 | 1:167:A:LEU:H    | 6        | 0.4           |
| (2,754)  | 1:167:A:LEU:HD22 | 1:167:A:LEU:H    | 6        | 0.4           |
| (2,754)  | 1:167:A:LEU:HD23 | 1:167:A:LEU:H    | 6        | 0.4           |
| (2,754)  | 1:167:A:LEU:HD21 | 1:167:A:LEU:H    | 8        | 0.4           |
| (2,754)  | 1:167:A:LEU:HD22 | 1:167:A:LEU:H    | 8        | 0.4           |
| (2,754)  | 1:167:A:LEU:HD23 | 1:167:A:LEU:H    | 8        | 0.4           |
| (2,754)  | 1:167:A:LEU:HD21 | 1:167:A:LEU:H    | 9        | 0.4           |
| (2,754)  | 1:167:A:LEU:HD22 | 1:167:A:LEU:H    | 9        | 0.4           |
| (2,754)  | 1:167:A:LEU:HD23 | 1:167:A:LEU:H    | 9        | 0.4           |
| (2,661)  | 1:125:A:LYS:HG2  | 1:126:A:THR:H    | 10       | 0.4           |
| (2,661)  | 1:125:A:LYS:HG3  | 1:126:A:THR:H    | 10       | 0.4           |
| (2,295)  | 1:52:A:LYS:HE2   | 1:54:A:GLN:HE22  | 2        | 0.4           |
| (2,295)  | 1:52:A:LYS:HE3   | 1:54:A:GLN:HE22  | 2        | 0.4           |
| (2,227)  | 1:43:A:ASP:HB3   | 1:46:A:TYR:HE1   | 8        | 0.4           |
| (2,227)  | 1:43:A:ASP:HB3   | 1:46:A:TYR:HE2   | 8        | 0.4           |
| (2,16)   | 1:17:A:GLN:HG2   | 1:18:A:ALA:H     | 6        | 0.4           |
| (2,16)   | 1:17:A:GLN:HG3   | 1:18:A:ALA:H     | 6        | 0.4           |
| (1,2327) | 1:171:A:LEU:HG   | 1:171:A:LEU:H    | 2        | 0.4           |
| (1,2320) | 1:171:A:LEU:HD11 | 1:171:A:LEU:HD21 | 3        | 0.4           |
| (1,2320) | 1:171:A:LEU:HD11 | 1:171:A:LEU:HD22 | 3        | 0.4           |
| (1,2320) | 1:171:A:LEU:HD11 | 1:171:A:LEU:HD23 | 3        | 0.4           |
| (1,2320) | 1:171:A:LEU:HD12 | 1:171:A:LEU:HD21 | 3        | 0.4           |
| (1,2320) | 1:171:A:LEU:HD12 | 1:171:A:LEU:HD22 | 3        | 0.4           |
| (1,2320) | 1:171:A:LEU:HD12 | 1:171:A:LEU:HD23 | 3        | 0.4           |
| (1,2320) | 1:171:A:LEU:HD13 | 1:171:A:LEU:HD21 | 3        | 0.4           |
| (1,2320) | 1:171:A:LEU:HD13 | 1:171:A:LEU:HD22 | 3        | 0.4           |
| (1,2320) | 1:171:A:LEU:HD13 | 1:171:A:LEU:HD23 | 3        | 0.4           |
| (1,2284) | 1:168:A:PHE:HB2  | 1:171:A:LEU:HD11 | 7        | 0.4           |
| (1,2284) | 1:168:A:PHE:HB2  | 1:171:A:LEU:HD12 | 7        | 0.4           |
| (1,2284) | 1:168:A:PHE:HB2  | 1:171:A:LEU:HD13 | 7        | 0.4           |
| (1,2191) | 1:158:A:ALA:HB1  | 1:160:A:TYR:HE1  | 10       | 0.4           |
| (1,2191) | 1:158:A:ALA:HB1  | 1:160:A:TYR:HE2  | 10       | 0.4           |
| (1,2191) | 1:158:A:ALA:HB2  | 1:160:A:TYR:HE1  | 10       | 0.4           |
| (1,2191) | 1:158:A:ALA:HB2  | 1:160:A:TYR:HE2  | 10       | 0.4           |
| (1,2191) | 1:158:A:ALA:HB3  | 1:160:A:TYR:HE1  | 10       | 0.4           |
| (1,2191) | 1:158:A:ALA:HB3  | 1:160:A:TYR:HE2  | 10       | 0.4           |
| (1,2110) | 1:154:A:LEU:HA   | 1:154:A:LEU:HD21 | 8        | 0.4           |
| (1,2110) | 1:154:A:LEU:HA   | 1:154:A:LEU:HD22 | 8        | 0.4           |
| (1,2110) | 1:154:A:LEU:HA   | 1:154:A:LEU:HD23 | 8        | 0.4           |
| (1,2038) | 1:144:A:VAL:HG21 | 1:144:A:VAL:H    | 1        | 0.4           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2038) | 1:144:A:VAL:HG22 | 1:144:A:VAL:H    | 1        | 0.4           |
| (1,2038) | 1:144:A:VAL:HG23 | 1:144:A:VAL:H    | 1        | 0.4           |
| (1,1953) | 1:136:A:PRO:HG3  | 1:155:A:ASN:HD21 | 4        | 0.4           |
| (1,1953) | 1:136:A:PRO:HG3  | 1:155:A:ASN:HD22 | 4        | 0.4           |
| (1,1941) | 1:135:A:VAL:HG21 | 1:135:A:VAL:H    | 4        | 0.4           |
| (1,1941) | 1:135:A:VAL:HG22 | 1:135:A:VAL:H    | 4        | 0.4           |
| (1,1941) | 1:135:A:VAL:HG23 | 1:135:A:VAL:H    | 4        | 0.4           |
| (1,1630) | 1:110:A:VAL:HG21 | 1:110:A:VAL:H    | 8        | 0.4           |
| (1,1630) | 1:110:A:VAL:HG22 | 1:110:A:VAL:H    | 8        | 0.4           |
| (1,1630) | 1:110:A:VAL:HG23 | 1:110:A:VAL:H    | 8        | 0.4           |
| (1,1475) | 1:95:A:PHE:HB2   | 1:96:A:SER:H     | 1        | 0.4           |
| (1,1475) | 1:95:A:PHE:HB3   | 1:96:A:SER:H     | 1        | 0.4           |
| (1,1475) | 1:95:A:PHE:HB2   | 1:96:A:SER:H     | 9        | 0.4           |
| (1,1475) | 1:95:A:PHE:HB3   | 1:96:A:SER:H     | 9        | 0.4           |
| (1,1451) | 1:91:A:ALA:HB1   | 1:91:A:ALA:H     | 9        | 0.4           |
| (1,1451) | 1:91:A:ALA:HB2   | 1:91:A:ALA:H     | 9        | 0.4           |
| (1,1451) | 1:91:A:ALA:HB3   | 1:91:A:ALA:H     | 9        | 0.4           |
| (1,1339) | 1:85:A:TYR:HD1   | 1:135:A:VAL:HA   | 5        | 0.4           |
| (1,1339) | 1:85:A:TYR:HD2   | 1:135:A:VAL:HA   | 5        | 0.4           |
| (1,1270) | 1:82:A:THR:HG21  | 1:83:A:SER:HA    | 7        | 0.4           |
| (1,1270) | 1:82:A:THR:HG22  | 1:83:A:SER:HA    | 7        | 0.4           |
| (1,1270) | 1:82:A:THR:HG23  | 1:83:A:SER:HA    | 7        | 0.4           |
| (1,1228) | 1:81:A:ILE:HG21  | 1:82:A:THR:HA    | 1        | 0.4           |
| (1,1228) | 1:81:A:ILE:HG22  | 1:82:A:THR:HA    | 1        | 0.4           |
| (1,1228) | 1:81:A:ILE:HG23  | 1:82:A:THR:HA    | 1        | 0.4           |
| (1,844)  | 1:66:A:ASN:HD21  | 1:70:A:LEU:HD21  | 7        | 0.4           |
| (1,844)  | 1:66:A:ASN:HD21  | 1:70:A:LEU:HD22  | 7        | 0.4           |
| (1,844)  | 1:66:A:ASN:HD21  | 1:70:A:LEU:HD23  | 7        | 0.4           |
| (1,605)  | 1:54:A:GLN:HG2   | 1:54:A:GLN:H     | 5        | 0.4           |
| (1,605)  | 1:54:A:GLN:HG3   | 1:54:A:GLN:H     | 5        | 0.4           |
| (1,520)  | 1:49:A:VAL:HB    | 1:152:A:ALA:HB1  | 10       | 0.4           |
| (1,520)  | 1:49:A:VAL:HB    | 1:152:A:ALA:HB2  | 10       | 0.4           |
| (1,520)  | 1:49:A:VAL:HB    | 1:152:A:ALA:HB3  | 10       | 0.4           |
| (1,487)  | 1:48:A:ILE:HG12  | 1:48:A:ILE:HG21  | 3        | 0.4           |
| (1,487)  | 1:48:A:ILE:HG12  | 1:48:A:ILE:HG22  | 3        | 0.4           |
| (1,487)  | 1:48:A:ILE:HG12  | 1:48:A:ILE:HG23  | 3        | 0.4           |
| (1,286)  | 1:36:A:ALA:HA    | 1:37:A:GLY:H     | 6        | 0.4           |
| (1,270)  | 1:34:A:PRO:HD3   | 1:168:A:PHE:HE1  | 2        | 0.4           |
| (1,270)  | 1:34:A:PRO:HD3   | 1:168:A:PHE:HE2  | 2        | 0.4           |
| (1,242)  | 1:32:A:ILE:HG21  | 1:160:A:TYR:HE1  | 6        | 0.4           |
| (1,242)  | 1:32:A:ILE:HG21  | 1:160:A:TYR:HE2  | 6        | 0.4           |
| (1,242)  | 1:32:A:ILE:HG22  | 1:160:A:TYR:HE1  | 6        | 0.4           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,242)  | 1:32:A:ILE:HG22  | 1:160:A:TYR:HE2  | 6        | 0.4           |
| (1,242)  | 1:32:A:ILE:HG23  | 1:160:A:TYR:HE1  | 6        | 0.4           |
| (1,242)  | 1:32:A:ILE:HG23  | 1:160:A:TYR:HE2  | 6        | 0.4           |
| (1,242)  | 1:32:A:ILE:HG21  | 1:160:A:TYR:HE1  | 7        | 0.4           |
| (1,242)  | 1:32:A:ILE:HG21  | 1:160:A:TYR:HE2  | 7        | 0.4           |
| (1,242)  | 1:32:A:ILE:HG22  | 1:160:A:TYR:HE1  | 7        | 0.4           |
| (1,242)  | 1:32:A:ILE:HG22  | 1:160:A:TYR:HE2  | 7        | 0.4           |
| (1,242)  | 1:32:A:ILE:HG23  | 1:160:A:TYR:HE1  | 7        | 0.4           |
| (1,242)  | 1:32:A:ILE:HG23  | 1:160:A:TYR:HE2  | 7        | 0.4           |
| (1,232)  | 1:32:A:ILE:HG21  | 1:32:A:ILE:HD11  | 1        | 0.4           |
| (1,232)  | 1:32:A:ILE:HG21  | 1:32:A:ILE:HD12  | 1        | 0.4           |
| (1,232)  | 1:32:A:ILE:HG21  | 1:32:A:ILE:HD13  | 1        | 0.4           |
| (1,232)  | 1:32:A:ILE:HG22  | 1:32:A:ILE:HD11  | 1        | 0.4           |
| (1,232)  | 1:32:A:ILE:HG22  | 1:32:A:ILE:HD12  | 1        | 0.4           |
| (1,232)  | 1:32:A:ILE:HG22  | 1:32:A:ILE:HD13  | 1        | 0.4           |
| (1,232)  | 1:32:A:ILE:HG23  | 1:32:A:ILE:HD11  | 1        | 0.4           |
| (1,232)  | 1:32:A:ILE:HG23  | 1:32:A:ILE:HD12  | 1        | 0.4           |
| (1,232)  | 1:32:A:ILE:HG23  | 1:32:A:ILE:HD13  | 1        | 0.4           |
| (1,166)  | 1:29:A:LEU:HD11  | 1:175:A:PHE:H    | 6        | 0.4           |
| (1,166)  | 1:29:A:LEU:HD12  | 1:175:A:PHE:H    | 6        | 0.4           |
| (1,166)  | 1:29:A:LEU:HD13  | 1:175:A:PHE:H    | 6        | 0.4           |
| (1,11)   | 1:20:A:SER:HB2   | 1:21:A:GLU:H     | 5        | 0.4           |
| (1,11)   | 1:20:A:SER:HB3   | 1:21:A:GLU:H     | 5        | 0.4           |
| (2,756)  | 1:167:A:LEU:H    | 1:167:A:LEU:HD21 | 5        | 0.39          |
| (2,756)  | 1:167:A:LEU:H    | 1:167:A:LEU:HD22 | 5        | 0.39          |
| (2,756)  | 1:167:A:LEU:H    | 1:167:A:LEU:HD23 | 5        | 0.39          |
| (2,755)  | 1:167:A:LEU:H    | 1:167:A:LEU:HD11 | 8        | 0.39          |
| (2,755)  | 1:167:A:LEU:H    | 1:167:A:LEU:HD12 | 8        | 0.39          |
| (2,755)  | 1:167:A:LEU:H    | 1:167:A:LEU:HD13 | 8        | 0.39          |
| (2,754)  | 1:167:A:LEU:HD21 | 1:167:A:LEU:H    | 5        | 0.39          |
| (2,754)  | 1:167:A:LEU:HD22 | 1:167:A:LEU:H    | 5        | 0.39          |
| (2,754)  | 1:167:A:LEU:HD23 | 1:167:A:LEU:H    | 5        | 0.39          |
| (2,753)  | 1:167:A:LEU:HD11 | 1:167:A:LEU:H    | 8        | 0.39          |
| (2,753)  | 1:167:A:LEU:HD12 | 1:167:A:LEU:H    | 8        | 0.39          |
| (2,753)  | 1:167:A:LEU:HD13 | 1:167:A:LEU:H    | 8        | 0.39          |
| (2,732)  | 1:155:A:ASN:H    | 1:156:A:PHE:HE1  | 6        | 0.39          |
| (2,732)  | 1:155:A:ASN:H    | 1:156:A:PHE:HE2  | 6        | 0.39          |
| (2,194)  | 1:38:A:ALA:HB1   | 1:39:A:GLN:HE21  | 6        | 0.39          |
| (2,194)  | 1:38:A:ALA:HB2   | 1:39:A:GLN:HE21  | 6        | 0.39          |
| (2,194)  | 1:38:A:ALA:HB3   | 1:39:A:GLN:HE21  | 6        | 0.39          |
| (1,2463) | 1:182:A:VAL:HG21 | 1:182:A:VAL:H    | 4        | 0.39          |
| (1,2463) | 1:182:A:VAL:HG22 | 1:182:A:VAL:H    | 4        | 0.39          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2463) | 1:182:A:VAL:HG23 | 1:182:A:VAL:H    | 4        | 0.39          |
| (1,2354) | 1:173:A:VAL:HG11 | 1:175:A:PHE:HE1  | 9        | 0.39          |
| (1,2354) | 1:173:A:VAL:HG11 | 1:175:A:PHE:HE2  | 9        | 0.39          |
| (1,2354) | 1:173:A:VAL:HG12 | 1:175:A:PHE:HE1  | 9        | 0.39          |
| (1,2354) | 1:173:A:VAL:HG12 | 1:175:A:PHE:HE2  | 9        | 0.39          |
| (1,2354) | 1:173:A:VAL:HG13 | 1:175:A:PHE:HE1  | 9        | 0.39          |
| (1,2354) | 1:173:A:VAL:HG13 | 1:175:A:PHE:HE2  | 9        | 0.39          |
| (1,2320) | 1:171:A:LEU:HD11 | 1:171:A:LEU:HD21 | 2        | 0.39          |
| (1,2320) | 1:171:A:LEU:HD11 | 1:171:A:LEU:HD22 | 2        | 0.39          |
| (1,2320) | 1:171:A:LEU:HD11 | 1:171:A:LEU:HD23 | 2        | 0.39          |
| (1,2320) | 1:171:A:LEU:HD12 | 1:171:A:LEU:HD21 | 2        | 0.39          |
| (1,2320) | 1:171:A:LEU:HD12 | 1:171:A:LEU:HD22 | 2        | 0.39          |
| (1,2320) | 1:171:A:LEU:HD12 | 1:171:A:LEU:HD23 | 2        | 0.39          |
| (1,2320) | 1:171:A:LEU:HD13 | 1:171:A:LEU:HD21 | 2        | 0.39          |
| (1,2320) | 1:171:A:LEU:HD13 | 1:171:A:LEU:HD22 | 2        | 0.39          |
| (1,2320) | 1:171:A:LEU:HD13 | 1:171:A:LEU:HD23 | 2        | 0.39          |
| (1,2110) | 1:154:A:LEU:HA   | 1:154:A:LEU:HD21 | 5        | 0.39          |
| (1,2110) | 1:154:A:LEU:HA   | 1:154:A:LEU:HD22 | 5        | 0.39          |
| (1,2110) | 1:154:A:LEU:HA   | 1:154:A:LEU:HD23 | 5        | 0.39          |
| (1,2015) | 1:142:A:ILE:HG21 | 1:144:A:VAL:H    | 9        | 0.39          |
| (1,2015) | 1:142:A:ILE:HG22 | 1:144:A:VAL:H    | 9        | 0.39          |
| (1,2015) | 1:142:A:ILE:HG23 | 1:144:A:VAL:H    | 9        | 0.39          |
| (1,2002) | 1:142:A:ILE:HA   | 1:142:A:ILE:HD11 | 1        | 0.39          |
| (1,2002) | 1:142:A:ILE:HA   | 1:142:A:ILE:HD12 | 1        | 0.39          |
| (1,2002) | 1:142:A:ILE:HA   | 1:142:A:ILE:HD13 | 1        | 0.39          |
| (1,1954) | 1:136:A:PRO:HG2  | 1:155:A:ASN:HD21 | 5        | 0.39          |
| (1,1954) | 1:136:A:PRO:HG2  | 1:155:A:ASN:HD22 | 5        | 0.39          |
| (1,1954) | 1:136:A:PRO:HG2  | 1:155:A:ASN:HD21 | 7        | 0.39          |
| (1,1954) | 1:136:A:PRO:HG2  | 1:155:A:ASN:HD22 | 7        | 0.39          |
| (1,1954) | 1:136:A:PRO:HG2  | 1:155:A:ASN:HD21 | 9        | 0.39          |
| (1,1954) | 1:136:A:PRO:HG2  | 1:155:A:ASN:HD22 | 9        | 0.39          |
| (1,1954) | 1:136:A:PRO:HG2  | 1:155:A:ASN:HD21 | 10       | 0.39          |
| (1,1954) | 1:136:A:PRO:HG2  | 1:155:A:ASN:HD22 | 10       | 0.39          |
| (1,1953) | 1:136:A:PRO:HG3  | 1:155:A:ASN:HD21 | 10       | 0.39          |
| (1,1953) | 1:136:A:PRO:HG3  | 1:155:A:ASN:HD22 | 10       | 0.39          |
| (1,1941) | 1:135:A:VAL:HG21 | 1:135:A:VAL:H    | 9        | 0.39          |
| (1,1941) | 1:135:A:VAL:HG22 | 1:135:A:VAL:H    | 9        | 0.39          |
| (1,1941) | 1:135:A:VAL:HG23 | 1:135:A:VAL:H    | 9        | 0.39          |
| (1,1777) | 1:121:A:LEU:HD21 | 1:121:A:LEU:H    | 6        | 0.39          |
| (1,1777) | 1:121:A:LEU:HD22 | 1:121:A:LEU:H    | 6        | 0.39          |
| (1,1777) | 1:121:A:LEU:HD23 | 1:121:A:LEU:H    | 6        | 0.39          |
| (1,1522) | 1:100:A:ALA:H    | 1:111:A:ILE:HD11 | 4        | 0.39          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1522) | 1:100:A:ALA:H   | 1:111:A:ILE:HD12 | 4        | 0.39          |
| (1,1522) | 1:100:A:ALA:H   | 1:111:A:ILE:HD13 | 4        | 0.39          |
| (1,1475) | 1:95:A:PHE:HB2  | 1:96:A:SER:H     | 8        | 0.39          |
| (1,1475) | 1:95:A:PHE:HB3  | 1:96:A:SER:H     | 8        | 0.39          |
| (1,1451) | 1:91:A:ALA:HB1  | 1:91:A:ALA:H     | 2        | 0.39          |
| (1,1451) | 1:91:A:ALA:HB2  | 1:91:A:ALA:H     | 2        | 0.39          |
| (1,1451) | 1:91:A:ALA:HB3  | 1:91:A:ALA:H     | 2        | 0.39          |
| (1,1338) | 1:85:A:TYR:HD1  | 1:86:A:GLU:H     | 1        | 0.39          |
| (1,1338) | 1:85:A:TYR:HD2  | 1:86:A:GLU:H     | 1        | 0.39          |
| (1,1270) | 1:82:A:THR:HG21 | 1:83:A:SER:HA    | 5        | 0.39          |
| (1,1270) | 1:82:A:THR:HG22 | 1:83:A:SER:HA    | 5        | 0.39          |
| (1,1270) | 1:82:A:THR:HG23 | 1:83:A:SER:HA    | 5        | 0.39          |
| (1,1270) | 1:82:A:THR:HG21 | 1:83:A:SER:HA    | 9        | 0.39          |
| (1,1270) | 1:82:A:THR:HG22 | 1:83:A:SER:HA    | 9        | 0.39          |
| (1,1270) | 1:82:A:THR:HG23 | 1:83:A:SER:HA    | 9        | 0.39          |
| (1,1236) | 1:81:A:ILE:HG21 | 1:154:A:LEU:HB3  | 4        | 0.39          |
| (1,1236) | 1:81:A:ILE:HG22 | 1:154:A:LEU:HB3  | 4        | 0.39          |
| (1,1236) | 1:81:A:ILE:HG23 | 1:154:A:LEU:HB3  | 4        | 0.39          |
| (1,1236) | 1:81:A:ILE:HG21 | 1:154:A:LEU:HB3  | 9        | 0.39          |
| (1,1236) | 1:81:A:ILE:HG22 | 1:154:A:LEU:HB3  | 9        | 0.39          |
| (1,1236) | 1:81:A:ILE:HG23 | 1:154:A:LEU:HB3  | 9        | 0.39          |
| (1,1228) | 1:81:A:ILE:HG21 | 1:82:A:THR:HA    | 2        | 0.39          |
| (1,1228) | 1:81:A:ILE:HG22 | 1:82:A:THR:HA    | 2        | 0.39          |
| (1,1228) | 1:81:A:ILE:HG23 | 1:82:A:THR:HA    | 2        | 0.39          |
| (1,1189) | 1:80:A:GLN:HG2  | 1:98:A:THR:HG21  | 2        | 0.39          |
| (1,1189) | 1:80:A:GLN:HG2  | 1:98:A:THR:HG22  | 2        | 0.39          |
| (1,1189) | 1:80:A:GLN:HG2  | 1:98:A:THR:HG23  | 2        | 0.39          |
| (1,1189) | 1:80:A:GLN:HG3  | 1:98:A:THR:HG21  | 2        | 0.39          |
| (1,1189) | 1:80:A:GLN:HG3  | 1:98:A:THR:HG22  | 2        | 0.39          |
| (1,1189) | 1:80:A:GLN:HG3  | 1:98:A:THR:HG23  | 2        | 0.39          |
| (1,1097) | 1:77:A:LEU:HD11 | 1:160:A:TYR:HB3  | 8        | 0.39          |
| (1,1097) | 1:77:A:LEU:HD12 | 1:160:A:TYR:HB3  | 8        | 0.39          |
| (1,1097) | 1:77:A:LEU:HD13 | 1:160:A:TYR:HB3  | 8        | 0.39          |
| (1,1097) | 1:77:A:LEU:HD21 | 1:160:A:TYR:HB3  | 8        | 0.39          |
| (1,1097) | 1:77:A:LEU:HD22 | 1:160:A:TYR:HB3  | 8        | 0.39          |
| (1,1097) | 1:77:A:LEU:HD23 | 1:160:A:TYR:HB3  | 8        | 0.39          |
| (1,1091) | 1:77:A:LEU:HD11 | 1:103:A:SER:HA   | 8        | 0.39          |
| (1,1091) | 1:77:A:LEU:HD12 | 1:103:A:SER:HA   | 8        | 0.39          |
| (1,1091) | 1:77:A:LEU:HD13 | 1:103:A:SER:HA   | 8        | 0.39          |
| (1,1091) | 1:77:A:LEU:HD21 | 1:103:A:SER:HA   | 8        | 0.39          |
| (1,1091) | 1:77:A:LEU:HD22 | 1:103:A:SER:HA   | 8        | 0.39          |
| (1,1091) | 1:77:A:LEU:HD23 | 1:103:A:SER:HA   | 8        | 0.39          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,731) | 1:62:A:VAL:HG21 | 1:177:A:PHE:HD1 | 2        | 0.39          |
| (1,731) | 1:62:A:VAL:HG21 | 1:177:A:PHE:HD2 | 2        | 0.39          |
| (1,731) | 1:62:A:VAL:HG22 | 1:177:A:PHE:HD1 | 2        | 0.39          |
| (1,731) | 1:62:A:VAL:HG22 | 1:177:A:PHE:HD2 | 2        | 0.39          |
| (1,731) | 1:62:A:VAL:HG23 | 1:177:A:PHE:HD1 | 2        | 0.39          |
| (1,731) | 1:62:A:VAL:HG23 | 1:177:A:PHE:HD2 | 2        | 0.39          |
| (1,731) | 1:62:A:VAL:HG21 | 1:177:A:PHE:HD1 | 10       | 0.39          |
| (1,731) | 1:62:A:VAL:HG21 | 1:177:A:PHE:HD2 | 10       | 0.39          |
| (1,731) | 1:62:A:VAL:HG22 | 1:177:A:PHE:HD1 | 10       | 0.39          |
| (1,731) | 1:62:A:VAL:HG22 | 1:177:A:PHE:HD2 | 10       | 0.39          |
| (1,731) | 1:62:A:VAL:HG23 | 1:177:A:PHE:HD1 | 10       | 0.39          |
| (1,731) | 1:62:A:VAL:HG23 | 1:177:A:PHE:HD2 | 10       | 0.39          |
| (1,599) | 1:53:A:ASP:H    | 1:55:A:VAL:HG11 | 3        | 0.39          |
| (1,599) | 1:53:A:ASP:H    | 1:55:A:VAL:HG12 | 3        | 0.39          |
| (1,599) | 1:53:A:ASP:H    | 1:55:A:VAL:HG13 | 3        | 0.39          |
| (1,582) | 1:51:A:ILE:HG21 | 1:55:A:VAL:H    | 1        | 0.39          |
| (1,582) | 1:51:A:ILE:HG22 | 1:55:A:VAL:H    | 1        | 0.39          |
| (1,582) | 1:51:A:ILE:HG23 | 1:55:A:VAL:H    | 1        | 0.39          |
| (1,581) | 1:51:A:ILE:HG21 | 1:53:A:ASP:H    | 6        | 0.39          |
| (1,581) | 1:51:A:ILE:HG22 | 1:53:A:ASP:H    | 6        | 0.39          |
| (1,581) | 1:51:A:ILE:HG23 | 1:53:A:ASP:H    | 6        | 0.39          |
| (1,580) | 1:51:A:ILE:HG21 | 1:53:A:ASP:H    | 6        | 0.39          |
| (1,580) | 1:51:A:ILE:HG22 | 1:53:A:ASP:H    | 6        | 0.39          |
| (1,580) | 1:51:A:ILE:HG23 | 1:53:A:ASP:H    | 6        | 0.39          |
| (1,485) | 1:48:A:ILE:HG13 | 1:48:A:ILE:HG21 | 5        | 0.39          |
| (1,485) | 1:48:A:ILE:HG13 | 1:48:A:ILE:HG22 | 5        | 0.39          |
| (1,485) | 1:48:A:ILE:HG13 | 1:48:A:ILE:HG23 | 5        | 0.39          |
| (1,296) | 1:38:A:ALA:HB1  | 1:39:A:GLN:H    | 7        | 0.39          |
| (1,296) | 1:38:A:ALA:HB2  | 1:39:A:GLN:H    | 7        | 0.39          |
| (1,296) | 1:38:A:ALA:HB3  | 1:39:A:GLN:H    | 7        | 0.39          |
| (1,289) | 1:37:A:GLY:HA3  | 1:37:A:GLY:H    | 3        | 0.39          |
| (1,289) | 1:37:A:GLY:HA3  | 1:37:A:GLY:H    | 9        | 0.39          |
| (1,286) | 1:36:A:ALA:HA   | 1:37:A:GLY:H    | 5        | 0.39          |
| (1,260) | 1:33:A:THR:HG21 | 1:34:A:PRO:HD3  | 2        | 0.39          |
| (1,260) | 1:33:A:THR:HG22 | 1:34:A:PRO:HD3  | 2        | 0.39          |
| (1,260) | 1:33:A:THR:HG23 | 1:34:A:PRO:HD3  | 2        | 0.39          |
| (1,209) | 1:32:A:ILE:HA   | 1:32:A:ILE:HG21 | 6        | 0.39          |
| (1,209) | 1:32:A:ILE:HA   | 1:32:A:ILE:HG22 | 6        | 0.39          |
| (1,209) | 1:32:A:ILE:HA   | 1:32:A:ILE:HG23 | 6        | 0.39          |
| (1,23)  | 1:23:A:ILE:HA   | 1:23:A:ILE:HD11 | 7        | 0.39          |
| (1,23)  | 1:23:A:ILE:HA   | 1:23:A:ILE:HD12 | 7        | 0.39          |
| (1,23)  | 1:23:A:ILE:HA   | 1:23:A:ILE:HD13 | 7        | 0.39          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,23)   | 1:23:A:ILE:HA    | 1:23:A:ILE:HD11  | 8        | 0.39          |
| (1,23)   | 1:23:A:ILE:HA    | 1:23:A:ILE:HD12  | 8        | 0.39          |
| (1,23)   | 1:23:A:ILE:HA    | 1:23:A:ILE:HD13  | 8        | 0.39          |
| (1,11)   | 1:20:A:SER:HB2   | 1:21:A:GLU:H     | 8        | 0.39          |
| (1,11)   | 1:20:A:SER:HB3   | 1:21:A:GLU:H     | 8        | 0.39          |
| (1,3)    | 1:16:A:ALA:HB1   | 1:16:A:ALA:H     | 6        | 0.39          |
| (1,3)    | 1:16:A:ALA:HB2   | 1:16:A:ALA:H     | 6        | 0.39          |
| (1,3)    | 1:16:A:ALA:HB3   | 1:16:A:ALA:H     | 6        | 0.39          |
| (2,756)  | 1:167:A:LEU:H    | 1:167:A:LEU:HD21 | 3        | 0.38          |
| (2,756)  | 1:167:A:LEU:H    | 1:167:A:LEU:HD22 | 3        | 0.38          |
| (2,756)  | 1:167:A:LEU:H    | 1:167:A:LEU:HD23 | 3        | 0.38          |
| (2,754)  | 1:167:A:LEU:HD21 | 1:167:A:LEU:H    | 3        | 0.38          |
| (2,754)  | 1:167:A:LEU:HD22 | 1:167:A:LEU:H    | 3        | 0.38          |
| (2,754)  | 1:167:A:LEU:HD23 | 1:167:A:LEU:H    | 3        | 0.38          |
| (2,729)  | 1:151:A:VAL:H    | 1:153:A:ILE:HD11 | 2        | 0.38          |
| (2,729)  | 1:151:A:VAL:H    | 1:153:A:ILE:HD12 | 2        | 0.38          |
| (2,729)  | 1:151:A:VAL:H    | 1:153:A:ILE:HD13 | 2        | 0.38          |
| (1,2098) | 1:153:A:ILE:HB   | 1:153:A:ILE:HG21 | 1        | 0.38          |
| (1,2098) | 1:153:A:ILE:HB   | 1:153:A:ILE:HG22 | 1        | 0.38          |
| (1,2098) | 1:153:A:ILE:HB   | 1:153:A:ILE:HG23 | 1        | 0.38          |
| (1,2098) | 1:153:A:ILE:HB   | 1:153:A:ILE:HG21 | 2        | 0.38          |
| (1,2098) | 1:153:A:ILE:HB   | 1:153:A:ILE:HG22 | 2        | 0.38          |
| (1,2098) | 1:153:A:ILE:HB   | 1:153:A:ILE:HG23 | 2        | 0.38          |
| (1,2098) | 1:153:A:ILE:HB   | 1:153:A:ILE:HG21 | 4        | 0.38          |
| (1,2098) | 1:153:A:ILE:HB   | 1:153:A:ILE:HG22 | 4        | 0.38          |
| (1,2098) | 1:153:A:ILE:HB   | 1:153:A:ILE:HG23 | 4        | 0.38          |
| (1,2098) | 1:153:A:ILE:HB   | 1:153:A:ILE:HG21 | 5        | 0.38          |
| (1,2098) | 1:153:A:ILE:HB   | 1:153:A:ILE:HG22 | 5        | 0.38          |
| (1,2098) | 1:153:A:ILE:HB   | 1:153:A:ILE:HG23 | 5        | 0.38          |
| (1,2098) | 1:153:A:ILE:HB   | 1:153:A:ILE:HG21 | 7        | 0.38          |
| (1,2098) | 1:153:A:ILE:HB   | 1:153:A:ILE:HG22 | 7        | 0.38          |
| (1,2098) | 1:153:A:ILE:HB   | 1:153:A:ILE:HG23 | 7        | 0.38          |
| (1,2093) | 1:153:A:ILE:HA   | 1:153:A:ILE:HG21 | 7        | 0.38          |
| (1,2093) | 1:153:A:ILE:HA   | 1:153:A:ILE:HG22 | 7        | 0.38          |
| (1,2093) | 1:153:A:ILE:HA   | 1:153:A:ILE:HG23 | 7        | 0.38          |
| (1,2067) | 1:148:A:THR:HB   | 1:148:A:THR:HG21 | 8        | 0.38          |
| (1,2067) | 1:148:A:THR:HB   | 1:148:A:THR:HG22 | 8        | 0.38          |
| (1,2067) | 1:148:A:THR:HB   | 1:148:A:THR:HG23 | 8        | 0.38          |
| (1,2015) | 1:142:A:ILE:HG21 | 1:144:A:VAL:H    | 6        | 0.38          |
| (1,2015) | 1:142:A:ILE:HG22 | 1:144:A:VAL:H    | 6        | 0.38          |
| (1,2015) | 1:142:A:ILE:HG23 | 1:144:A:VAL:H    | 6        | 0.38          |
| (1,1953) | 1:136:A:PRO:HG3  | 1:155:A:ASN:HD21 | 1        | 0.38          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1953) | 1:136:A:PRO:HG3  | 1:155:A:ASN:HD22 | 1        | 0.38          |
| (1,1941) | 1:135:A:VAL:HG21 | 1:135:A:VAL:H    | 1        | 0.38          |
| (1,1941) | 1:135:A:VAL:HG22 | 1:135:A:VAL:H    | 1        | 0.38          |
| (1,1941) | 1:135:A:VAL:HG23 | 1:135:A:VAL:H    | 1        | 0.38          |
| (1,1941) | 1:135:A:VAL:HG21 | 1:135:A:VAL:H    | 2        | 0.38          |
| (1,1941) | 1:135:A:VAL:HG22 | 1:135:A:VAL:H    | 2        | 0.38          |
| (1,1941) | 1:135:A:VAL:HG23 | 1:135:A:VAL:H    | 2        | 0.38          |
| (1,1941) | 1:135:A:VAL:HG21 | 1:135:A:VAL:H    | 5        | 0.38          |
| (1,1941) | 1:135:A:VAL:HG22 | 1:135:A:VAL:H    | 5        | 0.38          |
| (1,1941) | 1:135:A:VAL:HG23 | 1:135:A:VAL:H    | 5        | 0.38          |
| (1,1695) | 1:115:A:LYS:HA   | 1:118:A:ILE:HD11 | 9        | 0.38          |
| (1,1695) | 1:115:A:LYS:HA   | 1:118:A:ILE:HD12 | 9        | 0.38          |
| (1,1695) | 1:115:A:LYS:HA   | 1:118:A:ILE:HD13 | 9        | 0.38          |
| (1,1475) | 1:95:A:PHE:HB2   | 1:96:A:SER:H     | 4        | 0.38          |
| (1,1475) | 1:95:A:PHE:HB3   | 1:96:A:SER:H     | 4        | 0.38          |
| (1,1451) | 1:91:A:ALA:HB1   | 1:91:A:ALA:H     | 1        | 0.38          |
| (1,1451) | 1:91:A:ALA:HB2   | 1:91:A:ALA:H     | 1        | 0.38          |
| (1,1451) | 1:91:A:ALA:HB3   | 1:91:A:ALA:H     | 1        | 0.38          |
| (1,1451) | 1:91:A:ALA:HB1   | 1:91:A:ALA:H     | 4        | 0.38          |
| (1,1451) | 1:91:A:ALA:HB2   | 1:91:A:ALA:H     | 4        | 0.38          |
| (1,1451) | 1:91:A:ALA:HB3   | 1:91:A:ALA:H     | 4        | 0.38          |
| (1,1451) | 1:91:A:ALA:HB1   | 1:91:A:ALA:H     | 5        | 0.38          |
| (1,1451) | 1:91:A:ALA:HB2   | 1:91:A:ALA:H     | 5        | 0.38          |
| (1,1451) | 1:91:A:ALA:HB3   | 1:91:A:ALA:H     | 5        | 0.38          |
| (1,1451) | 1:91:A:ALA:HB1   | 1:91:A:ALA:H     | 8        | 0.38          |
| (1,1451) | 1:91:A:ALA:HB2   | 1:91:A:ALA:H     | 8        | 0.38          |
| (1,1451) | 1:91:A:ALA:HB3   | 1:91:A:ALA:H     | 8        | 0.38          |
| (1,1236) | 1:81:A:ILE:HG21  | 1:154:A:LEU:HB3  | 10       | 0.38          |
| (1,1236) | 1:81:A:ILE:HG22  | 1:154:A:LEU:HB3  | 10       | 0.38          |
| (1,1236) | 1:81:A:ILE:HG23  | 1:154:A:LEU:HB3  | 10       | 0.38          |
| (1,1162) | 1:79:A:ILE:HG13  | 1:80:A:GLN:H     | 4        | 0.38          |
| (1,1088) | 1:77:A:LEU:HD11  | 1:78:A:GLN:H     | 7        | 0.38          |
| (1,1088) | 1:77:A:LEU:HD12  | 1:78:A:GLN:H     | 7        | 0.38          |
| (1,1088) | 1:77:A:LEU:HD13  | 1:78:A:GLN:H     | 7        | 0.38          |
| (1,1088) | 1:77:A:LEU:HD21  | 1:78:A:GLN:H     | 7        | 0.38          |
| (1,1088) | 1:77:A:LEU:HD22  | 1:78:A:GLN:H     | 7        | 0.38          |
| (1,1088) | 1:77:A:LEU:HD23  | 1:78:A:GLN:H     | 7        | 0.38          |
| (1,837)  | 1:66:A:ASN:HB2   | 1:66:A:ASN:HD22  | 6        | 0.38          |
| (1,837)  | 1:66:A:ASN:HB2   | 1:66:A:ASN:HD22  | 7        | 0.38          |
| (1,520)  | 1:49:A:VAL:HB    | 1:152:A:ALA:HB1  | 2        | 0.38          |
| (1,520)  | 1:49:A:VAL:HB    | 1:152:A:ALA:HB2  | 2        | 0.38          |
| (1,520)  | 1:49:A:VAL:HB    | 1:152:A:ALA:HB3  | 2        | 0.38          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,520)  | 1:49:A:VAL:HB   | 1:152:A:ALA:HB1  | 9        | 0.38          |
| (1,520)  | 1:49:A:VAL:HB   | 1:152:A:ALA:HB2  | 9        | 0.38          |
| (1,520)  | 1:49:A:VAL:HB   | 1:152:A:ALA:HB3  | 9        | 0.38          |
| (1,269)  | 1:34:A:PRO:HD3  | 1:168:A:PHE:HD1  | 2        | 0.38          |
| (1,269)  | 1:34:A:PRO:HD3  | 1:168:A:PHE:HD2  | 2        | 0.38          |
| (1,232)  | 1:32:A:ILE:HG21 | 1:32:A:ILE:HD11  | 10       | 0.38          |
| (1,232)  | 1:32:A:ILE:HG21 | 1:32:A:ILE:HD12  | 10       | 0.38          |
| (1,232)  | 1:32:A:ILE:HG21 | 1:32:A:ILE:HD13  | 10       | 0.38          |
| (1,232)  | 1:32:A:ILE:HG22 | 1:32:A:ILE:HD11  | 10       | 0.38          |
| (1,232)  | 1:32:A:ILE:HG22 | 1:32:A:ILE:HD12  | 10       | 0.38          |
| (1,232)  | 1:32:A:ILE:HG22 | 1:32:A:ILE:HD13  | 10       | 0.38          |
| (1,232)  | 1:32:A:ILE:HG23 | 1:32:A:ILE:HD11  | 10       | 0.38          |
| (1,232)  | 1:32:A:ILE:HG23 | 1:32:A:ILE:HD12  | 10       | 0.38          |
| (1,232)  | 1:32:A:ILE:HG23 | 1:32:A:ILE:HD13  | 10       | 0.38          |
| (1,209)  | 1:32:A:ILE:HA   | 1:32:A:ILE:HG21  | 2        | 0.38          |
| (1,209)  | 1:32:A:ILE:HA   | 1:32:A:ILE:HG22  | 2        | 0.38          |
| (1,209)  | 1:32:A:ILE:HA   | 1:32:A:ILE:HG23  | 2        | 0.38          |
| (2,768)  | 1:173:A:VAL:HB  | 1:175:A:PHE:HE1  | 7        | 0.37          |
| (2,768)  | 1:173:A:VAL:HB  | 1:175:A:PHE:HE2  | 7        | 0.37          |
| (2,725)  | 1:145:A:TYR:HD1 | 1:147:A:GLU:H    | 10       | 0.37          |
| (2,725)  | 1:145:A:TYR:HD2 | 1:147:A:GLU:H    | 10       | 0.37          |
| (2,724)  | 1:145:A:TYR:HD1 | 1:147:A:GLU:HG2  | 7        | 0.37          |
| (2,724)  | 1:145:A:TYR:HD1 | 1:147:A:GLU:HG3  | 7        | 0.37          |
| (2,724)  | 1:145:A:TYR:HD2 | 1:147:A:GLU:HG2  | 7        | 0.37          |
| (2,724)  | 1:145:A:TYR:HD2 | 1:147:A:GLU:HG3  | 7        | 0.37          |
| (1,2286) | 1:168:A:PHE:HD1 | 1:168:A:PHE:H    | 10       | 0.37          |
| (1,2286) | 1:168:A:PHE:HD2 | 1:168:A:PHE:H    | 10       | 0.37          |
| (1,2098) | 1:153:A:ILE:HB  | 1:153:A:ILE:HG21 | 3        | 0.37          |
| (1,2098) | 1:153:A:ILE:HB  | 1:153:A:ILE:HG22 | 3        | 0.37          |
| (1,2098) | 1:153:A:ILE:HB  | 1:153:A:ILE:HG23 | 3        | 0.37          |
| (1,2098) | 1:153:A:ILE:HB  | 1:153:A:ILE:HG21 | 6        | 0.37          |
| (1,2098) | 1:153:A:ILE:HB  | 1:153:A:ILE:HG22 | 6        | 0.37          |
| (1,2098) | 1:153:A:ILE:HB  | 1:153:A:ILE:HG23 | 6        | 0.37          |
| (1,2098) | 1:153:A:ILE:HB  | 1:153:A:ILE:HG21 | 8        | 0.37          |
| (1,2098) | 1:153:A:ILE:HB  | 1:153:A:ILE:HG22 | 8        | 0.37          |
| (1,2098) | 1:153:A:ILE:HB  | 1:153:A:ILE:HG23 | 8        | 0.37          |
| (1,2098) | 1:153:A:ILE:HB  | 1:153:A:ILE:HG21 | 9        | 0.37          |
| (1,2098) | 1:153:A:ILE:HB  | 1:153:A:ILE:HG22 | 9        | 0.37          |
| (1,2098) | 1:153:A:ILE:HB  | 1:153:A:ILE:HG23 | 9        | 0.37          |
| (1,2093) | 1:153:A:ILE:HA  | 1:153:A:ILE:HG21 | 9        | 0.37          |
| (1,2093) | 1:153:A:ILE:HA  | 1:153:A:ILE:HG22 | 9        | 0.37          |
| (1,2093) | 1:153:A:ILE:HA  | 1:153:A:ILE:HG23 | 9        | 0.37          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2067) | 1:148:A:THR:HB   | 1:148:A:THR:HG21 | 1        | 0.37          |
| (1,2067) | 1:148:A:THR:HB   | 1:148:A:THR:HG22 | 1        | 0.37          |
| (1,2067) | 1:148:A:THR:HB   | 1:148:A:THR:HG23 | 1        | 0.37          |
| (1,2067) | 1:148:A:THR:HB   | 1:148:A:THR:HG21 | 2        | 0.37          |
| (1,2067) | 1:148:A:THR:HB   | 1:148:A:THR:HG22 | 2        | 0.37          |
| (1,2067) | 1:148:A:THR:HB   | 1:148:A:THR:HG23 | 2        | 0.37          |
| (1,2067) | 1:148:A:THR:HB   | 1:148:A:THR:HG21 | 4        | 0.37          |
| (1,2067) | 1:148:A:THR:HB   | 1:148:A:THR:HG22 | 4        | 0.37          |
| (1,2067) | 1:148:A:THR:HB   | 1:148:A:THR:HG23 | 4        | 0.37          |
| (1,2067) | 1:148:A:THR:HB   | 1:148:A:THR:HG21 | 5        | 0.37          |
| (1,2067) | 1:148:A:THR:HB   | 1:148:A:THR:HG22 | 5        | 0.37          |
| (1,2067) | 1:148:A:THR:HB   | 1:148:A:THR:HG23 | 5        | 0.37          |
| (1,2067) | 1:148:A:THR:HB   | 1:148:A:THR:HG21 | 6        | 0.37          |
| (1,2067) | 1:148:A:THR:HB   | 1:148:A:THR:HG22 | 6        | 0.37          |
| (1,2067) | 1:148:A:THR:HB   | 1:148:A:THR:HG23 | 6        | 0.37          |
| (1,2067) | 1:148:A:THR:HB   | 1:148:A:THR:HG21 | 7        | 0.37          |
| (1,2067) | 1:148:A:THR:HB   | 1:148:A:THR:HG22 | 7        | 0.37          |
| (1,2067) | 1:148:A:THR:HB   | 1:148:A:THR:HG23 | 7        | 0.37          |
| (1,2067) | 1:148:A:THR:HB   | 1:148:A:THR:HG21 | 9        | 0.37          |
| (1,2067) | 1:148:A:THR:HB   | 1:148:A:THR:HG22 | 9        | 0.37          |
| (1,2067) | 1:148:A:THR:HB   | 1:148:A:THR:HG23 | 9        | 0.37          |
| (1,2038) | 1:144:A:VAL:HG21 | 1:144:A:VAL:H    | 2        | 0.37          |
| (1,2038) | 1:144:A:VAL:HG22 | 1:144:A:VAL:H    | 2        | 0.37          |
| (1,2038) | 1:144:A:VAL:HG23 | 1:144:A:VAL:H    | 2        | 0.37          |
| (1,1953) | 1:136:A:PRO:HG3  | 1:155:A:ASN:HD21 | 7        | 0.37          |
| (1,1953) | 1:136:A:PRO:HG3  | 1:155:A:ASN:HD22 | 7        | 0.37          |
| (1,1818) | 1:131:A:THR:HG21 | 1:131:A:THR:H    | 4        | 0.37          |
| (1,1818) | 1:131:A:THR:HG22 | 1:131:A:THR:H    | 4        | 0.37          |
| (1,1818) | 1:131:A:THR:HG23 | 1:131:A:THR:H    | 4        | 0.37          |
| (1,1816) | 1:131:A:THR:HB   | 1:131:A:THR:HG21 | 1        | 0.37          |
| (1,1816) | 1:131:A:THR:HB   | 1:131:A:THR:HG22 | 1        | 0.37          |
| (1,1816) | 1:131:A:THR:HB   | 1:131:A:THR:HG23 | 1        | 0.37          |
| (1,1816) | 1:131:A:THR:HB   | 1:131:A:THR:HG21 | 2        | 0.37          |
| (1,1816) | 1:131:A:THR:HB   | 1:131:A:THR:HG22 | 2        | 0.37          |
| (1,1816) | 1:131:A:THR:HB   | 1:131:A:THR:HG23 | 2        | 0.37          |
| (1,1816) | 1:131:A:THR:HB   | 1:131:A:THR:HG21 | 3        | 0.37          |
| (1,1816) | 1:131:A:THR:HB   | 1:131:A:THR:HG22 | 3        | 0.37          |
| (1,1816) | 1:131:A:THR:HB   | 1:131:A:THR:HG23 | 3        | 0.37          |
| (1,1816) | 1:131:A:THR:HB   | 1:131:A:THR:HG21 | 4        | 0.37          |
| (1,1816) | 1:131:A:THR:HB   | 1:131:A:THR:HG22 | 4        | 0.37          |
| (1,1816) | 1:131:A:THR:HB   | 1:131:A:THR:HG23 | 4        | 0.37          |
| (1,1816) | 1:131:A:THR:HB   | 1:131:A:THR:HG21 | 5        | 0.37          |

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| Key      | Atom-1         | Atom-2           | Model ID | Violation (Å) |
|----------|----------------|------------------|----------|---------------|
| (1,1816) | 1:131:A:THR:HB | 1:131:A:THR:HG22 | 5        | 0.37          |
| (1,1816) | 1:131:A:THR:HB | 1:131:A:THR:HG23 | 5        | 0.37          |
| (1,1816) | 1:131:A:THR:HB | 1:131:A:THR:HG21 | 6        | 0.37          |
| (1,1816) | 1:131:A:THR:HB | 1:131:A:THR:HG22 | 6        | 0.37          |
| (1,1816) | 1:131:A:THR:HB | 1:131:A:THR:HG23 | 6        | 0.37          |
| (1,1816) | 1:131:A:THR:HB | 1:131:A:THR:HG21 | 7        | 0.37          |
| (1,1816) | 1:131:A:THR:HB | 1:131:A:THR:HG22 | 7        | 0.37          |
| (1,1816) | 1:131:A:THR:HB | 1:131:A:THR:HG23 | 7        | 0.37          |
| (1,1816) | 1:131:A:THR:HB | 1:131:A:THR:HG21 | 8        | 0.37          |
| (1,1816) | 1:131:A:THR:HB | 1:131:A:THR:HG22 | 8        | 0.37          |
| (1,1816) | 1:131:A:THR:HB | 1:131:A:THR:HG23 | 8        | 0.37          |
| (1,1816) | 1:131:A:THR:HB | 1:131:A:THR:HG21 | 9        | 0.37          |
| (1,1816) | 1:131:A:THR:HB | 1:131:A:THR:HG22 | 9        | 0.37          |
| (1,1816) | 1:131:A:THR:HB | 1:131:A:THR:HG23 | 9        | 0.37          |
| (1,1816) | 1:131:A:THR:HB | 1:131:A:THR:HG21 | 10       | 0.37          |
| (1,1816) | 1:131:A:THR:HB | 1:131:A:THR:HG22 | 10       | 0.37          |
| (1,1816) | 1:131:A:THR:HB | 1:131:A:THR:HG23 | 10       | 0.37          |
| (1,1451) | 1:91:A:ALA:HB1 | 1:91:A:ALA:H     | 3        | 0.37          |
| (1,1451) | 1:91:A:ALA:HB2 | 1:91:A:ALA:H     | 3        | 0.37          |
| (1,1451) | 1:91:A:ALA:HB3 | 1:91:A:ALA:H     | 3        | 0.37          |
| (1,1451) | 1:91:A:ALA:HB1 | 1:91:A:ALA:H     | 6        | 0.37          |
| (1,1451) | 1:91:A:ALA:HB2 | 1:91:A:ALA:H     | 6        | 0.37          |
| (1,1451) | 1:91:A:ALA:HB3 | 1:91:A:ALA:H     | 6        | 0.37          |
| (1,1451) | 1:91:A:ALA:HB1 | 1:91:A:ALA:H     | 7        | 0.37          |
| (1,1451) | 1:91:A:ALA:HB2 | 1:91:A:ALA:H     | 7        | 0.37          |
| (1,1451) | 1:91:A:ALA:HB3 | 1:91:A:ALA:H     | 7        | 0.37          |
| (1,1451) | 1:91:A:ALA:HB1 | 1:91:A:ALA:H     | 10       | 0.37          |
| (1,1451) | 1:91:A:ALA:HB2 | 1:91:A:ALA:H     | 10       | 0.37          |
| (1,1451) | 1:91:A:ALA:HB3 | 1:91:A:ALA:H     | 10       | 0.37          |
| (1,1447) | 1:90:A:THR:HB  | 1:90:A:THR:HG21  | 2        | 0.37          |
| (1,1447) | 1:90:A:THR:HB  | 1:90:A:THR:HG22  | 2        | 0.37          |
| (1,1447) | 1:90:A:THR:HB  | 1:90:A:THR:HG23  | 2        | 0.37          |
| (1,1447) | 1:90:A:THR:HB  | 1:90:A:THR:HG21  | 4        | 0.37          |
| (1,1447) | 1:90:A:THR:HB  | 1:90:A:THR:HG22  | 4        | 0.37          |
| (1,1447) | 1:90:A:THR:HB  | 1:90:A:THR:HG23  | 4        | 0.37          |
| (1,1447) | 1:90:A:THR:HB  | 1:90:A:THR:HG21  | 6        | 0.37          |
| (1,1447) | 1:90:A:THR:HB  | 1:90:A:THR:HG22  | 6        | 0.37          |
| (1,1447) | 1:90:A:THR:HB  | 1:90:A:THR:HG23  | 6        | 0.37          |
| (1,1447) | 1:90:A:THR:HB  | 1:90:A:THR:HG21  | 7        | 0.37          |
| (1,1447) | 1:90:A:THR:HB  | 1:90:A:THR:HG22  | 7        | 0.37          |
| (1,1447) | 1:90:A:THR:HB  | 1:90:A:THR:HG23  | 7        | 0.37          |
| (1,1447) | 1:90:A:THR:HB  | 1:90:A:THR:HG21  | 10       | 0.37          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1447) | 1:90:A:THR:HB   | 1:90:A:THR:HG22  | 10       | 0.37          |
| (1,1447) | 1:90:A:THR:HB   | 1:90:A:THR:HG23  | 10       | 0.37          |
| (1,1343) | 1:85:A:TYR:HE1  | 1:152:A:ALA:HA   | 1        | 0.37          |
| (1,1343) | 1:85:A:TYR:HE2  | 1:152:A:ALA:HA   | 1        | 0.37          |
| (1,1189) | 1:80:A:GLN:HG2  | 1:98:A:THR:HG21  | 9        | 0.37          |
| (1,1189) | 1:80:A:GLN:HG2  | 1:98:A:THR:HG22  | 9        | 0.37          |
| (1,1189) | 1:80:A:GLN:HG2  | 1:98:A:THR:HG23  | 9        | 0.37          |
| (1,1189) | 1:80:A:GLN:HG3  | 1:98:A:THR:HG21  | 9        | 0.37          |
| (1,1189) | 1:80:A:GLN:HG3  | 1:98:A:THR:HG22  | 9        | 0.37          |
| (1,1189) | 1:80:A:GLN:HG3  | 1:98:A:THR:HG23  | 9        | 0.37          |
| (1,1050) | 1:76:A:TYR:HA   | 1:76:A:TYR:HD1   | 10       | 0.37          |
| (1,1050) | 1:76:A:TYR:HA   | 1:76:A:TYR:HD2   | 10       | 0.37          |
| (1,731)  | 1:62:A:VAL:HG21 | 1:177:A:PHE:HD1  | 6        | 0.37          |
| (1,731)  | 1:62:A:VAL:HG21 | 1:177:A:PHE:HD2  | 6        | 0.37          |
| (1,731)  | 1:62:A:VAL:HG22 | 1:177:A:PHE:HD1  | 6        | 0.37          |
| (1,731)  | 1:62:A:VAL:HG22 | 1:177:A:PHE:HD2  | 6        | 0.37          |
| (1,731)  | 1:62:A:VAL:HG23 | 1:177:A:PHE:HD1  | 6        | 0.37          |
| (1,731)  | 1:62:A:VAL:HG23 | 1:177:A:PHE:HD2  | 6        | 0.37          |
| (1,655)  | 1:58:A:VAL:H    | 1:113:A:LEU:HD11 | 1        | 0.37          |
| (1,655)  | 1:58:A:VAL:H    | 1:113:A:LEU:HD12 | 1        | 0.37          |
| (1,655)  | 1:58:A:VAL:H    | 1:113:A:LEU:HD13 | 1        | 0.37          |
| (1,651)  | 1:58:A:VAL:HG11 | 1:59:A:LYS:H     | 2        | 0.37          |
| (1,651)  | 1:58:A:VAL:HG12 | 1:59:A:LYS:H     | 2        | 0.37          |
| (1,651)  | 1:58:A:VAL:HG13 | 1:59:A:LYS:H     | 2        | 0.37          |
| (1,651)  | 1:58:A:VAL:HG21 | 1:59:A:LYS:H     | 2        | 0.37          |
| (1,651)  | 1:58:A:VAL:HG22 | 1:59:A:LYS:H     | 2        | 0.37          |
| (1,651)  | 1:58:A:VAL:HG23 | 1:59:A:LYS:H     | 2        | 0.37          |
| (1,610)  | 1:55:A:VAL:HA   | 1:55:A:VAL:HG11  | 1        | 0.37          |
| (1,610)  | 1:55:A:VAL:HA   | 1:55:A:VAL:HG12  | 1        | 0.37          |
| (1,610)  | 1:55:A:VAL:HA   | 1:55:A:VAL:HG13  | 1        | 0.37          |
| (1,520)  | 1:49:A:VAL:HB   | 1:152:A:ALA:HB1  | 1        | 0.37          |
| (1,520)  | 1:49:A:VAL:HB   | 1:152:A:ALA:HB2  | 1        | 0.37          |
| (1,520)  | 1:49:A:VAL:HB   | 1:152:A:ALA:HB3  | 1        | 0.37          |
| (1,520)  | 1:49:A:VAL:HB   | 1:152:A:ALA:HB1  | 4        | 0.37          |
| (1,520)  | 1:49:A:VAL:HB   | 1:152:A:ALA:HB2  | 4        | 0.37          |
| (1,520)  | 1:49:A:VAL:HB   | 1:152:A:ALA:HB3  | 4        | 0.37          |
| (1,520)  | 1:49:A:VAL:HB   | 1:152:A:ALA:HB1  | 7        | 0.37          |
| (1,520)  | 1:49:A:VAL:HB   | 1:152:A:ALA:HB2  | 7        | 0.37          |
| (1,520)  | 1:49:A:VAL:HB   | 1:152:A:ALA:HB3  | 7        | 0.37          |
| (1,520)  | 1:49:A:VAL:HB   | 1:152:A:ALA:HB1  | 8        | 0.37          |
| (1,520)  | 1:49:A:VAL:HB   | 1:152:A:ALA:HB2  | 8        | 0.37          |
| (1,520)  | 1:49:A:VAL:HB   | 1:152:A:ALA:HB3  | 8        | 0.37          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,487)  | 1:48:A:ILE:HG12  | 1:48:A:ILE:HG21  | 2        | 0.37          |
| (1,487)  | 1:48:A:ILE:HG12  | 1:48:A:ILE:HG22  | 2        | 0.37          |
| (1,487)  | 1:48:A:ILE:HG12  | 1:48:A:ILE:HG23  | 2        | 0.37          |
| (1,487)  | 1:48:A:ILE:HG12  | 1:48:A:ILE:HG21  | 8        | 0.37          |
| (1,487)  | 1:48:A:ILE:HG12  | 1:48:A:ILE:HG22  | 8        | 0.37          |
| (1,487)  | 1:48:A:ILE:HG12  | 1:48:A:ILE:HG23  | 8        | 0.37          |
| (1,287)  | 1:36:A:ALA:HB1   | 1:36:A:ALA:H     | 4        | 0.37          |
| (1,287)  | 1:36:A:ALA:HB2   | 1:36:A:ALA:H     | 4        | 0.37          |
| (1,287)  | 1:36:A:ALA:HB3   | 1:36:A:ALA:H     | 4        | 0.37          |
| (1,286)  | 1:36:A:ALA:HA    | 1:37:A:GLY:H     | 1        | 0.37          |
| (1,209)  | 1:32:A:ILE:HA    | 1:32:A:ILE:HG21  | 1        | 0.37          |
| (1,209)  | 1:32:A:ILE:HA    | 1:32:A:ILE:HG22  | 1        | 0.37          |
| (1,209)  | 1:32:A:ILE:HA    | 1:32:A:ILE:HG23  | 1        | 0.37          |
| (1,209)  | 1:32:A:ILE:HA    | 1:32:A:ILE:HG21  | 8        | 0.37          |
| (1,209)  | 1:32:A:ILE:HA    | 1:32:A:ILE:HG22  | 8        | 0.37          |
| (1,209)  | 1:32:A:ILE:HA    | 1:32:A:ILE:HG23  | 8        | 0.37          |
| (1,123)  | 1:27:A:SER:HB2   | 1:27:A:SER:H     | 1        | 0.37          |
| (1,123)  | 1:27:A:SER:HB3   | 1:27:A:SER:H     | 1        | 0.37          |
| (1,123)  | 1:27:A:SER:HB2   | 1:27:A:SER:H     | 2        | 0.37          |
| (1,123)  | 1:27:A:SER:HB3   | 1:27:A:SER:H     | 2        | 0.37          |
| (1,123)  | 1:27:A:SER:HB2   | 1:27:A:SER:H     | 3        | 0.37          |
| (1,123)  | 1:27:A:SER:HB3   | 1:27:A:SER:H     | 3        | 0.37          |
| (1,123)  | 1:27:A:SER:HB2   | 1:27:A:SER:H     | 5        | 0.37          |
| (1,123)  | 1:27:A:SER:HB3   | 1:27:A:SER:H     | 5        | 0.37          |
| (1,123)  | 1:27:A:SER:HB2   | 1:27:A:SER:H     | 6        | 0.37          |
| (1,123)  | 1:27:A:SER:HB3   | 1:27:A:SER:H     | 6        | 0.37          |
| (2,755)  | 1:167:A:LEU:H    | 1:167:A:LEU:HD11 | 7        | 0.36          |
| (2,755)  | 1:167:A:LEU:H    | 1:167:A:LEU:HD12 | 7        | 0.36          |
| (2,755)  | 1:167:A:LEU:H    | 1:167:A:LEU:HD13 | 7        | 0.36          |
| (2,753)  | 1:167:A:LEU:HD11 | 1:167:A:LEU:H    | 7        | 0.36          |
| (2,753)  | 1:167:A:LEU:HD12 | 1:167:A:LEU:H    | 7        | 0.36          |
| (2,753)  | 1:167:A:LEU:HD13 | 1:167:A:LEU:H    | 7        | 0.36          |
| (2,725)  | 1:145:A:TYR:HD1  | 1:147:A:GLU:H    | 8        | 0.36          |
| (2,725)  | 1:145:A:TYR:HD2  | 1:147:A:GLU:H    | 8        | 0.36          |
| (2,628)  | 1:122:A:TYR:HB3  | 1:123:A:PRO:HD2  | 1        | 0.36          |
| (2,534)  | 1:85:A:TYR:HE1   | 1:151:A:VAL:H    | 1        | 0.36          |
| (2,534)  | 1:85:A:TYR:HE2   | 1:151:A:VAL:H    | 1        | 0.36          |
| (2,383)  | 1:70:A:LEU:HA    | 1:74:A:PHE:HD1   | 4        | 0.36          |
| (2,383)  | 1:70:A:LEU:HA    | 1:74:A:PHE:HD2   | 4        | 0.36          |
| (1,2371) | 1:174:A:ILE:HG21 | 1:175:A:PHE:H    | 8        | 0.36          |
| (1,2371) | 1:174:A:ILE:HG22 | 1:175:A:PHE:H    | 8        | 0.36          |
| (1,2371) | 1:174:A:ILE:HG23 | 1:175:A:PHE:H    | 8        | 0.36          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2067) | 1:148:A:THR:HB   | 1:148:A:THR:HG21 | 3        | 0.36          |
| (1,2067) | 1:148:A:THR:HB   | 1:148:A:THR:HG22 | 3        | 0.36          |
| (1,2067) | 1:148:A:THR:HB   | 1:148:A:THR:HG23 | 3        | 0.36          |
| (1,2067) | 1:148:A:THR:HB   | 1:148:A:THR:HG21 | 10       | 0.36          |
| (1,2067) | 1:148:A:THR:HB   | 1:148:A:THR:HG22 | 10       | 0.36          |
| (1,2067) | 1:148:A:THR:HB   | 1:148:A:THR:HG23 | 10       | 0.36          |
| (1,2054) | 1:145:A:TYR:HD1  | 1:146:A:ASN:H    | 2        | 0.36          |
| (1,2054) | 1:145:A:TYR:HD2  | 1:146:A:ASN:H    | 2        | 0.36          |
| (1,2032) | 1:143:A:ILE:HG21 | 1:144:A:VAL:H    | 6        | 0.36          |
| (1,2032) | 1:143:A:ILE:HG22 | 1:144:A:VAL:H    | 6        | 0.36          |
| (1,2032) | 1:143:A:ILE:HG23 | 1:144:A:VAL:H    | 6        | 0.36          |
| (1,1941) | 1:135:A:VAL:HG21 | 1:135:A:VAL:H    | 8        | 0.36          |
| (1,1941) | 1:135:A:VAL:HG22 | 1:135:A:VAL:H    | 8        | 0.36          |
| (1,1941) | 1:135:A:VAL:HG23 | 1:135:A:VAL:H    | 8        | 0.36          |
| (1,1941) | 1:135:A:VAL:HG21 | 1:135:A:VAL:H    | 10       | 0.36          |
| (1,1941) | 1:135:A:VAL:HG22 | 1:135:A:VAL:H    | 10       | 0.36          |
| (1,1941) | 1:135:A:VAL:HG23 | 1:135:A:VAL:H    | 10       | 0.36          |
| (1,1938) | 1:135:A:VAL:HG11 | 1:135:A:VAL:HG21 | 6        | 0.36          |
| (1,1938) | 1:135:A:VAL:HG11 | 1:135:A:VAL:HG22 | 6        | 0.36          |
| (1,1938) | 1:135:A:VAL:HG11 | 1:135:A:VAL:HG23 | 6        | 0.36          |
| (1,1938) | 1:135:A:VAL:HG12 | 1:135:A:VAL:HG21 | 6        | 0.36          |
| (1,1938) | 1:135:A:VAL:HG12 | 1:135:A:VAL:HG22 | 6        | 0.36          |
| (1,1938) | 1:135:A:VAL:HG12 | 1:135:A:VAL:HG23 | 6        | 0.36          |
| (1,1938) | 1:135:A:VAL:HG13 | 1:135:A:VAL:HG21 | 6        | 0.36          |
| (1,1938) | 1:135:A:VAL:HG13 | 1:135:A:VAL:HG22 | 6        | 0.36          |
| (1,1938) | 1:135:A:VAL:HG13 | 1:135:A:VAL:HG23 | 6        | 0.36          |
| (1,1707) | 1:115:A:LYS:HG2  | 1:116:A:GLU:H    | 2        | 0.36          |
| (1,1707) | 1:115:A:LYS:HG3  | 1:116:A:GLU:H    | 2        | 0.36          |
| (1,1707) | 1:115:A:LYS:HG2  | 1:116:A:GLU:H    | 6        | 0.36          |
| (1,1707) | 1:115:A:LYS:HG3  | 1:116:A:GLU:H    | 6        | 0.36          |
| (1,1447) | 1:90:A:THR:HB    | 1:90:A:THR:HG21  | 1        | 0.36          |
| (1,1447) | 1:90:A:THR:HB    | 1:90:A:THR:HG22  | 1        | 0.36          |
| (1,1447) | 1:90:A:THR:HB    | 1:90:A:THR:HG23  | 1        | 0.36          |
| (1,1447) | 1:90:A:THR:HB    | 1:90:A:THR:HG21  | 3        | 0.36          |
| (1,1447) | 1:90:A:THR:HB    | 1:90:A:THR:HG22  | 3        | 0.36          |
| (1,1447) | 1:90:A:THR:HB    | 1:90:A:THR:HG23  | 3        | 0.36          |
| (1,1447) | 1:90:A:THR:HB    | 1:90:A:THR:HG21  | 5        | 0.36          |
| (1,1447) | 1:90:A:THR:HB    | 1:90:A:THR:HG22  | 5        | 0.36          |
| (1,1447) | 1:90:A:THR:HB    | 1:90:A:THR:HG23  | 5        | 0.36          |
| (1,1447) | 1:90:A:THR:HB    | 1:90:A:THR:HG21  | 8        | 0.36          |
| (1,1447) | 1:90:A:THR:HB    | 1:90:A:THR:HG22  | 8        | 0.36          |
| (1,1447) | 1:90:A:THR:HB    | 1:90:A:THR:HG23  | 8        | 0.36          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1447) | 1:90:A:THR:HB   | 1:90:A:THR:HG21 | 9        | 0.36          |
| (1,1447) | 1:90:A:THR:HB   | 1:90:A:THR:HG22 | 9        | 0.36          |
| (1,1447) | 1:90:A:THR:HB   | 1:90:A:THR:HG23 | 9        | 0.36          |
| (1,1236) | 1:81:A:ILE:HG21 | 1:154:A:LEU:HB3 | 3        | 0.36          |
| (1,1236) | 1:81:A:ILE:HG22 | 1:154:A:LEU:HB3 | 3        | 0.36          |
| (1,1236) | 1:81:A:ILE:HG23 | 1:154:A:LEU:HB3 | 3        | 0.36          |
| (1,1189) | 1:80:A:GLN:HG2  | 1:98:A:THR:HG21 | 5        | 0.36          |
| (1,1189) | 1:80:A:GLN:HG2  | 1:98:A:THR:HG22 | 5        | 0.36          |
| (1,1189) | 1:80:A:GLN:HG2  | 1:98:A:THR:HG23 | 5        | 0.36          |
| (1,1189) | 1:80:A:GLN:HG3  | 1:98:A:THR:HG21 | 5        | 0.36          |
| (1,1189) | 1:80:A:GLN:HG3  | 1:98:A:THR:HG22 | 5        | 0.36          |
| (1,1189) | 1:80:A:GLN:HG3  | 1:98:A:THR:HG23 | 5        | 0.36          |
| (1,1162) | 1:79:A:ILE:HG13 | 1:80:A:GLN:H    | 7        | 0.36          |
| (1,582)  | 1:51:A:ILE:HG21 | 1:55:A:VAL:H    | 5        | 0.36          |
| (1,582)  | 1:51:A:ILE:HG22 | 1:55:A:VAL:H    | 5        | 0.36          |
| (1,582)  | 1:51:A:ILE:HG23 | 1:55:A:VAL:H    | 5        | 0.36          |
| (1,520)  | 1:49:A:VAL:HB   | 1:152:A:ALA:HB1 | 3        | 0.36          |
| (1,520)  | 1:49:A:VAL:HB   | 1:152:A:ALA:HB2 | 3        | 0.36          |
| (1,520)  | 1:49:A:VAL:HB   | 1:152:A:ALA:HB3 | 3        | 0.36          |
| (1,520)  | 1:49:A:VAL:HB   | 1:152:A:ALA:HB1 | 5        | 0.36          |
| (1,520)  | 1:49:A:VAL:HB   | 1:152:A:ALA:HB2 | 5        | 0.36          |
| (1,520)  | 1:49:A:VAL:HB   | 1:152:A:ALA:HB3 | 5        | 0.36          |
| (1,232)  | 1:32:A:ILE:HG21 | 1:32:A:ILE:HD11 | 9        | 0.36          |
| (1,232)  | 1:32:A:ILE:HG21 | 1:32:A:ILE:HD12 | 9        | 0.36          |
| (1,232)  | 1:32:A:ILE:HG21 | 1:32:A:ILE:HD13 | 9        | 0.36          |
| (1,232)  | 1:32:A:ILE:HG22 | 1:32:A:ILE:HD11 | 9        | 0.36          |
| (1,232)  | 1:32:A:ILE:HG22 | 1:32:A:ILE:HD12 | 9        | 0.36          |
| (1,232)  | 1:32:A:ILE:HG22 | 1:32:A:ILE:HD13 | 9        | 0.36          |
| (1,232)  | 1:32:A:ILE:HG23 | 1:32:A:ILE:HD11 | 9        | 0.36          |
| (1,232)  | 1:32:A:ILE:HG23 | 1:32:A:ILE:HD12 | 9        | 0.36          |
| (1,232)  | 1:32:A:ILE:HG23 | 1:32:A:ILE:HD13 | 9        | 0.36          |
| (1,212)  | 1:32:A:ILE:HB   | 1:32:A:ILE:HD11 | 7        | 0.36          |
| (1,212)  | 1:32:A:ILE:HB   | 1:32:A:ILE:HD12 | 7        | 0.36          |
| (1,212)  | 1:32:A:ILE:HB   | 1:32:A:ILE:HD13 | 7        | 0.36          |
| (2,768)  | 1:173:A:VAL:HB  | 1:175:A:PHE:HE1 | 2        | 0.35          |
| (2,768)  | 1:173:A:VAL:HB  | 1:175:A:PHE:HE2 | 2        | 0.35          |
| (2,731)  | 1:155:A:ASN:H   | 1:156:A:PHE:HD1 | 6        | 0.35          |
| (2,731)  | 1:155:A:ASN:H   | 1:156:A:PHE:HD2 | 6        | 0.35          |
| (2,714)  | 1:141:A:LYS:HD2 | 1:142:A:ILE:H   | 6        | 0.35          |
| (2,714)  | 1:141:A:LYS:HD3 | 1:142:A:ILE:H   | 6        | 0.35          |
| (2,593)  | 1:114:A:ASP:HB2 | 1:116:A:GLU:HG2 | 4        | 0.35          |
| (2,593)  | 1:114:A:ASP:HB2 | 1:116:A:GLU:HG3 | 4        | 0.35          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,178)  | 1:36:A:ALA:H     | 1:37:A:GLY:H     | 7        | 0.35          |
| (1,2327) | 1:171:A:LEU:HG   | 1:171:A:LEU:H    | 9        | 0.35          |
| (1,2320) | 1:171:A:LEU:HD11 | 1:171:A:LEU:HD21 | 9        | 0.35          |
| (1,2320) | 1:171:A:LEU:HD11 | 1:171:A:LEU:HD22 | 9        | 0.35          |
| (1,2320) | 1:171:A:LEU:HD11 | 1:171:A:LEU:HD23 | 9        | 0.35          |
| (1,2320) | 1:171:A:LEU:HD12 | 1:171:A:LEU:HD21 | 9        | 0.35          |
| (1,2320) | 1:171:A:LEU:HD12 | 1:171:A:LEU:HD22 | 9        | 0.35          |
| (1,2320) | 1:171:A:LEU:HD12 | 1:171:A:LEU:HD23 | 9        | 0.35          |
| (1,2320) | 1:171:A:LEU:HD13 | 1:171:A:LEU:HD21 | 9        | 0.35          |
| (1,2320) | 1:171:A:LEU:HD13 | 1:171:A:LEU:HD22 | 9        | 0.35          |
| (1,2320) | 1:171:A:LEU:HD13 | 1:171:A:LEU:HD23 | 9        | 0.35          |
| (1,2093) | 1:153:A:ILE:HA   | 1:153:A:ILE:HG21 | 2        | 0.35          |
| (1,2093) | 1:153:A:ILE:HA   | 1:153:A:ILE:HG22 | 2        | 0.35          |
| (1,2093) | 1:153:A:ILE:HA   | 1:153:A:ILE:HG23 | 2        | 0.35          |
| (1,2054) | 1:145:A:TYR:HD1  | 1:146:A:ASN:H    | 1        | 0.35          |
| (1,2054) | 1:145:A:TYR:HD2  | 1:146:A:ASN:H    | 1        | 0.35          |
| (1,2010) | 1:142:A:ILE:HD11 | 1:145:A:TYR:HD1  | 8        | 0.35          |
| (1,2010) | 1:142:A:ILE:HD11 | 1:145:A:TYR:HD2  | 8        | 0.35          |
| (1,2010) | 1:142:A:ILE:HD12 | 1:145:A:TYR:HD1  | 8        | 0.35          |
| (1,2010) | 1:142:A:ILE:HD12 | 1:145:A:TYR:HD2  | 8        | 0.35          |
| (1,2010) | 1:142:A:ILE:HD13 | 1:145:A:TYR:HD1  | 8        | 0.35          |
| (1,2010) | 1:142:A:ILE:HD13 | 1:145:A:TYR:HD2  | 8        | 0.35          |
| (1,1941) | 1:135:A:VAL:HG21 | 1:135:A:VAL:H    | 6        | 0.35          |
| (1,1941) | 1:135:A:VAL:HG22 | 1:135:A:VAL:H    | 6        | 0.35          |
| (1,1941) | 1:135:A:VAL:HG23 | 1:135:A:VAL:H    | 6        | 0.35          |
| (1,1765) | 1:120:A:VAL:HB   | 1:122:A:TYR:HE1  | 3        | 0.35          |
| (1,1765) | 1:120:A:VAL:HB   | 1:122:A:TYR:HE2  | 3        | 0.35          |
| (1,1747) | 1:118:A:ILE:HD11 | 1:118:A:ILE:H    | 10       | 0.35          |
| (1,1747) | 1:118:A:ILE:HD12 | 1:118:A:ILE:H    | 10       | 0.35          |
| (1,1747) | 1:118:A:ILE:HD13 | 1:118:A:ILE:H    | 10       | 0.35          |
| (1,1707) | 1:115:A:LYS:HG2  | 1:116:A:GLU:H    | 1        | 0.35          |
| (1,1707) | 1:115:A:LYS:HG3  | 1:116:A:GLU:H    | 1        | 0.35          |
| (1,1707) | 1:115:A:LYS:HG2  | 1:116:A:GLU:H    | 8        | 0.35          |
| (1,1707) | 1:115:A:LYS:HG3  | 1:116:A:GLU:H    | 8        | 0.35          |
| (1,1556) | 1:103:A:SER:HA   | 1:104:A:LEU:HB3  | 9        | 0.35          |
| (1,1556) | 1:103:A:SER:HA   | 1:104:A:LEU:HB3  | 10       | 0.35          |
| (1,1475) | 1:95:A:PHE:HB2   | 1:96:A:SER:H     | 10       | 0.35          |
| (1,1475) | 1:95:A:PHE:HB3   | 1:96:A:SER:H     | 10       | 0.35          |
| (1,1399) | 1:87:A:THR:HG21  | 1:87:A:THR:H     | 3        | 0.35          |
| (1,1399) | 1:87:A:THR:HG22  | 1:87:A:THR:H     | 3        | 0.35          |
| (1,1399) | 1:87:A:THR:HG23  | 1:87:A:THR:H     | 3        | 0.35          |
| (1,1270) | 1:82:A:THR:HG21  | 1:83:A:SER:HA    | 2        | 0.35          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1270) | 1:82:A:THR:HG22 | 1:83:A:SER:HA   | 2        | 0.35          |
| (1,1270) | 1:82:A:THR:HG23 | 1:83:A:SER:HA   | 2        | 0.35          |
| (1,1162) | 1:79:A:ILE:HG13 | 1:80:A:GLN:H    | 3        | 0.35          |
| (1,1162) | 1:79:A:ILE:HG13 | 1:80:A:GLN:H    | 8        | 0.35          |
| (1,1090) | 1:77:A:LEU:HD11 | 1:79:A:ILE:H    | 5        | 0.35          |
| (1,1090) | 1:77:A:LEU:HD12 | 1:79:A:ILE:H    | 5        | 0.35          |
| (1,1090) | 1:77:A:LEU:HD13 | 1:79:A:ILE:H    | 5        | 0.35          |
| (1,1090) | 1:77:A:LEU:HD21 | 1:79:A:ILE:H    | 5        | 0.35          |
| (1,1090) | 1:77:A:LEU:HD22 | 1:79:A:ILE:H    | 5        | 0.35          |
| (1,1090) | 1:77:A:LEU:HD23 | 1:79:A:ILE:H    | 5        | 0.35          |
| (1,1090) | 1:77:A:LEU:HD11 | 1:79:A:ILE:H    | 6        | 0.35          |
| (1,1090) | 1:77:A:LEU:HD12 | 1:79:A:ILE:H    | 6        | 0.35          |
| (1,1090) | 1:77:A:LEU:HD13 | 1:79:A:ILE:H    | 6        | 0.35          |
| (1,1090) | 1:77:A:LEU:HD21 | 1:79:A:ILE:H    | 6        | 0.35          |
| (1,1090) | 1:77:A:LEU:HD22 | 1:79:A:ILE:H    | 6        | 0.35          |
| (1,1090) | 1:77:A:LEU:HD23 | 1:79:A:ILE:H    | 6        | 0.35          |
| (1,965)  | 1:72:A:PRO:HB2  | 1:73:A:TYR:HD1  | 10       | 0.35          |
| (1,965)  | 1:72:A:PRO:HB2  | 1:73:A:TYR:HD2  | 10       | 0.35          |
| (1,922)  | 1:70:A:LEU:HD11 | 1:70:A:LEU:H    | 6        | 0.35          |
| (1,922)  | 1:70:A:LEU:HD12 | 1:70:A:LEU:H    | 6        | 0.35          |
| (1,922)  | 1:70:A:LEU:HD13 | 1:70:A:LEU:H    | 6        | 0.35          |
| (1,621)  | 1:55:A:VAL:H    | 1:55:A:VAL:HG21 | 1        | 0.35          |
| (1,621)  | 1:55:A:VAL:H    | 1:55:A:VAL:HG22 | 1        | 0.35          |
| (1,621)  | 1:55:A:VAL:H    | 1:55:A:VAL:HG23 | 1        | 0.35          |
| (1,610)  | 1:55:A:VAL:HA   | 1:55:A:VAL:HG11 | 2        | 0.35          |
| (1,610)  | 1:55:A:VAL:HA   | 1:55:A:VAL:HG12 | 2        | 0.35          |
| (1,610)  | 1:55:A:VAL:HA   | 1:55:A:VAL:HG13 | 2        | 0.35          |
| (1,599)  | 1:53:A:ASP:H    | 1:55:A:VAL:HG11 | 2        | 0.35          |
| (1,599)  | 1:53:A:ASP:H    | 1:55:A:VAL:HG12 | 2        | 0.35          |
| (1,599)  | 1:53:A:ASP:H    | 1:55:A:VAL:HG13 | 2        | 0.35          |
| (1,389)  | 1:44:A:ILE:HG21 | 1:44:A:ILE:H    | 5        | 0.35          |
| (1,389)  | 1:44:A:ILE:HG22 | 1:44:A:ILE:H    | 5        | 0.35          |
| (1,389)  | 1:44:A:ILE:HG23 | 1:44:A:ILE:H    | 5        | 0.35          |
| (1,356)  | 1:42:A:ASP:HB2  | 1:160:A:TYR:HE1 | 6        | 0.35          |
| (1,356)  | 1:42:A:ASP:HB2  | 1:160:A:TYR:HE2 | 6        | 0.35          |
| (1,356)  | 1:42:A:ASP:HB3  | 1:160:A:TYR:HE1 | 6        | 0.35          |
| (1,356)  | 1:42:A:ASP:HB3  | 1:160:A:TYR:HE2 | 6        | 0.35          |
| (1,286)  | 1:36:A:ALA:HA   | 1:37:A:GLY:H    | 2        | 0.35          |
| (1,232)  | 1:32:A:ILE:HG21 | 1:32:A:ILE:HD11 | 5        | 0.35          |
| (1,232)  | 1:32:A:ILE:HG21 | 1:32:A:ILE:HD12 | 5        | 0.35          |
| (1,232)  | 1:32:A:ILE:HG21 | 1:32:A:ILE:HD13 | 5        | 0.35          |
| (1,232)  | 1:32:A:ILE:HG22 | 1:32:A:ILE:HD11 | 5        | 0.35          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,232)  | 1:32:A:ILE:HG22  | 1:32:A:ILE:HD12  | 5        | 0.35          |
| (1,232)  | 1:32:A:ILE:HG22  | 1:32:A:ILE:HD13  | 5        | 0.35          |
| (1,232)  | 1:32:A:ILE:HG23  | 1:32:A:ILE:HD11  | 5        | 0.35          |
| (1,232)  | 1:32:A:ILE:HG23  | 1:32:A:ILE:HD12  | 5        | 0.35          |
| (1,232)  | 1:32:A:ILE:HG23  | 1:32:A:ILE:HD13  | 5        | 0.35          |
| (2,732)  | 1:155:A:ASN:H    | 1:156:A:PHE:HE1  | 3        | 0.34          |
| (2,732)  | 1:155:A:ASN:H    | 1:156:A:PHE:HE2  | 3        | 0.34          |
| (2,129)  | 1:28:A:HIS:H     | 1:156:A:PHE:HE1  | 1        | 0.34          |
| (2,129)  | 1:28:A:HIS:H     | 1:156:A:PHE:HE2  | 1        | 0.34          |
| (1,2352) | 1:173:A:VAL:HG11 | 1:173:A:VAL:HG21 | 2        | 0.34          |
| (1,2352) | 1:173:A:VAL:HG11 | 1:173:A:VAL:HG22 | 2        | 0.34          |
| (1,2352) | 1:173:A:VAL:HG11 | 1:173:A:VAL:HG23 | 2        | 0.34          |
| (1,2352) | 1:173:A:VAL:HG12 | 1:173:A:VAL:HG21 | 2        | 0.34          |
| (1,2352) | 1:173:A:VAL:HG12 | 1:173:A:VAL:HG22 | 2        | 0.34          |
| (1,2352) | 1:173:A:VAL:HG12 | 1:173:A:VAL:HG23 | 2        | 0.34          |
| (1,2352) | 1:173:A:VAL:HG13 | 1:173:A:VAL:HG21 | 2        | 0.34          |
| (1,2352) | 1:173:A:VAL:HG13 | 1:173:A:VAL:HG22 | 2        | 0.34          |
| (1,2352) | 1:173:A:VAL:HG13 | 1:173:A:VAL:HG23 | 2        | 0.34          |
| (1,2327) | 1:171:A:LEU:HG   | 1:171:A:LEU:H    | 7        | 0.34          |
| (1,2321) | 1:171:A:LEU:HD11 | 1:171:A:LEU:H    | 6        | 0.34          |
| (1,2321) | 1:171:A:LEU:HD12 | 1:171:A:LEU:H    | 6        | 0.34          |
| (1,2321) | 1:171:A:LEU:HD13 | 1:171:A:LEU:H    | 6        | 0.34          |
| (1,2320) | 1:171:A:LEU:HD11 | 1:171:A:LEU:HD21 | 1        | 0.34          |
| (1,2320) | 1:171:A:LEU:HD11 | 1:171:A:LEU:HD22 | 1        | 0.34          |
| (1,2320) | 1:171:A:LEU:HD11 | 1:171:A:LEU:HD23 | 1        | 0.34          |
| (1,2320) | 1:171:A:LEU:HD12 | 1:171:A:LEU:HD21 | 1        | 0.34          |
| (1,2320) | 1:171:A:LEU:HD12 | 1:171:A:LEU:HD22 | 1        | 0.34          |
| (1,2320) | 1:171:A:LEU:HD12 | 1:171:A:LEU:HD23 | 1        | 0.34          |
| (1,2320) | 1:171:A:LEU:HD13 | 1:171:A:LEU:HD21 | 1        | 0.34          |
| (1,2320) | 1:171:A:LEU:HD13 | 1:171:A:LEU:HD22 | 1        | 0.34          |
| (1,2320) | 1:171:A:LEU:HD13 | 1:171:A:LEU:HD23 | 1        | 0.34          |
| (1,2320) | 1:171:A:LEU:HD11 | 1:171:A:LEU:HD21 | 10       | 0.34          |
| (1,2320) | 1:171:A:LEU:HD11 | 1:171:A:LEU:HD22 | 10       | 0.34          |
| (1,2320) | 1:171:A:LEU:HD11 | 1:171:A:LEU:HD23 | 10       | 0.34          |
| (1,2320) | 1:171:A:LEU:HD12 | 1:171:A:LEU:HD21 | 10       | 0.34          |
| (1,2320) | 1:171:A:LEU:HD12 | 1:171:A:LEU:HD22 | 10       | 0.34          |
| (1,2320) | 1:171:A:LEU:HD12 | 1:171:A:LEU:HD23 | 10       | 0.34          |
| (1,2320) | 1:171:A:LEU:HD13 | 1:171:A:LEU:HD21 | 10       | 0.34          |
| (1,2320) | 1:171:A:LEU:HD13 | 1:171:A:LEU:HD22 | 10       | 0.34          |
| (1,2320) | 1:171:A:LEU:HD13 | 1:171:A:LEU:HD23 | 10       | 0.34          |
| (1,2106) | 1:153:A:ILE:HG21 | 1:155:A:ASN:HD21 | 8        | 0.34          |
| (1,2106) | 1:153:A:ILE:HG21 | 1:155:A:ASN:HD22 | 8        | 0.34          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2106) | 1:153:A:ILE:HG22 | 1:155:A:ASN:HD21 | 8        | 0.34          |
| (1,2106) | 1:153:A:ILE:HG22 | 1:155:A:ASN:HD22 | 8        | 0.34          |
| (1,2106) | 1:153:A:ILE:HG23 | 1:155:A:ASN:HD21 | 8        | 0.34          |
| (1,2106) | 1:153:A:ILE:HG23 | 1:155:A:ASN:HD22 | 8        | 0.34          |
| (1,2093) | 1:153:A:ILE:HA   | 1:153:A:ILE:HG21 | 5        | 0.34          |
| (1,2093) | 1:153:A:ILE:HA   | 1:153:A:ILE:HG22 | 5        | 0.34          |
| (1,2093) | 1:153:A:ILE:HA   | 1:153:A:ILE:HG23 | 5        | 0.34          |
| (1,2054) | 1:145:A:TYR:HD1  | 1:146:A:ASN:H    | 4        | 0.34          |
| (1,2054) | 1:145:A:TYR:HD2  | 1:146:A:ASN:H    | 4        | 0.34          |
| (1,2054) | 1:145:A:TYR:HD1  | 1:146:A:ASN:H    | 9        | 0.34          |
| (1,2054) | 1:145:A:TYR:HD2  | 1:146:A:ASN:H    | 9        | 0.34          |
| (1,2038) | 1:144:A:VAL:HG21 | 1:144:A:VAL:H    | 3        | 0.34          |
| (1,2038) | 1:144:A:VAL:HG22 | 1:144:A:VAL:H    | 3        | 0.34          |
| (1,2038) | 1:144:A:VAL:HG23 | 1:144:A:VAL:H    | 3        | 0.34          |
| (1,1940) | 1:135:A:VAL:HG11 | 1:155:A:ASN:HD21 | 2        | 0.34          |
| (1,1940) | 1:135:A:VAL:HG11 | 1:155:A:ASN:HD22 | 2        | 0.34          |
| (1,1940) | 1:135:A:VAL:HG12 | 1:155:A:ASN:HD21 | 2        | 0.34          |
| (1,1940) | 1:135:A:VAL:HG12 | 1:155:A:ASN:HD22 | 2        | 0.34          |
| (1,1940) | 1:135:A:VAL:HG13 | 1:155:A:ASN:HD21 | 2        | 0.34          |
| (1,1940) | 1:135:A:VAL:HG13 | 1:155:A:ASN:HD22 | 2        | 0.34          |
| (1,1938) | 1:135:A:VAL:HG11 | 1:135:A:VAL:HG21 | 3        | 0.34          |
| (1,1938) | 1:135:A:VAL:HG11 | 1:135:A:VAL:HG22 | 3        | 0.34          |
| (1,1938) | 1:135:A:VAL:HG11 | 1:135:A:VAL:HG23 | 3        | 0.34          |
| (1,1938) | 1:135:A:VAL:HG12 | 1:135:A:VAL:HG21 | 3        | 0.34          |
| (1,1938) | 1:135:A:VAL:HG12 | 1:135:A:VAL:HG22 | 3        | 0.34          |
| (1,1938) | 1:135:A:VAL:HG12 | 1:135:A:VAL:HG23 | 3        | 0.34          |
| (1,1938) | 1:135:A:VAL:HG13 | 1:135:A:VAL:HG21 | 3        | 0.34          |
| (1,1938) | 1:135:A:VAL:HG13 | 1:135:A:VAL:HG22 | 3        | 0.34          |
| (1,1938) | 1:135:A:VAL:HG13 | 1:135:A:VAL:HG23 | 3        | 0.34          |
| (1,1844) | 1:132:A:SER:HB2  | 1:142:A:ILE:HG21 | 2        | 0.34          |
| (1,1844) | 1:132:A:SER:HB2  | 1:142:A:ILE:HG22 | 2        | 0.34          |
| (1,1844) | 1:132:A:SER:HB2  | 1:142:A:ILE:HG23 | 2        | 0.34          |
| (1,1706) | 1:115:A:LYS:HG2  | 1:115:A:LYS:H    | 4        | 0.34          |
| (1,1706) | 1:115:A:LYS:HG3  | 1:115:A:LYS:H    | 4        | 0.34          |
| (1,1706) | 1:115:A:LYS:HG2  | 1:115:A:LYS:H    | 10       | 0.34          |
| (1,1706) | 1:115:A:LYS:HG3  | 1:115:A:LYS:H    | 10       | 0.34          |
| (1,1556) | 1:103:A:SER:HA   | 1:104:A:LEU:HB3  | 2        | 0.34          |
| (1,1546) | 1:102:A:ILE:HG21 | 1:108:A:SER:HA   | 1        | 0.34          |
| (1,1546) | 1:102:A:ILE:HG22 | 1:108:A:SER:HA   | 1        | 0.34          |
| (1,1546) | 1:102:A:ILE:HG23 | 1:108:A:SER:HA   | 1        | 0.34          |
| (1,1537) | 1:102:A:ILE:HD11 | 1:107:A:PRO:HA   | 3        | 0.34          |
| (1,1537) | 1:102:A:ILE:HD12 | 1:107:A:PRO:HA   | 3        | 0.34          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1537) | 1:102:A:ILE:HD13 | 1:107:A:PRO:HA   | 3        | 0.34          |
| (1,1162) | 1:79:A:ILE:HG13  | 1:80:A:GLN:H     | 10       | 0.34          |
| (1,844)  | 1:66:A:ASN:HD21  | 1:70:A:LEU:HD21  | 6        | 0.34          |
| (1,844)  | 1:66:A:ASN:HD21  | 1:70:A:LEU:HD22  | 6        | 0.34          |
| (1,844)  | 1:66:A:ASN:HD21  | 1:70:A:LEU:HD23  | 6        | 0.34          |
| (1,837)  | 1:66:A:ASN:HB2   | 1:66:A:ASN:HD22  | 1        | 0.34          |
| (1,597)  | 1:53:A:ASP:HB2   | 1:54:A:GLN:H     | 6        | 0.34          |
| (1,597)  | 1:53:A:ASP:HB3   | 1:54:A:GLN:H     | 6        | 0.34          |
| (1,495)  | 1:48:A:ILE:HG21  | 1:50:A:TRP:HE1   | 8        | 0.34          |
| (1,495)  | 1:48:A:ILE:HG22  | 1:50:A:TRP:HE1   | 8        | 0.34          |
| (1,495)  | 1:48:A:ILE:HG23  | 1:50:A:TRP:HE1   | 8        | 0.34          |
| (1,487)  | 1:48:A:ILE:HG12  | 1:48:A:ILE:HG21  | 6        | 0.34          |
| (1,487)  | 1:48:A:ILE:HG12  | 1:48:A:ILE:HG22  | 6        | 0.34          |
| (1,487)  | 1:48:A:ILE:HG12  | 1:48:A:ILE:HG23  | 6        | 0.34          |
| (1,389)  | 1:44:A:ILE:HG21  | 1:44:A:ILE:H     | 2        | 0.34          |
| (1,389)  | 1:44:A:ILE:HG22  | 1:44:A:ILE:H     | 2        | 0.34          |
| (1,389)  | 1:44:A:ILE:HG23  | 1:44:A:ILE:H     | 2        | 0.34          |
| (1,389)  | 1:44:A:ILE:HG21  | 1:44:A:ILE:H     | 4        | 0.34          |
| (1,389)  | 1:44:A:ILE:HG22  | 1:44:A:ILE:H     | 4        | 0.34          |
| (1,389)  | 1:44:A:ILE:HG23  | 1:44:A:ILE:H     | 4        | 0.34          |
| (1,270)  | 1:34:A:PRO:HD3   | 1:168:A:PHE:HE1  | 8        | 0.34          |
| (1,270)  | 1:34:A:PRO:HD3   | 1:168:A:PHE:HE2  | 8        | 0.34          |
| (1,242)  | 1:32:A:ILE:HG21  | 1:160:A:TYR:HE1  | 4        | 0.34          |
| (1,242)  | 1:32:A:ILE:HG21  | 1:160:A:TYR:HE2  | 4        | 0.34          |
| (1,242)  | 1:32:A:ILE:HG22  | 1:160:A:TYR:HE1  | 4        | 0.34          |
| (1,242)  | 1:32:A:ILE:HG22  | 1:160:A:TYR:HE2  | 4        | 0.34          |
| (1,242)  | 1:32:A:ILE:HG23  | 1:160:A:TYR:HE1  | 4        | 0.34          |
| (1,242)  | 1:32:A:ILE:HG23  | 1:160:A:TYR:HE2  | 4        | 0.34          |
| (2,735)  | 1:158:A:ALA:H    | 1:160:A:TYR:HE1  | 2        | 0.33          |
| (2,735)  | 1:158:A:ALA:H    | 1:160:A:TYR:HE2  | 2        | 0.33          |
| (2,734)  | 1:158:A:ALA:H    | 1:159:A:PHE:HD1  | 10       | 0.33          |
| (2,734)  | 1:158:A:ALA:H    | 1:159:A:PHE:HD2  | 10       | 0.33          |
| (1,2463) | 1:182:A:VAL:HG21 | 1:182:A:VAL:H    | 2        | 0.33          |
| (1,2463) | 1:182:A:VAL:HG22 | 1:182:A:VAL:H    | 2        | 0.33          |
| (1,2463) | 1:182:A:VAL:HG23 | 1:182:A:VAL:H    | 2        | 0.33          |
| (1,2352) | 1:173:A:VAL:HG11 | 1:173:A:VAL:HG21 | 7        | 0.33          |
| (1,2352) | 1:173:A:VAL:HG11 | 1:173:A:VAL:HG22 | 7        | 0.33          |
| (1,2352) | 1:173:A:VAL:HG11 | 1:173:A:VAL:HG23 | 7        | 0.33          |
| (1,2352) | 1:173:A:VAL:HG12 | 1:173:A:VAL:HG21 | 7        | 0.33          |
| (1,2352) | 1:173:A:VAL:HG12 | 1:173:A:VAL:HG22 | 7        | 0.33          |
| (1,2352) | 1:173:A:VAL:HG12 | 1:173:A:VAL:HG23 | 7        | 0.33          |
| (1,2352) | 1:173:A:VAL:HG13 | 1:173:A:VAL:HG21 | 7        | 0.33          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2352) | 1:173:A:VAL:HG13 | 1:173:A:VAL:HG22 | 7        | 0.33          |
| (1,2352) | 1:173:A:VAL:HG13 | 1:173:A:VAL:HG23 | 7        | 0.33          |
| (1,2320) | 1:171:A:LEU:HD11 | 1:171:A:LEU:HD21 | 7        | 0.33          |
| (1,2320) | 1:171:A:LEU:HD11 | 1:171:A:LEU:HD22 | 7        | 0.33          |
| (1,2320) | 1:171:A:LEU:HD11 | 1:171:A:LEU:HD23 | 7        | 0.33          |
| (1,2320) | 1:171:A:LEU:HD12 | 1:171:A:LEU:HD21 | 7        | 0.33          |
| (1,2320) | 1:171:A:LEU:HD12 | 1:171:A:LEU:HD22 | 7        | 0.33          |
| (1,2320) | 1:171:A:LEU:HD12 | 1:171:A:LEU:HD23 | 7        | 0.33          |
| (1,2320) | 1:171:A:LEU:HD13 | 1:171:A:LEU:HD21 | 7        | 0.33          |
| (1,2320) | 1:171:A:LEU:HD13 | 1:171:A:LEU:HD22 | 7        | 0.33          |
| (1,2320) | 1:171:A:LEU:HD13 | 1:171:A:LEU:HD23 | 7        | 0.33          |
| (1,2286) | 1:168:A:PHE:HD1  | 1:168:A:PHE:H    | 1        | 0.33          |
| (1,2286) | 1:168:A:PHE:HD2  | 1:168:A:PHE:H    | 1        | 0.33          |
| (1,2286) | 1:168:A:PHE:HD1  | 1:168:A:PHE:H    | 3        | 0.33          |
| (1,2286) | 1:168:A:PHE:HD2  | 1:168:A:PHE:H    | 3        | 0.33          |
| (1,2286) | 1:168:A:PHE:HD1  | 1:168:A:PHE:H    | 5        | 0.33          |
| (1,2286) | 1:168:A:PHE:HD2  | 1:168:A:PHE:H    | 5        | 0.33          |
| (1,2191) | 1:158:A:ALA:HB1  | 1:160:A:TYR:HE1  | 2        | 0.33          |
| (1,2191) | 1:158:A:ALA:HB1  | 1:160:A:TYR:HE2  | 2        | 0.33          |
| (1,2191) | 1:158:A:ALA:HB2  | 1:160:A:TYR:HE1  | 2        | 0.33          |
| (1,2191) | 1:158:A:ALA:HB2  | 1:160:A:TYR:HE2  | 2        | 0.33          |
| (1,2191) | 1:158:A:ALA:HB3  | 1:160:A:TYR:HE1  | 2        | 0.33          |
| (1,2191) | 1:158:A:ALA:HB3  | 1:160:A:TYR:HE2  | 2        | 0.33          |
| (1,2120) | 1:154:A:LEU:HG   | 1:154:A:LEU:H    | 2        | 0.33          |
| (1,2038) | 1:144:A:VAL:HG21 | 1:144:A:VAL:H    | 8        | 0.33          |
| (1,2038) | 1:144:A:VAL:HG22 | 1:144:A:VAL:H    | 8        | 0.33          |
| (1,2038) | 1:144:A:VAL:HG23 | 1:144:A:VAL:H    | 8        | 0.33          |
| (1,2032) | 1:143:A:ILE:HG21 | 1:144:A:VAL:H    | 9        | 0.33          |
| (1,2032) | 1:143:A:ILE:HG22 | 1:144:A:VAL:H    | 9        | 0.33          |
| (1,2032) | 1:143:A:ILE:HG23 | 1:144:A:VAL:H    | 9        | 0.33          |
| (1,2022) | 1:143:A:ILE:HA   | 1:143:A:ILE:HG21 | 5        | 0.33          |
| (1,2022) | 1:143:A:ILE:HA   | 1:143:A:ILE:HG22 | 5        | 0.33          |
| (1,2022) | 1:143:A:ILE:HA   | 1:143:A:ILE:HG23 | 5        | 0.33          |
| (1,1938) | 1:135:A:VAL:HG11 | 1:135:A:VAL:HG21 | 8        | 0.33          |
| (1,1938) | 1:135:A:VAL:HG11 | 1:135:A:VAL:HG22 | 8        | 0.33          |
| (1,1938) | 1:135:A:VAL:HG11 | 1:135:A:VAL:HG23 | 8        | 0.33          |
| (1,1938) | 1:135:A:VAL:HG12 | 1:135:A:VAL:HG21 | 8        | 0.33          |
| (1,1938) | 1:135:A:VAL:HG12 | 1:135:A:VAL:HG22 | 8        | 0.33          |
| (1,1938) | 1:135:A:VAL:HG12 | 1:135:A:VAL:HG23 | 8        | 0.33          |
| (1,1938) | 1:135:A:VAL:HG13 | 1:135:A:VAL:HG21 | 8        | 0.33          |
| (1,1938) | 1:135:A:VAL:HG13 | 1:135:A:VAL:HG22 | 8        | 0.33          |
| (1,1938) | 1:135:A:VAL:HG13 | 1:135:A:VAL:HG23 | 8        | 0.33          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1836) | 1:132:A:SER:HA  | 1:145:A:TYR:HD1  | 4        | 0.33          |
| (1,1836) | 1:132:A:SER:HA  | 1:145:A:TYR:HD2  | 4        | 0.33          |
| (1,1706) | 1:115:A:LYS:HG2 | 1:115:A:LYS:H    | 3        | 0.33          |
| (1,1706) | 1:115:A:LYS:HG3 | 1:115:A:LYS:H    | 3        | 0.33          |
| (1,1653) | 1:113:A:LEU:HA  | 1:113:A:LEU:HD21 | 4        | 0.33          |
| (1,1653) | 1:113:A:LEU:HA  | 1:113:A:LEU:HD22 | 4        | 0.33          |
| (1,1653) | 1:113:A:LEU:HA  | 1:113:A:LEU:HD23 | 4        | 0.33          |
| (1,1557) | 1:103:A:SER:HA  | 1:104:A:LEU:HB2  | 8        | 0.33          |
| (1,1556) | 1:103:A:SER:HA  | 1:104:A:LEU:HB3  | 1        | 0.33          |
| (1,1556) | 1:103:A:SER:HA  | 1:104:A:LEU:HB3  | 3        | 0.33          |
| (1,1338) | 1:85:A:TYR:HD1  | 1:86:A:GLU:H     | 4        | 0.33          |
| (1,1338) | 1:85:A:TYR:HD2  | 1:86:A:GLU:H     | 4        | 0.33          |
| (1,1216) | 1:81:A:ILE:HD11 | 1:100:A:ALA:H    | 7        | 0.33          |
| (1,1216) | 1:81:A:ILE:HD12 | 1:100:A:ALA:H    | 7        | 0.33          |
| (1,1216) | 1:81:A:ILE:HD13 | 1:100:A:ALA:H    | 7        | 0.33          |
| (1,1215) | 1:81:A:ILE:HD11 | 1:100:A:ALA:HB1  | 8        | 0.33          |
| (1,1215) | 1:81:A:ILE:HD11 | 1:100:A:ALA:HB2  | 8        | 0.33          |
| (1,1215) | 1:81:A:ILE:HD11 | 1:100:A:ALA:HB3  | 8        | 0.33          |
| (1,1215) | 1:81:A:ILE:HD12 | 1:100:A:ALA:HB1  | 8        | 0.33          |
| (1,1215) | 1:81:A:ILE:HD12 | 1:100:A:ALA:HB2  | 8        | 0.33          |
| (1,1215) | 1:81:A:ILE:HD12 | 1:100:A:ALA:HB3  | 8        | 0.33          |
| (1,1215) | 1:81:A:ILE:HD13 | 1:100:A:ALA:HB1  | 8        | 0.33          |
| (1,1215) | 1:81:A:ILE:HD13 | 1:100:A:ALA:HB2  | 8        | 0.33          |
| (1,1215) | 1:81:A:ILE:HD13 | 1:100:A:ALA:HB3  | 8        | 0.33          |
| (1,610)  | 1:55:A:VAL:HA   | 1:55:A:VAL:HG11  | 6        | 0.33          |
| (1,610)  | 1:55:A:VAL:HA   | 1:55:A:VAL:HG12  | 6        | 0.33          |
| (1,610)  | 1:55:A:VAL:HA   | 1:55:A:VAL:HG13  | 6        | 0.33          |
| (1,487)  | 1:48:A:ILE:HG12 | 1:48:A:ILE:HG21  | 7        | 0.33          |
| (1,487)  | 1:48:A:ILE:HG12 | 1:48:A:ILE:HG22  | 7        | 0.33          |
| (1,487)  | 1:48:A:ILE:HG12 | 1:48:A:ILE:HG23  | 7        | 0.33          |
| (1,427)  | 1:46:A:TYR:HA   | 1:156:A:PHE:HE1  | 7        | 0.33          |
| (1,427)  | 1:46:A:TYR:HA   | 1:156:A:PHE:HE2  | 7        | 0.33          |
| (1,270)  | 1:34:A:PRO:HD3  | 1:168:A:PHE:HE1  | 3        | 0.33          |
| (1,270)  | 1:34:A:PRO:HD3  | 1:168:A:PHE:HE2  | 3        | 0.33          |
| (1,238)  | 1:32:A:ILE:HG21 | 1:42:A:ASP:HB2   | 9        | 0.33          |
| (1,238)  | 1:32:A:ILE:HG21 | 1:42:A:ASP:HB3   | 9        | 0.33          |
| (1,238)  | 1:32:A:ILE:HG22 | 1:42:A:ASP:HB2   | 9        | 0.33          |
| (1,238)  | 1:32:A:ILE:HG22 | 1:42:A:ASP:HB3   | 9        | 0.33          |
| (1,238)  | 1:32:A:ILE:HG23 | 1:42:A:ASP:HB2   | 9        | 0.33          |
| (1,238)  | 1:32:A:ILE:HG23 | 1:42:A:ASP:HB3   | 9        | 0.33          |
| (1,3)    | 1:16:A:ALA:HB1  | 1:16:A:ALA:H     | 3        | 0.33          |
| (1,3)    | 1:16:A:ALA:HB2  | 1:16:A:ALA:H     | 3        | 0.33          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3)    | 1:16:A:ALA:HB3   | 1:16:A:ALA:H     | 3        | 0.33          |
| (1,3)    | 1:16:A:ALA:HB1   | 1:16:A:ALA:H     | 9        | 0.33          |
| (1,3)    | 1:16:A:ALA:HB2   | 1:16:A:ALA:H     | 9        | 0.33          |
| (1,3)    | 1:16:A:ALA:HB3   | 1:16:A:ALA:H     | 9        | 0.33          |
| (3,4)    | 1:57:A:ASP:HA    | 1:114:A:ASP:HA   | 6        | 0.32          |
| (2,765)  | 1:169:A:ASP:H    | 1:171:A:LEU:HD11 | 7        | 0.32          |
| (2,765)  | 1:169:A:ASP:H    | 1:171:A:LEU:HD12 | 7        | 0.32          |
| (2,765)  | 1:169:A:ASP:H    | 1:171:A:LEU:HD13 | 7        | 0.32          |
| (2,732)  | 1:155:A:ASN:H    | 1:156:A:PHE:HE1  | 5        | 0.32          |
| (2,732)  | 1:155:A:ASN:H    | 1:156:A:PHE:HE2  | 5        | 0.32          |
| (2,614)  | 1:118:A:ILE:HG21 | 1:151:A:VAL:HA   | 3        | 0.32          |
| (2,614)  | 1:118:A:ILE:HG22 | 1:151:A:VAL:HA   | 3        | 0.32          |
| (2,614)  | 1:118:A:ILE:HG23 | 1:151:A:VAL:HA   | 3        | 0.32          |
| (2,601)  | 1:115:A:LYS:HE2  | 1:116:A:GLU:H    | 7        | 0.32          |
| (2,601)  | 1:115:A:LYS:HE3  | 1:116:A:GLU:H    | 7        | 0.32          |
| (2,523)  | 1:85:A:TYR:HD1   | 1:134:A:TRP:H    | 6        | 0.32          |
| (2,523)  | 1:85:A:TYR:HD2   | 1:134:A:TRP:H    | 6        | 0.32          |
| (2,397)  | 1:73:A:TYR:HD1   | 1:74:A:PHE:HA    | 2        | 0.32          |
| (2,397)  | 1:73:A:TYR:HD2   | 1:74:A:PHE:HA    | 2        | 0.32          |
| (1,2448) | 1:179:A:VAL:HG11 | 1:179:A:VAL:H    | 2        | 0.32          |
| (1,2448) | 1:179:A:VAL:HG12 | 1:179:A:VAL:H    | 2        | 0.32          |
| (1,2448) | 1:179:A:VAL:HG13 | 1:179:A:VAL:H    | 2        | 0.32          |
| (1,2446) | 1:179:A:VAL:HB   | 1:179:A:VAL:H    | 10       | 0.32          |
| (1,2352) | 1:173:A:VAL:HG11 | 1:173:A:VAL:HG21 | 1        | 0.32          |
| (1,2352) | 1:173:A:VAL:HG11 | 1:173:A:VAL:HG22 | 1        | 0.32          |
| (1,2352) | 1:173:A:VAL:HG11 | 1:173:A:VAL:HG23 | 1        | 0.32          |
| (1,2352) | 1:173:A:VAL:HG12 | 1:173:A:VAL:HG21 | 1        | 0.32          |
| (1,2352) | 1:173:A:VAL:HG12 | 1:173:A:VAL:HG22 | 1        | 0.32          |
| (1,2352) | 1:173:A:VAL:HG12 | 1:173:A:VAL:HG23 | 1        | 0.32          |
| (1,2352) | 1:173:A:VAL:HG13 | 1:173:A:VAL:HG21 | 1        | 0.32          |
| (1,2352) | 1:173:A:VAL:HG13 | 1:173:A:VAL:HG22 | 1        | 0.32          |
| (1,2352) | 1:173:A:VAL:HG13 | 1:173:A:VAL:HG23 | 1        | 0.32          |
| (1,2352) | 1:173:A:VAL:HG11 | 1:173:A:VAL:HG21 | 3        | 0.32          |
| (1,2352) | 1:173:A:VAL:HG11 | 1:173:A:VAL:HG22 | 3        | 0.32          |
| (1,2352) | 1:173:A:VAL:HG11 | 1:173:A:VAL:HG23 | 3        | 0.32          |
| (1,2352) | 1:173:A:VAL:HG12 | 1:173:A:VAL:HG21 | 3        | 0.32          |
| (1,2352) | 1:173:A:VAL:HG12 | 1:173:A:VAL:HG22 | 3        | 0.32          |
| (1,2352) | 1:173:A:VAL:HG12 | 1:173:A:VAL:HG23 | 3        | 0.32          |
| (1,2352) | 1:173:A:VAL:HG13 | 1:173:A:VAL:HG21 | 3        | 0.32          |
| (1,2352) | 1:173:A:VAL:HG13 | 1:173:A:VAL:HG22 | 3        | 0.32          |
| (1,2352) | 1:173:A:VAL:HG13 | 1:173:A:VAL:HG23 | 3        | 0.32          |
| (1,2327) | 1:171:A:LEU:HG   | 1:171:A:LEU:H    | 1        | 0.32          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2320) | 1:171:A:LEU:HD11 | 1:171:A:LEU:HD21 | 6        | 0.32          |
| (1,2320) | 1:171:A:LEU:HD11 | 1:171:A:LEU:HD22 | 6        | 0.32          |
| (1,2320) | 1:171:A:LEU:HD11 | 1:171:A:LEU:HD23 | 6        | 0.32          |
| (1,2320) | 1:171:A:LEU:HD12 | 1:171:A:LEU:HD21 | 6        | 0.32          |
| (1,2320) | 1:171:A:LEU:HD12 | 1:171:A:LEU:HD22 | 6        | 0.32          |
| (1,2320) | 1:171:A:LEU:HD12 | 1:171:A:LEU:HD23 | 6        | 0.32          |
| (1,2320) | 1:171:A:LEU:HD13 | 1:171:A:LEU:HD21 | 6        | 0.32          |
| (1,2320) | 1:171:A:LEU:HD13 | 1:171:A:LEU:HD22 | 6        | 0.32          |
| (1,2320) | 1:171:A:LEU:HD13 | 1:171:A:LEU:HD23 | 6        | 0.32          |
| (1,2286) | 1:168:A:PHE:HD1  | 1:168:A:PHE:H    | 7        | 0.32          |
| (1,2286) | 1:168:A:PHE:HD2  | 1:168:A:PHE:H    | 7        | 0.32          |
| (1,2246) | 1:162:A:ALA:HB1  | 1:168:A:PHE:HZ   | 1        | 0.32          |
| (1,2246) | 1:162:A:ALA:HB2  | 1:168:A:PHE:HZ   | 1        | 0.32          |
| (1,2246) | 1:162:A:ALA:HB3  | 1:168:A:PHE:HZ   | 1        | 0.32          |
| (1,2245) | 1:162:A:ALA:HB1  | 1:168:A:PHE:HE1  | 8        | 0.32          |
| (1,2245) | 1:162:A:ALA:HB1  | 1:168:A:PHE:HE2  | 8        | 0.32          |
| (1,2245) | 1:162:A:ALA:HB2  | 1:168:A:PHE:HE1  | 8        | 0.32          |
| (1,2245) | 1:162:A:ALA:HB2  | 1:168:A:PHE:HE2  | 8        | 0.32          |
| (1,2245) | 1:162:A:ALA:HB3  | 1:168:A:PHE:HE1  | 8        | 0.32          |
| (1,2245) | 1:162:A:ALA:HB3  | 1:168:A:PHE:HE2  | 8        | 0.32          |
| (1,2110) | 1:154:A:LEU:HA   | 1:154:A:LEU:HD21 | 4        | 0.32          |
| (1,2110) | 1:154:A:LEU:HA   | 1:154:A:LEU:HD22 | 4        | 0.32          |
| (1,2110) | 1:154:A:LEU:HA   | 1:154:A:LEU:HD23 | 4        | 0.32          |
| (1,2038) | 1:144:A:VAL:HG21 | 1:144:A:VAL:H    | 6        | 0.32          |
| (1,2038) | 1:144:A:VAL:HG22 | 1:144:A:VAL:H    | 6        | 0.32          |
| (1,2038) | 1:144:A:VAL:HG23 | 1:144:A:VAL:H    | 6        | 0.32          |
| (1,1970) | 1:138:A:GLU:HB2  | 1:138:A:GLU:H    | 7        | 0.32          |
| (1,1970) | 1:138:A:GLU:HB3  | 1:138:A:GLU:H    | 7        | 0.32          |
| (1,1938) | 1:135:A:VAL:HG11 | 1:135:A:VAL:HG21 | 4        | 0.32          |
| (1,1938) | 1:135:A:VAL:HG11 | 1:135:A:VAL:HG22 | 4        | 0.32          |
| (1,1938) | 1:135:A:VAL:HG11 | 1:135:A:VAL:HG23 | 4        | 0.32          |
| (1,1938) | 1:135:A:VAL:HG12 | 1:135:A:VAL:HG21 | 4        | 0.32          |
| (1,1938) | 1:135:A:VAL:HG12 | 1:135:A:VAL:HG22 | 4        | 0.32          |
| (1,1938) | 1:135:A:VAL:HG12 | 1:135:A:VAL:HG23 | 4        | 0.32          |
| (1,1938) | 1:135:A:VAL:HG13 | 1:135:A:VAL:HG21 | 4        | 0.32          |
| (1,1938) | 1:135:A:VAL:HG13 | 1:135:A:VAL:HG22 | 4        | 0.32          |
| (1,1938) | 1:135:A:VAL:HG13 | 1:135:A:VAL:HG23 | 4        | 0.32          |
| (1,1938) | 1:135:A:VAL:HG11 | 1:135:A:VAL:HG21 | 5        | 0.32          |
| (1,1938) | 1:135:A:VAL:HG11 | 1:135:A:VAL:HG22 | 5        | 0.32          |
| (1,1938) | 1:135:A:VAL:HG11 | 1:135:A:VAL:HG23 | 5        | 0.32          |
| (1,1938) | 1:135:A:VAL:HG12 | 1:135:A:VAL:HG21 | 5        | 0.32          |
| (1,1938) | 1:135:A:VAL:HG12 | 1:135:A:VAL:HG22 | 5        | 0.32          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1938) | 1:135:A:VAL:HG12 | 1:135:A:VAL:HG23 | 5        | 0.32          |
| (1,1938) | 1:135:A:VAL:HG13 | 1:135:A:VAL:HG21 | 5        | 0.32          |
| (1,1938) | 1:135:A:VAL:HG13 | 1:135:A:VAL:HG22 | 5        | 0.32          |
| (1,1938) | 1:135:A:VAL:HG13 | 1:135:A:VAL:HG23 | 5        | 0.32          |
| (1,1938) | 1:135:A:VAL:HG11 | 1:135:A:VAL:HG21 | 10       | 0.32          |
| (1,1938) | 1:135:A:VAL:HG11 | 1:135:A:VAL:HG22 | 10       | 0.32          |
| (1,1938) | 1:135:A:VAL:HG11 | 1:135:A:VAL:HG23 | 10       | 0.32          |
| (1,1938) | 1:135:A:VAL:HG12 | 1:135:A:VAL:HG21 | 10       | 0.32          |
| (1,1938) | 1:135:A:VAL:HG12 | 1:135:A:VAL:HG22 | 10       | 0.32          |
| (1,1938) | 1:135:A:VAL:HG12 | 1:135:A:VAL:HG23 | 10       | 0.32          |
| (1,1938) | 1:135:A:VAL:HG13 | 1:135:A:VAL:HG21 | 10       | 0.32          |
| (1,1938) | 1:135:A:VAL:HG13 | 1:135:A:VAL:HG22 | 10       | 0.32          |
| (1,1938) | 1:135:A:VAL:HG13 | 1:135:A:VAL:HG23 | 10       | 0.32          |
| (1,1557) | 1:103:A:SER:HA   | 1:104:A:LEU:HB2  | 7        | 0.32          |
| (1,1485) | 1:95:A:PHE:HE1   | 1:117:A:ASP:HA   | 2        | 0.32          |
| (1,1485) | 1:95:A:PHE:HE2   | 1:117:A:ASP:HA   | 2        | 0.32          |
| (1,1400) | 1:87:A:THR:HG21  | 1:88:A:ASN:HA    | 2        | 0.32          |
| (1,1400) | 1:87:A:THR:HG22  | 1:88:A:ASN:HA    | 2        | 0.32          |
| (1,1400) | 1:87:A:THR:HG23  | 1:88:A:ASN:HA    | 2        | 0.32          |
| (1,1399) | 1:87:A:THR:HG21  | 1:87:A:THR:H     | 6        | 0.32          |
| (1,1399) | 1:87:A:THR:HG22  | 1:87:A:THR:H     | 6        | 0.32          |
| (1,1399) | 1:87:A:THR:HG23  | 1:87:A:THR:H     | 6        | 0.32          |
| (1,1236) | 1:81:A:ILE:HG21  | 1:154:A:LEU:HB3  | 6        | 0.32          |
| (1,1236) | 1:81:A:ILE:HG22  | 1:154:A:LEU:HB3  | 6        | 0.32          |
| (1,1236) | 1:81:A:ILE:HG23  | 1:154:A:LEU:HB3  | 6        | 0.32          |
| (1,1233) | 1:81:A:ILE:HG21  | 1:100:A:ALA:HB1  | 9        | 0.32          |
| (1,1233) | 1:81:A:ILE:HG21  | 1:100:A:ALA:HB2  | 9        | 0.32          |
| (1,1233) | 1:81:A:ILE:HG21  | 1:100:A:ALA:HB3  | 9        | 0.32          |
| (1,1233) | 1:81:A:ILE:HG22  | 1:100:A:ALA:HB1  | 9        | 0.32          |
| (1,1233) | 1:81:A:ILE:HG22  | 1:100:A:ALA:HB2  | 9        | 0.32          |
| (1,1233) | 1:81:A:ILE:HG22  | 1:100:A:ALA:HB3  | 9        | 0.32          |
| (1,1233) | 1:81:A:ILE:HG23  | 1:100:A:ALA:HB1  | 9        | 0.32          |
| (1,1233) | 1:81:A:ILE:HG23  | 1:100:A:ALA:HB2  | 9        | 0.32          |
| (1,1233) | 1:81:A:ILE:HG23  | 1:100:A:ALA:HB3  | 9        | 0.32          |
| (1,1180) | 1:80:A:GLN:HA    | 1:101:A:VAL:H    | 9        | 0.32          |
| (1,915)  | 1:69:A:GLN:HG3   | 1:70:A:LEU:H     | 10       | 0.32          |
| (1,909)  | 1:69:A:GLN:HB2   | 1:70:A:LEU:H     | 9        | 0.32          |
| (1,852)  | 1:66:A:ASN:HD22  | 1:70:A:LEU:HD21  | 10       | 0.32          |
| (1,852)  | 1:66:A:ASN:HD22  | 1:70:A:LEU:HD22  | 10       | 0.32          |
| (1,852)  | 1:66:A:ASN:HD22  | 1:70:A:LEU:HD23  | 10       | 0.32          |
| (1,731)  | 1:62:A:VAL:HG21  | 1:177:A:PHE:HD1  | 5        | 0.32          |
| (1,731)  | 1:62:A:VAL:HG21  | 1:177:A:PHE:HD2  | 5        | 0.32          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,731) | 1:62:A:VAL:HG22 | 1:177:A:PHE:HD1 | 5        | 0.32          |
| (1,731) | 1:62:A:VAL:HG22 | 1:177:A:PHE:HD2 | 5        | 0.32          |
| (1,731) | 1:62:A:VAL:HG23 | 1:177:A:PHE:HD1 | 5        | 0.32          |
| (1,731) | 1:62:A:VAL:HG23 | 1:177:A:PHE:HD2 | 5        | 0.32          |
| (1,679) | 1:60:A:LEU:HD11 | 1:177:A:PHE:HD1 | 4        | 0.32          |
| (1,679) | 1:60:A:LEU:HD11 | 1:177:A:PHE:HD2 | 4        | 0.32          |
| (1,679) | 1:60:A:LEU:HD12 | 1:177:A:PHE:HD1 | 4        | 0.32          |
| (1,679) | 1:60:A:LEU:HD12 | 1:177:A:PHE:HD2 | 4        | 0.32          |
| (1,679) | 1:60:A:LEU:HD13 | 1:177:A:PHE:HD1 | 4        | 0.32          |
| (1,679) | 1:60:A:LEU:HD13 | 1:177:A:PHE:HD2 | 4        | 0.32          |
| (1,621) | 1:55:A:VAL:H    | 1:55:A:VAL:HG21 | 8        | 0.32          |
| (1,621) | 1:55:A:VAL:H    | 1:55:A:VAL:HG22 | 8        | 0.32          |
| (1,621) | 1:55:A:VAL:H    | 1:55:A:VAL:HG23 | 8        | 0.32          |
| (1,495) | 1:48:A:ILE:HG21 | 1:50:A:TRP:HE1  | 1        | 0.32          |
| (1,495) | 1:48:A:ILE:HG22 | 1:50:A:TRP:HE1  | 1        | 0.32          |
| (1,495) | 1:48:A:ILE:HG23 | 1:50:A:TRP:HE1  | 1        | 0.32          |
| (1,487) | 1:48:A:ILE:HG12 | 1:48:A:ILE:HG21 | 10       | 0.32          |
| (1,487) | 1:48:A:ILE:HG12 | 1:48:A:ILE:HG22 | 10       | 0.32          |
| (1,487) | 1:48:A:ILE:HG12 | 1:48:A:ILE:HG23 | 10       | 0.32          |
| (1,467) | 1:47:A:ALA:H    | 1:156:A:PHE:HE1 | 4        | 0.32          |
| (1,467) | 1:47:A:ALA:H    | 1:156:A:PHE:HE2 | 4        | 0.32          |
| (1,286) | 1:36:A:ALA:HA   | 1:37:A:GLY:H    | 3        | 0.32          |
| (1,286) | 1:36:A:ALA:HA   | 1:37:A:GLY:H    | 4        | 0.32          |
| (1,286) | 1:36:A:ALA:HA   | 1:37:A:GLY:H    | 8        | 0.32          |
| (1,286) | 1:36:A:ALA:HA   | 1:37:A:GLY:H    | 9        | 0.32          |
| (1,232) | 1:32:A:ILE:HG21 | 1:32:A:ILE:HD11 | 2        | 0.32          |
| (1,232) | 1:32:A:ILE:HG21 | 1:32:A:ILE:HD12 | 2        | 0.32          |
| (1,232) | 1:32:A:ILE:HG21 | 1:32:A:ILE:HD13 | 2        | 0.32          |
| (1,232) | 1:32:A:ILE:HG22 | 1:32:A:ILE:HD11 | 2        | 0.32          |
| (1,232) | 1:32:A:ILE:HG22 | 1:32:A:ILE:HD12 | 2        | 0.32          |
| (1,232) | 1:32:A:ILE:HG22 | 1:32:A:ILE:HD13 | 2        | 0.32          |
| (1,232) | 1:32:A:ILE:HG23 | 1:32:A:ILE:HD11 | 2        | 0.32          |
| (1,232) | 1:32:A:ILE:HG23 | 1:32:A:ILE:HD12 | 2        | 0.32          |
| (1,232) | 1:32:A:ILE:HG23 | 1:32:A:ILE:HD13 | 2        | 0.32          |
| (1,232) | 1:32:A:ILE:HG21 | 1:32:A:ILE:HD11 | 6        | 0.32          |
| (1,232) | 1:32:A:ILE:HG21 | 1:32:A:ILE:HD12 | 6        | 0.32          |
| (1,232) | 1:32:A:ILE:HG21 | 1:32:A:ILE:HD13 | 6        | 0.32          |
| (1,232) | 1:32:A:ILE:HG22 | 1:32:A:ILE:HD11 | 6        | 0.32          |
| (1,232) | 1:32:A:ILE:HG22 | 1:32:A:ILE:HD12 | 6        | 0.32          |
| (1,232) | 1:32:A:ILE:HG22 | 1:32:A:ILE:HD13 | 6        | 0.32          |
| (1,232) | 1:32:A:ILE:HG23 | 1:32:A:ILE:HD11 | 6        | 0.32          |
| (1,232) | 1:32:A:ILE:HG23 | 1:32:A:ILE:HD12 | 6        | 0.32          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,232)  | 1:32:A:ILE:HG23  | 1:32:A:ILE:HD13  | 6        | 0.32          |
| (1,123)  | 1:27:A:SER:HB2   | 1:27:A:SER:H     | 7        | 0.32          |
| (1,123)  | 1:27:A:SER:HB3   | 1:27:A:SER:H     | 7        | 0.32          |
| (1,123)  | 1:27:A:SER:HB2   | 1:27:A:SER:H     | 8        | 0.32          |
| (1,123)  | 1:27:A:SER:HB3   | 1:27:A:SER:H     | 8        | 0.32          |
| (1,3)    | 1:16:A:ALA:HB1   | 1:16:A:ALA:H     | 1        | 0.32          |
| (1,3)    | 1:16:A:ALA:HB2   | 1:16:A:ALA:H     | 1        | 0.32          |
| (1,3)    | 1:16:A:ALA:HB3   | 1:16:A:ALA:H     | 1        | 0.32          |
| (2,755)  | 1:167:A:LEU:H    | 1:167:A:LEU:HD11 | 1        | 0.31          |
| (2,755)  | 1:167:A:LEU:H    | 1:167:A:LEU:HD12 | 1        | 0.31          |
| (2,755)  | 1:167:A:LEU:H    | 1:167:A:LEU:HD13 | 1        | 0.31          |
| (2,753)  | 1:167:A:LEU:HD11 | 1:167:A:LEU:H    | 1        | 0.31          |
| (2,753)  | 1:167:A:LEU:HD12 | 1:167:A:LEU:H    | 1        | 0.31          |
| (2,753)  | 1:167:A:LEU:HD13 | 1:167:A:LEU:H    | 1        | 0.31          |
| (2,592)  | 1:114:A:ASP:HB3  | 1:116:A:GLU:HG2  | 3        | 0.31          |
| (2,592)  | 1:114:A:ASP:HB3  | 1:116:A:GLU:HG3  | 3        | 0.31          |
| (2,490)  | 1:81:A:ILE:HD11  | 1:101:A:VAL:H    | 5        | 0.31          |
| (2,490)  | 1:81:A:ILE:HD12  | 1:101:A:VAL:H    | 5        | 0.31          |
| (2,490)  | 1:81:A:ILE:HD13  | 1:101:A:VAL:H    | 5        | 0.31          |
| (2,425)  | 1:74:A:PHE:HZ    | 1:160:A:TYR:HE1  | 6        | 0.31          |
| (2,425)  | 1:74:A:PHE:HZ    | 1:160:A:TYR:HE2  | 6        | 0.31          |
| (2,355)  | 1:64:A:LEU:H     | 1:175:A:PHE:HE1  | 9        | 0.31          |
| (2,355)  | 1:64:A:LEU:H     | 1:175:A:PHE:HE2  | 9        | 0.31          |
| (2,295)  | 1:52:A:LYS:HE2   | 1:54:A:GLN:HE22  | 3        | 0.31          |
| (2,295)  | 1:52:A:LYS:HE3   | 1:54:A:GLN:HE22  | 3        | 0.31          |
| (1,2446) | 1:179:A:VAL:HB   | 1:179:A:VAL:H    | 2        | 0.31          |
| (1,2352) | 1:173:A:VAL:HG11 | 1:173:A:VAL:HG21 | 6        | 0.31          |
| (1,2352) | 1:173:A:VAL:HG11 | 1:173:A:VAL:HG22 | 6        | 0.31          |
| (1,2352) | 1:173:A:VAL:HG11 | 1:173:A:VAL:HG23 | 6        | 0.31          |
| (1,2352) | 1:173:A:VAL:HG12 | 1:173:A:VAL:HG21 | 6        | 0.31          |
| (1,2352) | 1:173:A:VAL:HG12 | 1:173:A:VAL:HG22 | 6        | 0.31          |
| (1,2352) | 1:173:A:VAL:HG12 | 1:173:A:VAL:HG23 | 6        | 0.31          |
| (1,2352) | 1:173:A:VAL:HG13 | 1:173:A:VAL:HG21 | 6        | 0.31          |
| (1,2352) | 1:173:A:VAL:HG13 | 1:173:A:VAL:HG22 | 6        | 0.31          |
| (1,2352) | 1:173:A:VAL:HG13 | 1:173:A:VAL:HG23 | 6        | 0.31          |
| (1,2352) | 1:173:A:VAL:HG11 | 1:173:A:VAL:HG21 | 10       | 0.31          |
| (1,2352) | 1:173:A:VAL:HG11 | 1:173:A:VAL:HG22 | 10       | 0.31          |
| (1,2352) | 1:173:A:VAL:HG11 | 1:173:A:VAL:HG23 | 10       | 0.31          |
| (1,2352) | 1:173:A:VAL:HG12 | 1:173:A:VAL:HG21 | 10       | 0.31          |
| (1,2352) | 1:173:A:VAL:HG12 | 1:173:A:VAL:HG22 | 10       | 0.31          |
| (1,2352) | 1:173:A:VAL:HG12 | 1:173:A:VAL:HG23 | 10       | 0.31          |
| (1,2352) | 1:173:A:VAL:HG13 | 1:173:A:VAL:HG21 | 10       | 0.31          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2352) | 1:173:A:VAL:HG13 | 1:173:A:VAL:HG22 | 10       | 0.31          |
| (1,2352) | 1:173:A:VAL:HG13 | 1:173:A:VAL:HG23 | 10       | 0.31          |
| (1,2093) | 1:153:A:ILE:HA   | 1:153:A:ILE:HG21 | 8        | 0.31          |
| (1,2093) | 1:153:A:ILE:HA   | 1:153:A:ILE:HG22 | 8        | 0.31          |
| (1,2093) | 1:153:A:ILE:HA   | 1:153:A:ILE:HG23 | 8        | 0.31          |
| (1,1938) | 1:135:A:VAL:HG11 | 1:135:A:VAL:HG21 | 1        | 0.31          |
| (1,1938) | 1:135:A:VAL:HG11 | 1:135:A:VAL:HG22 | 1        | 0.31          |
| (1,1938) | 1:135:A:VAL:HG11 | 1:135:A:VAL:HG23 | 1        | 0.31          |
| (1,1938) | 1:135:A:VAL:HG12 | 1:135:A:VAL:HG21 | 1        | 0.31          |
| (1,1938) | 1:135:A:VAL:HG12 | 1:135:A:VAL:HG22 | 1        | 0.31          |
| (1,1938) | 1:135:A:VAL:HG12 | 1:135:A:VAL:HG23 | 1        | 0.31          |
| (1,1938) | 1:135:A:VAL:HG13 | 1:135:A:VAL:HG21 | 1        | 0.31          |
| (1,1938) | 1:135:A:VAL:HG13 | 1:135:A:VAL:HG22 | 1        | 0.31          |
| (1,1938) | 1:135:A:VAL:HG13 | 1:135:A:VAL:HG23 | 1        | 0.31          |
| (1,1938) | 1:135:A:VAL:HG11 | 1:135:A:VAL:HG21 | 2        | 0.31          |
| (1,1938) | 1:135:A:VAL:HG11 | 1:135:A:VAL:HG22 | 2        | 0.31          |
| (1,1938) | 1:135:A:VAL:HG11 | 1:135:A:VAL:HG23 | 2        | 0.31          |
| (1,1938) | 1:135:A:VAL:HG12 | 1:135:A:VAL:HG21 | 2        | 0.31          |
| (1,1938) | 1:135:A:VAL:HG12 | 1:135:A:VAL:HG22 | 2        | 0.31          |
| (1,1938) | 1:135:A:VAL:HG12 | 1:135:A:VAL:HG23 | 2        | 0.31          |
| (1,1938) | 1:135:A:VAL:HG13 | 1:135:A:VAL:HG21 | 2        | 0.31          |
| (1,1938) | 1:135:A:VAL:HG13 | 1:135:A:VAL:HG22 | 2        | 0.31          |
| (1,1938) | 1:135:A:VAL:HG13 | 1:135:A:VAL:HG23 | 2        | 0.31          |
| (1,1938) | 1:135:A:VAL:HG11 | 1:135:A:VAL:HG21 | 7        | 0.31          |
| (1,1938) | 1:135:A:VAL:HG11 | 1:135:A:VAL:HG22 | 7        | 0.31          |
| (1,1938) | 1:135:A:VAL:HG11 | 1:135:A:VAL:HG23 | 7        | 0.31          |
| (1,1938) | 1:135:A:VAL:HG12 | 1:135:A:VAL:HG21 | 7        | 0.31          |
| (1,1938) | 1:135:A:VAL:HG12 | 1:135:A:VAL:HG22 | 7        | 0.31          |
| (1,1938) | 1:135:A:VAL:HG12 | 1:135:A:VAL:HG23 | 7        | 0.31          |
| (1,1938) | 1:135:A:VAL:HG13 | 1:135:A:VAL:HG21 | 7        | 0.31          |
| (1,1938) | 1:135:A:VAL:HG13 | 1:135:A:VAL:HG22 | 7        | 0.31          |
| (1,1938) | 1:135:A:VAL:HG13 | 1:135:A:VAL:HG23 | 7        | 0.31          |
| (1,1938) | 1:135:A:VAL:HG11 | 1:135:A:VAL:HG21 | 9        | 0.31          |
| (1,1938) | 1:135:A:VAL:HG11 | 1:135:A:VAL:HG22 | 9        | 0.31          |
| (1,1938) | 1:135:A:VAL:HG11 | 1:135:A:VAL:HG23 | 9        | 0.31          |
| (1,1938) | 1:135:A:VAL:HG12 | 1:135:A:VAL:HG21 | 9        | 0.31          |
| (1,1938) | 1:135:A:VAL:HG12 | 1:135:A:VAL:HG22 | 9        | 0.31          |
| (1,1938) | 1:135:A:VAL:HG12 | 1:135:A:VAL:HG23 | 9        | 0.31          |
| (1,1938) | 1:135:A:VAL:HG13 | 1:135:A:VAL:HG21 | 9        | 0.31          |
| (1,1938) | 1:135:A:VAL:HG13 | 1:135:A:VAL:HG22 | 9        | 0.31          |
| (1,1938) | 1:135:A:VAL:HG13 | 1:135:A:VAL:HG23 | 9        | 0.31          |
| (1,1845) | 1:132:A:SER:HB2  | 1:145:A:TYR:HD1  | 3        | 0.31          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1845) | 1:132:A:SER:HB2  | 1:145:A:TYR:HD2 | 3        | 0.31          |
| (1,1841) | 1:132:A:SER:HB3  | 1:145:A:TYR:HD1 | 2        | 0.31          |
| (1,1841) | 1:132:A:SER:HB3  | 1:145:A:TYR:HD2 | 2        | 0.31          |
| (1,1777) | 1:121:A:LEU:HD21 | 1:121:A:LEU:H   | 10       | 0.31          |
| (1,1777) | 1:121:A:LEU:HD22 | 1:121:A:LEU:H   | 10       | 0.31          |
| (1,1777) | 1:121:A:LEU:HD23 | 1:121:A:LEU:H   | 10       | 0.31          |
| (1,1770) | 1:120:A:VAL:HG21 | 1:121:A:LEU:H   | 4        | 0.31          |
| (1,1770) | 1:120:A:VAL:HG22 | 1:121:A:LEU:H   | 4        | 0.31          |
| (1,1770) | 1:120:A:VAL:HG23 | 1:121:A:LEU:H   | 4        | 0.31          |
| (1,1767) | 1:120:A:VAL:HG11 | 1:121:A:LEU:H   | 6        | 0.31          |
| (1,1767) | 1:120:A:VAL:HG12 | 1:121:A:LEU:H   | 6        | 0.31          |
| (1,1767) | 1:120:A:VAL:HG13 | 1:121:A:LEU:H   | 6        | 0.31          |
| (1,1557) | 1:103:A:SER:HA   | 1:104:A:LEU:HB2 | 4        | 0.31          |
| (1,1556) | 1:103:A:SER:HA   | 1:104:A:LEU:HB3 | 6        | 0.31          |
| (1,1483) | 1:95:A:PHE:HE1   | 1:116:A:GLU:HB3 | 5        | 0.31          |
| (1,1483) | 1:95:A:PHE:HE2   | 1:116:A:GLU:HB3 | 5        | 0.31          |
| (1,1236) | 1:81:A:ILE:HG21  | 1:154:A:LEU:HB3 | 5        | 0.31          |
| (1,1236) | 1:81:A:ILE:HG22  | 1:154:A:LEU:HB3 | 5        | 0.31          |
| (1,1236) | 1:81:A:ILE:HG23  | 1:154:A:LEU:HB3 | 5        | 0.31          |
| (1,1236) | 1:81:A:ILE:HG21  | 1:154:A:LEU:HB3 | 8        | 0.31          |
| (1,1236) | 1:81:A:ILE:HG22  | 1:154:A:LEU:HB3 | 8        | 0.31          |
| (1,1236) | 1:81:A:ILE:HG23  | 1:154:A:LEU:HB3 | 8        | 0.31          |
| (1,1189) | 1:80:A:GLN:HG2   | 1:98:A:THR:HG21 | 1        | 0.31          |
| (1,1189) | 1:80:A:GLN:HG2   | 1:98:A:THR:HG22 | 1        | 0.31          |
| (1,1189) | 1:80:A:GLN:HG2   | 1:98:A:THR:HG23 | 1        | 0.31          |
| (1,1189) | 1:80:A:GLN:HG3   | 1:98:A:THR:HG21 | 1        | 0.31          |
| (1,1189) | 1:80:A:GLN:HG3   | 1:98:A:THR:HG22 | 1        | 0.31          |
| (1,1189) | 1:80:A:GLN:HG3   | 1:98:A:THR:HG23 | 1        | 0.31          |
| (1,1189) | 1:80:A:GLN:HG2   | 1:98:A:THR:HG21 | 8        | 0.31          |
| (1,1189) | 1:80:A:GLN:HG2   | 1:98:A:THR:HG22 | 8        | 0.31          |
| (1,1189) | 1:80:A:GLN:HG2   | 1:98:A:THR:HG23 | 8        | 0.31          |
| (1,1189) | 1:80:A:GLN:HG3   | 1:98:A:THR:HG21 | 8        | 0.31          |
| (1,1189) | 1:80:A:GLN:HG3   | 1:98:A:THR:HG22 | 8        | 0.31          |
| (1,1189) | 1:80:A:GLN:HG3   | 1:98:A:THR:HG23 | 8        | 0.31          |
| (1,1032) | 1:74:A:PHE:HE1   | 1:168:A:PHE:HZ  | 8        | 0.31          |
| (1,1032) | 1:74:A:PHE:HE2   | 1:168:A:PHE:HZ  | 8        | 0.31          |
| (1,1013) | 1:74:A:PHE:HB2   | 1:163:A:LYS:H   | 10       | 0.31          |
| (1,843)  | 1:66:A:ASN:HD21  | 1:70:A:LEU:HD11 | 9        | 0.31          |
| (1,843)  | 1:66:A:ASN:HD21  | 1:70:A:LEU:HD12 | 9        | 0.31          |
| (1,843)  | 1:66:A:ASN:HD21  | 1:70:A:LEU:HD13 | 9        | 0.31          |
| (1,681)  | 1:60:A:LEU:HD21  | 1:177:A:PHE:HD1 | 2        | 0.31          |
| (1,681)  | 1:60:A:LEU:HD21  | 1:177:A:PHE:HD2 | 2        | 0.31          |

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| Key     | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,681) | 1:60:A:LEU:HD22 | 1:177:A:PHE:HD1  | 2        | 0.31          |
| (1,681) | 1:60:A:LEU:HD22 | 1:177:A:PHE:HD2  | 2        | 0.31          |
| (1,681) | 1:60:A:LEU:HD23 | 1:177:A:PHE:HD1  | 2        | 0.31          |
| (1,681) | 1:60:A:LEU:HD23 | 1:177:A:PHE:HD2  | 2        | 0.31          |
| (1,610) | 1:55:A:VAL:HA   | 1:55:A:VAL:HG11  | 7        | 0.31          |
| (1,610) | 1:55:A:VAL:HA   | 1:55:A:VAL:HG12  | 7        | 0.31          |
| (1,610) | 1:55:A:VAL:HA   | 1:55:A:VAL:HG13  | 7        | 0.31          |
| (1,556) | 1:50:A:TRP:HD1  | 1:151:A:VAL:HG21 | 7        | 0.31          |
| (1,556) | 1:50:A:TRP:HD1  | 1:151:A:VAL:HG22 | 7        | 0.31          |
| (1,556) | 1:50:A:TRP:HD1  | 1:151:A:VAL:HG23 | 7        | 0.31          |
| (1,495) | 1:48:A:ILE:HG21 | 1:50:A:TRP:HE1   | 4        | 0.31          |
| (1,495) | 1:48:A:ILE:HG22 | 1:50:A:TRP:HE1   | 4        | 0.31          |
| (1,495) | 1:48:A:ILE:HG23 | 1:50:A:TRP:HE1   | 4        | 0.31          |
| (1,487) | 1:48:A:ILE:HG12 | 1:48:A:ILE:HG21  | 4        | 0.31          |
| (1,487) | 1:48:A:ILE:HG12 | 1:48:A:ILE:HG22  | 4        | 0.31          |
| (1,487) | 1:48:A:ILE:HG12 | 1:48:A:ILE:HG23  | 4        | 0.31          |
| (1,487) | 1:48:A:ILE:HG12 | 1:48:A:ILE:HG21  | 9        | 0.31          |
| (1,487) | 1:48:A:ILE:HG12 | 1:48:A:ILE:HG22  | 9        | 0.31          |
| (1,487) | 1:48:A:ILE:HG12 | 1:48:A:ILE:HG23  | 9        | 0.31          |
| (1,467) | 1:47:A:ALA:H    | 1:156:A:PHE:HE1  | 2        | 0.31          |
| (1,467) | 1:47:A:ALA:H    | 1:156:A:PHE:HE2  | 2        | 0.31          |
| (1,445) | 1:46:A:TYR:HE1  | 1:141:A:LYS:HE3  | 6        | 0.31          |
| (1,445) | 1:46:A:TYR:HE2  | 1:141:A:LYS:HE3  | 6        | 0.31          |
| (1,427) | 1:46:A:TYR:HA   | 1:156:A:PHE:HE1  | 2        | 0.31          |
| (1,427) | 1:46:A:TYR:HA   | 1:156:A:PHE:HE2  | 2        | 0.31          |
| (1,389) | 1:44:A:ILE:HG21 | 1:44:A:ILE:H     | 1        | 0.31          |
| (1,389) | 1:44:A:ILE:HG22 | 1:44:A:ILE:H     | 1        | 0.31          |
| (1,389) | 1:44:A:ILE:HG23 | 1:44:A:ILE:H     | 1        | 0.31          |
| (1,389) | 1:44:A:ILE:HG21 | 1:44:A:ILE:H     | 8        | 0.31          |
| (1,389) | 1:44:A:ILE:HG22 | 1:44:A:ILE:H     | 8        | 0.31          |
| (1,389) | 1:44:A:ILE:HG23 | 1:44:A:ILE:H     | 8        | 0.31          |
| (1,270) | 1:34:A:PRO:HD3  | 1:168:A:PHE:HE1  | 10       | 0.31          |
| (1,270) | 1:34:A:PRO:HD3  | 1:168:A:PHE:HE2  | 10       | 0.31          |
| (1,238) | 1:32:A:ILE:HG21 | 1:42:A:ASP:HB2   | 6        | 0.31          |
| (1,238) | 1:32:A:ILE:HG21 | 1:42:A:ASP:HB3   | 6        | 0.31          |
| (1,238) | 1:32:A:ILE:HG22 | 1:42:A:ASP:HB2   | 6        | 0.31          |
| (1,238) | 1:32:A:ILE:HG22 | 1:42:A:ASP:HB3   | 6        | 0.31          |
| (1,238) | 1:32:A:ILE:HG23 | 1:42:A:ASP:HB2   | 6        | 0.31          |
| (1,238) | 1:32:A:ILE:HG23 | 1:42:A:ASP:HB3   | 6        | 0.31          |
| (1,123) | 1:27:A:SER:HB2  | 1:27:A:SER:H     | 4        | 0.31          |
| (1,123) | 1:27:A:SER:HB3  | 1:27:A:SER:H     | 4        | 0.31          |
| (1,123) | 1:27:A:SER:HB2  | 1:27:A:SER:H     | 9        | 0.31          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,123)  | 1:27:A:SER:HB3   | 1:27:A:SER:H     | 9        | 0.31          |
| (1,3)    | 1:16:A:ALA:HB1   | 1:16:A:ALA:H     | 7        | 0.31          |
| (1,3)    | 1:16:A:ALA:HB2   | 1:16:A:ALA:H     | 7        | 0.31          |
| (1,3)    | 1:16:A:ALA:HB3   | 1:16:A:ALA:H     | 7        | 0.31          |
| (2,724)  | 1:145:A:TYR:HD1  | 1:147:A:GLU:HG2  | 5        | 0.3           |
| (2,724)  | 1:145:A:TYR:HD1  | 1:147:A:GLU:HG3  | 5        | 0.3           |
| (2,724)  | 1:145:A:TYR:HD2  | 1:147:A:GLU:HG2  | 5        | 0.3           |
| (2,724)  | 1:145:A:TYR:HD2  | 1:147:A:GLU:HG3  | 5        | 0.3           |
| (2,702)  | 1:132:A:SER:HB2  | 1:145:A:TYR:HE1  | 3        | 0.3           |
| (2,702)  | 1:132:A:SER:HB2  | 1:145:A:TYR:HE2  | 3        | 0.3           |
| (1,2352) | 1:173:A:VAL:HG11 | 1:173:A:VAL:HG21 | 4        | 0.3           |
| (1,2352) | 1:173:A:VAL:HG11 | 1:173:A:VAL:HG22 | 4        | 0.3           |
| (1,2352) | 1:173:A:VAL:HG11 | 1:173:A:VAL:HG23 | 4        | 0.3           |
| (1,2352) | 1:173:A:VAL:HG12 | 1:173:A:VAL:HG21 | 4        | 0.3           |
| (1,2352) | 1:173:A:VAL:HG12 | 1:173:A:VAL:HG22 | 4        | 0.3           |
| (1,2352) | 1:173:A:VAL:HG12 | 1:173:A:VAL:HG23 | 4        | 0.3           |
| (1,2352) | 1:173:A:VAL:HG13 | 1:173:A:VAL:HG21 | 4        | 0.3           |
| (1,2352) | 1:173:A:VAL:HG13 | 1:173:A:VAL:HG22 | 4        | 0.3           |
| (1,2352) | 1:173:A:VAL:HG13 | 1:173:A:VAL:HG23 | 4        | 0.3           |
| (1,2352) | 1:173:A:VAL:HG11 | 1:173:A:VAL:HG21 | 5        | 0.3           |
| (1,2352) | 1:173:A:VAL:HG11 | 1:173:A:VAL:HG22 | 5        | 0.3           |
| (1,2352) | 1:173:A:VAL:HG11 | 1:173:A:VAL:HG23 | 5        | 0.3           |
| (1,2352) | 1:173:A:VAL:HG12 | 1:173:A:VAL:HG21 | 5        | 0.3           |
| (1,2352) | 1:173:A:VAL:HG12 | 1:173:A:VAL:HG22 | 5        | 0.3           |
| (1,2352) | 1:173:A:VAL:HG12 | 1:173:A:VAL:HG23 | 5        | 0.3           |
| (1,2352) | 1:173:A:VAL:HG13 | 1:173:A:VAL:HG21 | 5        | 0.3           |
| (1,2352) | 1:173:A:VAL:HG13 | 1:173:A:VAL:HG22 | 5        | 0.3           |
| (1,2352) | 1:173:A:VAL:HG13 | 1:173:A:VAL:HG23 | 5        | 0.3           |
| (1,2352) | 1:173:A:VAL:HG11 | 1:173:A:VAL:HG21 | 8        | 0.3           |
| (1,2352) | 1:173:A:VAL:HG11 | 1:173:A:VAL:HG22 | 8        | 0.3           |
| (1,2352) | 1:173:A:VAL:HG11 | 1:173:A:VAL:HG23 | 8        | 0.3           |
| (1,2352) | 1:173:A:VAL:HG12 | 1:173:A:VAL:HG21 | 8        | 0.3           |
| (1,2352) | 1:173:A:VAL:HG12 | 1:173:A:VAL:HG22 | 8        | 0.3           |
| (1,2352) | 1:173:A:VAL:HG12 | 1:173:A:VAL:HG23 | 8        | 0.3           |
| (1,2352) | 1:173:A:VAL:HG13 | 1:173:A:VAL:HG21 | 8        | 0.3           |
| (1,2352) | 1:173:A:VAL:HG13 | 1:173:A:VAL:HG22 | 8        | 0.3           |
| (1,2352) | 1:173:A:VAL:HG13 | 1:173:A:VAL:HG23 | 8        | 0.3           |
| (1,2352) | 1:173:A:VAL:HG11 | 1:173:A:VAL:HG21 | 9        | 0.3           |
| (1,2352) | 1:173:A:VAL:HG11 | 1:173:A:VAL:HG22 | 9        | 0.3           |
| (1,2352) | 1:173:A:VAL:HG11 | 1:173:A:VAL:HG23 | 9        | 0.3           |
| (1,2352) | 1:173:A:VAL:HG12 | 1:173:A:VAL:HG21 | 9        | 0.3           |
| (1,2352) | 1:173:A:VAL:HG12 | 1:173:A:VAL:HG22 | 9        | 0.3           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2352) | 1:173:A:VAL:HG12 | 1:173:A:VAL:HG23 | 9        | 0.3           |
| (1,2352) | 1:173:A:VAL:HG13 | 1:173:A:VAL:HG21 | 9        | 0.3           |
| (1,2352) | 1:173:A:VAL:HG13 | 1:173:A:VAL:HG22 | 9        | 0.3           |
| (1,2352) | 1:173:A:VAL:HG13 | 1:173:A:VAL:HG23 | 9        | 0.3           |
| (1,2286) | 1:168:A:PHE:HD1  | 1:168:A:PHE:H    | 4        | 0.3           |
| (1,2286) | 1:168:A:PHE:HD2  | 1:168:A:PHE:H    | 4        | 0.3           |
| (1,2286) | 1:168:A:PHE:HD1  | 1:168:A:PHE:H    | 9        | 0.3           |
| (1,2286) | 1:168:A:PHE:HD2  | 1:168:A:PHE:H    | 9        | 0.3           |
| (1,2246) | 1:162:A:ALA:HB1  | 1:168:A:PHE:HZ   | 7        | 0.3           |
| (1,2246) | 1:162:A:ALA:HB2  | 1:168:A:PHE:HZ   | 7        | 0.3           |
| (1,2246) | 1:162:A:ALA:HB3  | 1:168:A:PHE:HZ   | 7        | 0.3           |
| (1,2106) | 1:153:A:ILE:HG21 | 1:155:A:ASN:HD21 | 5        | 0.3           |
| (1,2106) | 1:153:A:ILE:HG21 | 1:155:A:ASN:HD22 | 5        | 0.3           |
| (1,2106) | 1:153:A:ILE:HG22 | 1:155:A:ASN:HD21 | 5        | 0.3           |
| (1,2106) | 1:153:A:ILE:HG22 | 1:155:A:ASN:HD22 | 5        | 0.3           |
| (1,2106) | 1:153:A:ILE:HG23 | 1:155:A:ASN:HD21 | 5        | 0.3           |
| (1,2106) | 1:153:A:ILE:HG23 | 1:155:A:ASN:HD22 | 5        | 0.3           |
| (1,2038) | 1:144:A:VAL:HG21 | 1:144:A:VAL:H    | 4        | 0.3           |
| (1,2038) | 1:144:A:VAL:HG22 | 1:144:A:VAL:H    | 4        | 0.3           |
| (1,2038) | 1:144:A:VAL:HG23 | 1:144:A:VAL:H    | 4        | 0.3           |
| (1,2038) | 1:144:A:VAL:HG21 | 1:144:A:VAL:H    | 5        | 0.3           |
| (1,2038) | 1:144:A:VAL:HG22 | 1:144:A:VAL:H    | 5        | 0.3           |
| (1,2038) | 1:144:A:VAL:HG23 | 1:144:A:VAL:H    | 5        | 0.3           |
| (1,1941) | 1:135:A:VAL:HG21 | 1:135:A:VAL:H    | 3        | 0.3           |
| (1,1941) | 1:135:A:VAL:HG22 | 1:135:A:VAL:H    | 3        | 0.3           |
| (1,1941) | 1:135:A:VAL:HG23 | 1:135:A:VAL:H    | 3        | 0.3           |
| (1,1845) | 1:132:A:SER:HB2  | 1:145:A:TYR:HD1  | 7        | 0.3           |
| (1,1845) | 1:132:A:SER:HB2  | 1:145:A:TYR:HD2  | 7        | 0.3           |
| (1,1841) | 1:132:A:SER:HB3  | 1:145:A:TYR:HD1  | 1        | 0.3           |
| (1,1841) | 1:132:A:SER:HB3  | 1:145:A:TYR:HD2  | 1        | 0.3           |
| (1,1640) | 1:111:A:ILE:HG21 | 1:112:A:VAL:H    | 1        | 0.3           |
| (1,1640) | 1:111:A:ILE:HG22 | 1:112:A:VAL:H    | 1        | 0.3           |
| (1,1640) | 1:111:A:ILE:HG23 | 1:112:A:VAL:H    | 1        | 0.3           |
| (1,1556) | 1:103:A:SER:HA   | 1:104:A:LEU:HB3  | 5        | 0.3           |
| (1,1546) | 1:102:A:ILE:HG21 | 1:108:A:SER:HA   | 5        | 0.3           |
| (1,1546) | 1:102:A:ILE:HG22 | 1:108:A:SER:HA   | 5        | 0.3           |
| (1,1546) | 1:102:A:ILE:HG23 | 1:108:A:SER:HA   | 5        | 0.3           |
| (1,1343) | 1:85:A:TYR:HE1   | 1:152:A:ALA:HA   | 7        | 0.3           |
| (1,1343) | 1:85:A:TYR:HE2   | 1:152:A:ALA:HA   | 7        | 0.3           |
| (1,1342) | 1:85:A:TYR:HE1   | 1:143:A:ILE:HG21 | 4        | 0.3           |
| (1,1342) | 1:85:A:TYR:HE1   | 1:143:A:ILE:HG22 | 4        | 0.3           |
| (1,1342) | 1:85:A:TYR:HE1   | 1:143:A:ILE:HG23 | 4        | 0.3           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1342) | 1:85:A:TYR:HE2   | 1:143:A:ILE:HG21 | 4        | 0.3           |
| (1,1342) | 1:85:A:TYR:HE2   | 1:143:A:ILE:HG22 | 4        | 0.3           |
| (1,1342) | 1:85:A:TYR:HE2   | 1:143:A:ILE:HG23 | 4        | 0.3           |
| (1,1338) | 1:85:A:TYR:HD1   | 1:86:A:GLU:H     | 10       | 0.3           |
| (1,1338) | 1:85:A:TYR:HD2   | 1:86:A:GLU:H     | 10       | 0.3           |
| (1,1236) | 1:81:A:ILE:HG21  | 1:154:A:LEU:HB3  | 7        | 0.3           |
| (1,1236) | 1:81:A:ILE:HG22  | 1:154:A:LEU:HB3  | 7        | 0.3           |
| (1,1236) | 1:81:A:ILE:HG23  | 1:154:A:LEU:HB3  | 7        | 0.3           |
| (1,1232) | 1:81:A:ILE:HG21  | 1:99:A:LYS:H     | 3        | 0.3           |
| (1,1232) | 1:81:A:ILE:HG22  | 1:99:A:LYS:H     | 3        | 0.3           |
| (1,1232) | 1:81:A:ILE:HG23  | 1:99:A:LYS:H     | 3        | 0.3           |
| (1,1180) | 1:80:A:GLN:HA    | 1:101:A:VAL:H    | 4        | 0.3           |
| (1,1162) | 1:79:A:ILE:HG13  | 1:80:A:GLN:H     | 5        | 0.3           |
| (1,621)  | 1:55:A:VAL:H     | 1:55:A:VAL:HG21  | 2        | 0.3           |
| (1,621)  | 1:55:A:VAL:H     | 1:55:A:VAL:HG22  | 2        | 0.3           |
| (1,621)  | 1:55:A:VAL:H     | 1:55:A:VAL:HG23  | 2        | 0.3           |
| (1,610)  | 1:55:A:VAL:HA    | 1:55:A:VAL:HG11  | 5        | 0.3           |
| (1,610)  | 1:55:A:VAL:HA    | 1:55:A:VAL:HG12  | 5        | 0.3           |
| (1,610)  | 1:55:A:VAL:HA    | 1:55:A:VAL:HG13  | 5        | 0.3           |
| (1,242)  | 1:32:A:ILE:HG21  | 1:160:A:TYR:HE1  | 3        | 0.3           |
| (1,242)  | 1:32:A:ILE:HG21  | 1:160:A:TYR:HE2  | 3        | 0.3           |
| (1,242)  | 1:32:A:ILE:HG22  | 1:160:A:TYR:HE1  | 3        | 0.3           |
| (1,242)  | 1:32:A:ILE:HG22  | 1:160:A:TYR:HE2  | 3        | 0.3           |
| (1,242)  | 1:32:A:ILE:HG23  | 1:160:A:TYR:HE1  | 3        | 0.3           |
| (1,242)  | 1:32:A:ILE:HG23  | 1:160:A:TYR:HE2  | 3        | 0.3           |
| (1,212)  | 1:32:A:ILE:HB    | 1:32:A:ILE:HD11  | 4        | 0.3           |
| (1,212)  | 1:32:A:ILE:HB    | 1:32:A:ILE:HD12  | 4        | 0.3           |
| (1,212)  | 1:32:A:ILE:HB    | 1:32:A:ILE:HD13  | 4        | 0.3           |
| (1,123)  | 1:27:A:SER:HB2   | 1:27:A:SER:H     | 10       | 0.3           |
| (1,123)  | 1:27:A:SER:HB3   | 1:27:A:SER:H     | 10       | 0.3           |
| (1,3)    | 1:16:A:ALA:HB1   | 1:16:A:ALA:H     | 5        | 0.3           |
| (1,3)    | 1:16:A:ALA:HB2   | 1:16:A:ALA:H     | 5        | 0.3           |
| (1,3)    | 1:16:A:ALA:HB3   | 1:16:A:ALA:H     | 5        | 0.3           |
| (2,755)  | 1:167:A:LEU:H    | 1:167:A:LEU:HD11 | 4        | 0.29          |
| (2,755)  | 1:167:A:LEU:H    | 1:167:A:LEU:HD12 | 4        | 0.29          |
| (2,755)  | 1:167:A:LEU:H    | 1:167:A:LEU:HD13 | 4        | 0.29          |
| (2,755)  | 1:167:A:LEU:H    | 1:167:A:LEU:HD11 | 10       | 0.29          |
| (2,755)  | 1:167:A:LEU:H    | 1:167:A:LEU:HD12 | 10       | 0.29          |
| (2,755)  | 1:167:A:LEU:H    | 1:167:A:LEU:HD13 | 10       | 0.29          |
| (2,753)  | 1:167:A:LEU:HD11 | 1:167:A:LEU:H    | 4        | 0.29          |
| (2,753)  | 1:167:A:LEU:HD12 | 1:167:A:LEU:H    | 4        | 0.29          |
| (2,753)  | 1:167:A:LEU:HD13 | 1:167:A:LEU:H    | 4        | 0.29          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,753)  | 1:167:A:LEU:HD11 | 1:167:A:LEU:H    | 10       | 0.29          |
| (2,753)  | 1:167:A:LEU:HD12 | 1:167:A:LEU:H    | 10       | 0.29          |
| (2,753)  | 1:167:A:LEU:HD13 | 1:167:A:LEU:H    | 10       | 0.29          |
| (2,735)  | 1:158:A:ALA:H    | 1:160:A:TYR:HE1  | 10       | 0.29          |
| (2,735)  | 1:158:A:ALA:H    | 1:160:A:TYR:HE2  | 10       | 0.29          |
| (2,383)  | 1:70:A:LEU:HA    | 1:74:A:PHE:HD1   | 3        | 0.29          |
| (2,383)  | 1:70:A:LEU:HA    | 1:74:A:PHE:HD2   | 3        | 0.29          |
| (1,2327) | 1:171:A:LEU:HG   | 1:171:A:LEU:H    | 6        | 0.29          |
| (1,2262) | 1:164:A:GLU:HA   | 1:164:A:GLU:HG2  | 4        | 0.29          |
| (1,2262) | 1:164:A:GLU:HA   | 1:164:A:GLU:HG3  | 4        | 0.29          |
| (1,2106) | 1:153:A:ILE:HG21 | 1:155:A:ASN:HD21 | 1        | 0.29          |
| (1,2106) | 1:153:A:ILE:HG21 | 1:155:A:ASN:HD22 | 1        | 0.29          |
| (1,2106) | 1:153:A:ILE:HG22 | 1:155:A:ASN:HD21 | 1        | 0.29          |
| (1,2106) | 1:153:A:ILE:HG22 | 1:155:A:ASN:HD22 | 1        | 0.29          |
| (1,2106) | 1:153:A:ILE:HG23 | 1:155:A:ASN:HD21 | 1        | 0.29          |
| (1,2106) | 1:153:A:ILE:HG23 | 1:155:A:ASN:HD22 | 1        | 0.29          |
| (1,2028) | 1:143:A:ILE:HD11 | 1:143:A:ILE:H    | 5        | 0.29          |
| (1,2028) | 1:143:A:ILE:HD12 | 1:143:A:ILE:H    | 5        | 0.29          |
| (1,2028) | 1:143:A:ILE:HD13 | 1:143:A:ILE:H    | 5        | 0.29          |
| (1,1546) | 1:102:A:ILE:HG21 | 1:108:A:SER:HA   | 6        | 0.29          |
| (1,1546) | 1:102:A:ILE:HG22 | 1:108:A:SER:HA   | 6        | 0.29          |
| (1,1546) | 1:102:A:ILE:HG23 | 1:108:A:SER:HA   | 6        | 0.29          |
| (1,1485) | 1:95:A:PHE:HE1   | 1:117:A:ASP:HA   | 9        | 0.29          |
| (1,1485) | 1:95:A:PHE:HE2   | 1:117:A:ASP:HA   | 9        | 0.29          |
| (1,1485) | 1:95:A:PHE:HE1   | 1:117:A:ASP:HA   | 10       | 0.29          |
| (1,1485) | 1:95:A:PHE:HE2   | 1:117:A:ASP:HA   | 10       | 0.29          |
| (1,1483) | 1:95:A:PHE:HE1   | 1:116:A:GLU:HB3  | 1        | 0.29          |
| (1,1483) | 1:95:A:PHE:HE2   | 1:116:A:GLU:HB3  | 1        | 0.29          |
| (1,1483) | 1:95:A:PHE:HE1   | 1:116:A:GLU:HB3  | 4        | 0.29          |
| (1,1483) | 1:95:A:PHE:HE2   | 1:116:A:GLU:HB3  | 4        | 0.29          |
| (1,1399) | 1:87:A:THR:HG21  | 1:87:A:THR:H     | 5        | 0.29          |
| (1,1399) | 1:87:A:THR:HG22  | 1:87:A:THR:H     | 5        | 0.29          |
| (1,1399) | 1:87:A:THR:HG23  | 1:87:A:THR:H     | 5        | 0.29          |
| (1,1343) | 1:85:A:TYR:HE1   | 1:152:A:ALA:HA   | 8        | 0.29          |
| (1,1343) | 1:85:A:TYR:HE2   | 1:152:A:ALA:HA   | 8        | 0.29          |
| (1,1252) | 1:82:A:THR:HA    | 1:82:A:THR:HG21  | 2        | 0.29          |
| (1,1252) | 1:82:A:THR:HA    | 1:82:A:THR:HG22  | 2        | 0.29          |
| (1,1252) | 1:82:A:THR:HA    | 1:82:A:THR:HG23  | 2        | 0.29          |
| (1,1180) | 1:80:A:GLN:HA    | 1:101:A:VAL:H    | 1        | 0.29          |
| (1,1162) | 1:79:A:ILE:HG13  | 1:80:A:GLN:H     | 6        | 0.29          |
| (1,1071) | 1:76:A:TYR:HE1   | 1:160:A:TYR:HA   | 7        | 0.29          |
| (1,1071) | 1:76:A:TYR:HE2   | 1:160:A:TYR:HA   | 7        | 0.29          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1020) | 1:74:A:PHE:HD1  | 1:162:A:ALA:HA  | 8        | 0.29          |
| (1,1020) | 1:74:A:PHE:HD2  | 1:162:A:ALA:HA  | 8        | 0.29          |
| (1,852)  | 1:66:A:ASN:HD22 | 1:70:A:LEU:HD21 | 5        | 0.29          |
| (1,852)  | 1:66:A:ASN:HD22 | 1:70:A:LEU:HD22 | 5        | 0.29          |
| (1,852)  | 1:66:A:ASN:HD22 | 1:70:A:LEU:HD23 | 5        | 0.29          |
| (1,852)  | 1:66:A:ASN:HD22 | 1:70:A:LEU:HD21 | 7        | 0.29          |
| (1,852)  | 1:66:A:ASN:HD22 | 1:70:A:LEU:HD22 | 7        | 0.29          |
| (1,852)  | 1:66:A:ASN:HD22 | 1:70:A:LEU:HD23 | 7        | 0.29          |
| (1,495)  | 1:48:A:ILE:HG21 | 1:50:A:TRP:HE1  | 9        | 0.29          |
| (1,495)  | 1:48:A:ILE:HG22 | 1:50:A:TRP:HE1  | 9        | 0.29          |
| (1,495)  | 1:48:A:ILE:HG23 | 1:50:A:TRP:HE1  | 9        | 0.29          |
| (1,487)  | 1:48:A:ILE:HG12 | 1:48:A:ILE:HG21 | 1        | 0.29          |
| (1,487)  | 1:48:A:ILE:HG12 | 1:48:A:ILE:HG22 | 1        | 0.29          |
| (1,487)  | 1:48:A:ILE:HG12 | 1:48:A:ILE:HG23 | 1        | 0.29          |
| (1,467)  | 1:47:A:ALA:H    | 1:156:A:PHE:HE1 | 5        | 0.29          |
| (1,467)  | 1:47:A:ALA:H    | 1:156:A:PHE:HE2 | 5        | 0.29          |
| (1,467)  | 1:47:A:ALA:H    | 1:156:A:PHE:HE1 | 7        | 0.29          |
| (1,467)  | 1:47:A:ALA:H    | 1:156:A:PHE:HE2 | 7        | 0.29          |
| (1,456)  | 1:47:A:ALA:HB1  | 1:156:A:PHE:HZ  | 1        | 0.29          |
| (1,456)  | 1:47:A:ALA:HB2  | 1:156:A:PHE:HZ  | 1        | 0.29          |
| (1,456)  | 1:47:A:ALA:HB3  | 1:156:A:PHE:HZ  | 1        | 0.29          |
| (1,455)  | 1:47:A:ALA:HB1  | 1:48:A:ILE:H    | 1        | 0.29          |
| (1,455)  | 1:47:A:ALA:HB2  | 1:48:A:ILE:H    | 1        | 0.29          |
| (1,455)  | 1:47:A:ALA:HB3  | 1:48:A:ILE:H    | 1        | 0.29          |
| (1,353)  | 1:42:A:ASP:HB2  | 1:158:A:ALA:HB1 | 3        | 0.29          |
| (1,353)  | 1:42:A:ASP:HB2  | 1:158:A:ALA:HB2 | 3        | 0.29          |
| (1,353)  | 1:42:A:ASP:HB2  | 1:158:A:ALA:HB3 | 3        | 0.29          |
| (1,353)  | 1:42:A:ASP:HB3  | 1:158:A:ALA:HB1 | 3        | 0.29          |
| (1,353)  | 1:42:A:ASP:HB3  | 1:158:A:ALA:HB2 | 3        | 0.29          |
| (1,353)  | 1:42:A:ASP:HB3  | 1:158:A:ALA:HB3 | 3        | 0.29          |
| (1,257)  | 1:33:A:THR:HB   | 1:33:A:THR:HG21 | 2        | 0.29          |
| (1,257)  | 1:33:A:THR:HB   | 1:33:A:THR:HG22 | 2        | 0.29          |
| (1,257)  | 1:33:A:THR:HB   | 1:33:A:THR:HG23 | 2        | 0.29          |
| (1,166)  | 1:29:A:LEU:HD11 | 1:175:A:PHE:H   | 10       | 0.29          |
| (1,166)  | 1:29:A:LEU:HD12 | 1:175:A:PHE:H   | 10       | 0.29          |
| (1,166)  | 1:29:A:LEU:HD13 | 1:175:A:PHE:H   | 10       | 0.29          |
| (1,11)   | 1:20:A:SER:HB2  | 1:21:A:GLU:H    | 1        | 0.29          |
| (1,11)   | 1:20:A:SER:HB3  | 1:21:A:GLU:H    | 1        | 0.29          |
| (1,3)    | 1:16:A:ALA:HB1  | 1:16:A:ALA:H    | 8        | 0.29          |
| (1,3)    | 1:16:A:ALA:HB2  | 1:16:A:ALA:H    | 8        | 0.29          |
| (1,3)    | 1:16:A:ALA:HB3  | 1:16:A:ALA:H    | 8        | 0.29          |
| (2,714)  | 1:141:A:LYS:HD2 | 1:142:A:ILE:H   | 1        | 0.28          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,714)  | 1:141:A:LYS:HD3  | 1:142:A:ILE:H    | 1        | 0.28          |
| (2,628)  | 1:122:A:TYR:HB3  | 1:123:A:PRO:HD2  | 6        | 0.28          |
| (2,625)  | 1:121:A:LEU:H    | 1:122:A:TYR:HD1  | 7        | 0.28          |
| (2,625)  | 1:121:A:LEU:H    | 1:122:A:TYR:HD2  | 7        | 0.28          |
| (2,567)  | 1:90:A:THR:HG21  | 1:92:A:LEU:H     | 9        | 0.28          |
| (2,567)  | 1:90:A:THR:HG22  | 1:92:A:LEU:H     | 9        | 0.28          |
| (2,567)  | 1:90:A:THR:HG23  | 1:92:A:LEU:H     | 9        | 0.28          |
| (2,547)  | 1:87:A:THR:HG21  | 1:91:A:ALA:H     | 2        | 0.28          |
| (2,547)  | 1:87:A:THR:HG22  | 1:91:A:ALA:H     | 2        | 0.28          |
| (2,547)  | 1:87:A:THR:HG23  | 1:91:A:ALA:H     | 2        | 0.28          |
| (2,522)  | 1:85:A:TYR:HD1   | 1:134:A:TRP:HA   | 3        | 0.28          |
| (2,522)  | 1:85:A:TYR:HD2   | 1:134:A:TRP:HA   | 3        | 0.28          |
| (2,517)  | 1:84:A:GLY:HA2   | 1:85:A:TYR:HD1   | 4        | 0.28          |
| (2,517)  | 1:84:A:GLY:HA2   | 1:85:A:TYR:HD2   | 4        | 0.28          |
| (2,517)  | 1:84:A:GLY:HA3   | 1:85:A:TYR:HD1   | 4        | 0.28          |
| (2,517)  | 1:84:A:GLY:HA3   | 1:85:A:TYR:HD2   | 4        | 0.28          |
| (2,481)  | 1:80:A:GLN:HE22  | 1:98:A:THR:HG21  | 2        | 0.28          |
| (2,481)  | 1:80:A:GLN:HE22  | 1:98:A:THR:HG22  | 2        | 0.28          |
| (2,481)  | 1:80:A:GLN:HE22  | 1:98:A:THR:HG23  | 2        | 0.28          |
| (1,2371) | 1:174:A:ILE:HG21 | 1:175:A:PHE:H    | 5        | 0.28          |
| (1,2371) | 1:174:A:ILE:HG22 | 1:175:A:PHE:H    | 5        | 0.28          |
| (1,2371) | 1:174:A:ILE:HG23 | 1:175:A:PHE:H    | 5        | 0.28          |
| (1,2303) | 1:170:A:SER:HA   | 1:171:A:LEU:HD11 | 1        | 0.28          |
| (1,2303) | 1:170:A:SER:HA   | 1:171:A:LEU:HD12 | 1        | 0.28          |
| (1,2303) | 1:170:A:SER:HA   | 1:171:A:LEU:HD13 | 1        | 0.28          |
| (1,2246) | 1:162:A:ALA:HB1  | 1:168:A:PHE:HZ   | 4        | 0.28          |
| (1,2246) | 1:162:A:ALA:HB2  | 1:168:A:PHE:HZ   | 4        | 0.28          |
| (1,2246) | 1:162:A:ALA:HB3  | 1:168:A:PHE:HZ   | 4        | 0.28          |
| (1,2177) | 1:157:A:LYS:H    | 1:158:A:ALA:HA   | 6        | 0.28          |
| (1,2177) | 1:157:A:LYS:H    | 1:158:A:ALA:HA   | 9        | 0.28          |
| (1,2053) | 1:145:A:TYR:HD1  | 1:145:A:TYR:H    | 6        | 0.28          |
| (1,2053) | 1:145:A:TYR:HD2  | 1:145:A:TYR:H    | 6        | 0.28          |
| (1,2015) | 1:142:A:ILE:HG21 | 1:144:A:VAL:H    | 2        | 0.28          |
| (1,2015) | 1:142:A:ILE:HG22 | 1:144:A:VAL:H    | 2        | 0.28          |
| (1,2015) | 1:142:A:ILE:HG23 | 1:144:A:VAL:H    | 2        | 0.28          |
| (1,2013) | 1:142:A:ILE:HG21 | 1:143:A:ILE:H    | 3        | 0.28          |
| (1,2013) | 1:142:A:ILE:HG22 | 1:143:A:ILE:H    | 3        | 0.28          |
| (1,2013) | 1:142:A:ILE:HG23 | 1:143:A:ILE:H    | 3        | 0.28          |
| (1,2003) | 1:142:A:ILE:HA   | 1:142:A:ILE:HG21 | 4        | 0.28          |
| (1,2003) | 1:142:A:ILE:HA   | 1:142:A:ILE:HG22 | 4        | 0.28          |
| (1,2003) | 1:142:A:ILE:HA   | 1:142:A:ILE:HG23 | 4        | 0.28          |
| (1,2003) | 1:142:A:ILE:HA   | 1:142:A:ILE:HG21 | 7        | 0.28          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2003) | 1:142:A:ILE:HA   | 1:142:A:ILE:HG22 | 7        | 0.28          |
| (1,2003) | 1:142:A:ILE:HA   | 1:142:A:ILE:HG23 | 7        | 0.28          |
| (1,2003) | 1:142:A:ILE:HA   | 1:142:A:ILE:HG21 | 9        | 0.28          |
| (1,2003) | 1:142:A:ILE:HA   | 1:142:A:ILE:HG22 | 9        | 0.28          |
| (1,2003) | 1:142:A:ILE:HA   | 1:142:A:ILE:HG23 | 9        | 0.28          |
| (1,1954) | 1:136:A:PRO:HG2  | 1:155:A:ASN:HD21 | 1        | 0.28          |
| (1,1954) | 1:136:A:PRO:HG2  | 1:155:A:ASN:HD22 | 1        | 0.28          |
| (1,1954) | 1:136:A:PRO:HG2  | 1:155:A:ASN:HD21 | 4        | 0.28          |
| (1,1954) | 1:136:A:PRO:HG2  | 1:155:A:ASN:HD22 | 4        | 0.28          |
| (1,1859) | 1:133:A:ILE:HD11 | 1:144:A:VAL:HB   | 8        | 0.28          |
| (1,1859) | 1:133:A:ILE:HD12 | 1:144:A:VAL:HB   | 8        | 0.28          |
| (1,1859) | 1:133:A:ILE:HD13 | 1:144:A:VAL:HB   | 8        | 0.28          |
| (1,1767) | 1:120:A:VAL:HG11 | 1:121:A:LEU:H    | 3        | 0.28          |
| (1,1767) | 1:120:A:VAL:HG12 | 1:121:A:LEU:H    | 3        | 0.28          |
| (1,1767) | 1:120:A:VAL:HG13 | 1:121:A:LEU:H    | 3        | 0.28          |
| (1,1706) | 1:115:A:LYS:HG2  | 1:115:A:LYS:H    | 1        | 0.28          |
| (1,1706) | 1:115:A:LYS:HG3  | 1:115:A:LYS:H    | 1        | 0.28          |
| (1,1706) | 1:115:A:LYS:HG2  | 1:115:A:LYS:H    | 8        | 0.28          |
| (1,1706) | 1:115:A:LYS:HG3  | 1:115:A:LYS:H    | 8        | 0.28          |
| (1,1653) | 1:113:A:LEU:HA   | 1:113:A:LEU:HD21 | 10       | 0.28          |
| (1,1653) | 1:113:A:LEU:HA   | 1:113:A:LEU:HD22 | 10       | 0.28          |
| (1,1653) | 1:113:A:LEU:HA   | 1:113:A:LEU:HD23 | 10       | 0.28          |
| (1,1252) | 1:82:A:THR:HA    | 1:82:A:THR:HG21  | 9        | 0.28          |
| (1,1252) | 1:82:A:THR:HA    | 1:82:A:THR:HG22  | 9        | 0.28          |
| (1,1252) | 1:82:A:THR:HA    | 1:82:A:THR:HG23  | 9        | 0.28          |
| (1,1180) | 1:80:A:GLN:HA    | 1:101:A:VAL:H    | 2        | 0.28          |
| (1,1162) | 1:79:A:ILE:HG13  | 1:80:A:GLN:H     | 1        | 0.28          |
| (1,1162) | 1:79:A:ILE:HG13  | 1:80:A:GLN:H     | 9        | 0.28          |
| (1,999)  | 1:74:A:PHE:HA    | 1:74:A:PHE:HD1   | 8        | 0.28          |
| (1,999)  | 1:74:A:PHE:HA    | 1:74:A:PHE:HD2   | 8        | 0.28          |
| (1,908)  | 1:69:A:GLN:HB3   | 1:70:A:LEU:H     | 10       | 0.28          |
| (1,873)  | 1:67:A:ALA:HB1   | 1:68:A:GLU:H     | 4        | 0.28          |
| (1,873)  | 1:67:A:ALA:HB2   | 1:68:A:GLU:H     | 4        | 0.28          |
| (1,873)  | 1:67:A:ALA:HB3   | 1:68:A:GLU:H     | 4        | 0.28          |
| (1,844)  | 1:66:A:ASN:HD21  | 1:70:A:LEU:HD21  | 1        | 0.28          |
| (1,844)  | 1:66:A:ASN:HD21  | 1:70:A:LEU:HD22  | 1        | 0.28          |
| (1,844)  | 1:66:A:ASN:HD21  | 1:70:A:LEU:HD23  | 1        | 0.28          |
| (1,755)  | 1:63:A:THR:HG21  | 1:108:A:SER:HA   | 10       | 0.28          |
| (1,755)  | 1:63:A:THR:HG22  | 1:108:A:SER:HA   | 10       | 0.28          |
| (1,755)  | 1:63:A:THR:HG23  | 1:108:A:SER:HA   | 10       | 0.28          |
| (1,727)  | 1:62:A:VAL:HG11  | 1:177:A:PHE:HE1  | 5        | 0.28          |
| (1,727)  | 1:62:A:VAL:HG11  | 1:177:A:PHE:HE2  | 5        | 0.28          |

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| Key     | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,727) | 1:62:A:VAL:HG12 | 1:177:A:PHE:HE1  | 5        | 0.28          |
| (1,727) | 1:62:A:VAL:HG12 | 1:177:A:PHE:HE2  | 5        | 0.28          |
| (1,727) | 1:62:A:VAL:HG13 | 1:177:A:PHE:HE1  | 5        | 0.28          |
| (1,727) | 1:62:A:VAL:HG13 | 1:177:A:PHE:HE2  | 5        | 0.28          |
| (1,724) | 1:62:A:VAL:HG11 | 1:63:A:THR:H     | 5        | 0.28          |
| (1,724) | 1:62:A:VAL:HG12 | 1:63:A:THR:H     | 5        | 0.28          |
| (1,724) | 1:62:A:VAL:HG13 | 1:63:A:THR:H     | 5        | 0.28          |
| (1,709) | 1:62:A:VAL:HA   | 1:62:A:VAL:HG11  | 3        | 0.28          |
| (1,709) | 1:62:A:VAL:HA   | 1:62:A:VAL:HG12  | 3        | 0.28          |
| (1,709) | 1:62:A:VAL:HA   | 1:62:A:VAL:HG13  | 3        | 0.28          |
| (1,610) | 1:55:A:VAL:HA   | 1:55:A:VAL:HG11  | 3        | 0.28          |
| (1,610) | 1:55:A:VAL:HA   | 1:55:A:VAL:HG12  | 3        | 0.28          |
| (1,610) | 1:55:A:VAL:HA   | 1:55:A:VAL:HG13  | 3        | 0.28          |
| (1,610) | 1:55:A:VAL:HA   | 1:55:A:VAL:HG11  | 4        | 0.28          |
| (1,610) | 1:55:A:VAL:HA   | 1:55:A:VAL:HG12  | 4        | 0.28          |
| (1,610) | 1:55:A:VAL:HA   | 1:55:A:VAL:HG13  | 4        | 0.28          |
| (1,610) | 1:55:A:VAL:HA   | 1:55:A:VAL:HG11  | 8        | 0.28          |
| (1,610) | 1:55:A:VAL:HA   | 1:55:A:VAL:HG12  | 8        | 0.28          |
| (1,610) | 1:55:A:VAL:HA   | 1:55:A:VAL:HG13  | 8        | 0.28          |
| (1,597) | 1:53:A:ASP:HB2  | 1:54:A:GLN:H     | 5        | 0.28          |
| (1,597) | 1:53:A:ASP:HB3  | 1:54:A:GLN:H     | 5        | 0.28          |
| (1,568) | 1:51:A:ILE:HA   | 1:51:A:ILE:HG21  | 5        | 0.28          |
| (1,568) | 1:51:A:ILE:HA   | 1:51:A:ILE:HG22  | 5        | 0.28          |
| (1,568) | 1:51:A:ILE:HA   | 1:51:A:ILE:HG23  | 5        | 0.28          |
| (1,436) | 1:46:A:TYR:HB2  | 1:153:A:ILE:HG21 | 3        | 0.28          |
| (1,436) | 1:46:A:TYR:HB2  | 1:153:A:ILE:HG22 | 3        | 0.28          |
| (1,436) | 1:46:A:TYR:HB2  | 1:153:A:ILE:HG23 | 3        | 0.28          |
| (1,362) | 1:42:A:ASP:H    | 1:160:A:TYR:HE1  | 1        | 0.28          |
| (1,362) | 1:42:A:ASP:H    | 1:160:A:TYR:HE2  | 1        | 0.28          |
| (1,286) | 1:36:A:ALA:HA   | 1:37:A:GLY:H     | 10       | 0.28          |
| (1,257) | 1:33:A:THR:HB   | 1:33:A:THR:HG21  | 3        | 0.28          |
| (1,257) | 1:33:A:THR:HB   | 1:33:A:THR:HG22  | 3        | 0.28          |
| (1,257) | 1:33:A:THR:HB   | 1:33:A:THR:HG23  | 3        | 0.28          |
| (1,257) | 1:33:A:THR:HB   | 1:33:A:THR:HG21  | 4        | 0.28          |
| (1,257) | 1:33:A:THR:HB   | 1:33:A:THR:HG22  | 4        | 0.28          |
| (1,257) | 1:33:A:THR:HB   | 1:33:A:THR:HG23  | 4        | 0.28          |
| (1,257) | 1:33:A:THR:HB   | 1:33:A:THR:HG21  | 5        | 0.28          |
| (1,257) | 1:33:A:THR:HB   | 1:33:A:THR:HG22  | 5        | 0.28          |
| (1,257) | 1:33:A:THR:HB   | 1:33:A:THR:HG23  | 5        | 0.28          |
| (1,257) | 1:33:A:THR:HB   | 1:33:A:THR:HG21  | 6        | 0.28          |
| (1,257) | 1:33:A:THR:HB   | 1:33:A:THR:HG22  | 6        | 0.28          |
| (1,257) | 1:33:A:THR:HB   | 1:33:A:THR:HG23  | 6        | 0.28          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,257) | 1:33:A:THR:HB    | 1:33:A:THR:HG21 | 7        | 0.28          |
| (1,257) | 1:33:A:THR:HB    | 1:33:A:THR:HG22 | 7        | 0.28          |
| (1,257) | 1:33:A:THR:HB    | 1:33:A:THR:HG23 | 7        | 0.28          |
| (1,257) | 1:33:A:THR:HB    | 1:33:A:THR:HG21 | 8        | 0.28          |
| (1,257) | 1:33:A:THR:HB    | 1:33:A:THR:HG22 | 8        | 0.28          |
| (1,257) | 1:33:A:THR:HB    | 1:33:A:THR:HG23 | 8        | 0.28          |
| (1,212) | 1:32:A:ILE:HB    | 1:32:A:ILE:HD11 | 3        | 0.28          |
| (1,212) | 1:32:A:ILE:HB    | 1:32:A:ILE:HD12 | 3        | 0.28          |
| (1,212) | 1:32:A:ILE:HB    | 1:32:A:ILE:HD13 | 3        | 0.28          |
| (1,171) | 1:29:A:LEU:HD21  | 1:175:A:PHE:H   | 2        | 0.28          |
| (1,171) | 1:29:A:LEU:HD22  | 1:175:A:PHE:H   | 2        | 0.28          |
| (1,171) | 1:29:A:LEU:HD23  | 1:175:A:PHE:H   | 2        | 0.28          |
| (1,170) | 1:29:A:LEU:HD21  | 1:175:A:PHE:HD1 | 5        | 0.28          |
| (1,170) | 1:29:A:LEU:HD21  | 1:175:A:PHE:HD2 | 5        | 0.28          |
| (1,170) | 1:29:A:LEU:HD22  | 1:175:A:PHE:HD1 | 5        | 0.28          |
| (1,170) | 1:29:A:LEU:HD22  | 1:175:A:PHE:HD2 | 5        | 0.28          |
| (1,170) | 1:29:A:LEU:HD23  | 1:175:A:PHE:HD1 | 5        | 0.28          |
| (1,170) | 1:29:A:LEU:HD23  | 1:175:A:PHE:HD2 | 5        | 0.28          |
| (1,170) | 1:29:A:LEU:HD21  | 1:175:A:PHE:HD1 | 8        | 0.28          |
| (1,170) | 1:29:A:LEU:HD21  | 1:175:A:PHE:HD2 | 8        | 0.28          |
| (1,170) | 1:29:A:LEU:HD22  | 1:175:A:PHE:HD1 | 8        | 0.28          |
| (1,170) | 1:29:A:LEU:HD22  | 1:175:A:PHE:HD2 | 8        | 0.28          |
| (1,170) | 1:29:A:LEU:HD23  | 1:175:A:PHE:HD1 | 8        | 0.28          |
| (1,170) | 1:29:A:LEU:HD23  | 1:175:A:PHE:HD2 | 8        | 0.28          |
| (2,628) | 1:122:A:TYR:HB3  | 1:123:A:PRO:HD2 | 3        | 0.27          |
| (2,628) | 1:122:A:TYR:HB3  | 1:123:A:PRO:HD2 | 9        | 0.27          |
| (2,614) | 1:118:A:ILE:HG21 | 1:151:A:VAL:HA  | 9        | 0.27          |
| (2,614) | 1:118:A:ILE:HG22 | 1:151:A:VAL:HA  | 9        | 0.27          |
| (2,614) | 1:118:A:ILE:HG23 | 1:151:A:VAL:HA  | 9        | 0.27          |
| (2,607) | 1:115:A:LYS:H    | 1:116:A:GLU:HG2 | 6        | 0.27          |
| (2,607) | 1:115:A:LYS:H    | 1:116:A:GLU:HG3 | 6        | 0.27          |
| (2,523) | 1:85:A:TYR:HD1   | 1:134:A:TRP:H   | 9        | 0.27          |
| (2,523) | 1:85:A:TYR:HD2   | 1:134:A:TRP:H   | 9        | 0.27          |
| (2,468) | 1:79:A:ILE:HG21  | 1:156:A:PHE:HE1 | 6        | 0.27          |
| (2,468) | 1:79:A:ILE:HG21  | 1:156:A:PHE:HE2 | 6        | 0.27          |
| (2,468) | 1:79:A:ILE:HG22  | 1:156:A:PHE:HE1 | 6        | 0.27          |
| (2,468) | 1:79:A:ILE:HG22  | 1:156:A:PHE:HE2 | 6        | 0.27          |
| (2,468) | 1:79:A:ILE:HG23  | 1:156:A:PHE:HE1 | 6        | 0.27          |
| (2,468) | 1:79:A:ILE:HG23  | 1:156:A:PHE:HE2 | 6        | 0.27          |
| (2,397) | 1:73:A:TYR:HD1   | 1:74:A:PHE:HA   | 9        | 0.27          |
| (2,397) | 1:73:A:TYR:HD2   | 1:74:A:PHE:HA   | 9        | 0.27          |
| (2,383) | 1:70:A:LEU:HA    | 1:74:A:PHE:HD1  | 5        | 0.27          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,383)  | 1:70:A:LEU:HA    | 1:74:A:PHE:HD2   | 5        | 0.27          |
| (2,178)  | 1:36:A:ALA:H     | 1:37:A:GLY:H     | 10       | 0.27          |
| (2,125)  | 1:28:A:HIS:HE1   | 1:46:A:TYR:HE1   | 7        | 0.27          |
| (2,125)  | 1:28:A:HIS:HE1   | 1:46:A:TYR:HE2   | 7        | 0.27          |
| (1,2262) | 1:164:A:GLU:HA   | 1:164:A:GLU:HG2  | 2        | 0.27          |
| (1,2262) | 1:164:A:GLU:HA   | 1:164:A:GLU:HG3  | 2        | 0.27          |
| (1,2262) | 1:164:A:GLU:HA   | 1:164:A:GLU:HG2  | 5        | 0.27          |
| (1,2262) | 1:164:A:GLU:HA   | 1:164:A:GLU:HG3  | 5        | 0.27          |
| (1,2246) | 1:162:A:ALA:HB1  | 1:168:A:PHE:HZ   | 9        | 0.27          |
| (1,2246) | 1:162:A:ALA:HB2  | 1:168:A:PHE:HZ   | 9        | 0.27          |
| (1,2246) | 1:162:A:ALA:HB3  | 1:168:A:PHE:HZ   | 9        | 0.27          |
| (1,2177) | 1:157:A:LYS:H    | 1:158:A:ALA:HA   | 1        | 0.27          |
| (1,2177) | 1:157:A:LYS:H    | 1:158:A:ALA:HA   | 4        | 0.27          |
| (1,2177) | 1:157:A:LYS:H    | 1:158:A:ALA:HA   | 8        | 0.27          |
| (1,2066) | 1:148:A:THR:HA   | 1:149:A:LYS:H    | 9        | 0.27          |
| (1,2043) | 1:145:A:TYR:HA   | 1:145:A:TYR:HD1  | 4        | 0.27          |
| (1,2043) | 1:145:A:TYR:HA   | 1:145:A:TYR:HD2  | 4        | 0.27          |
| (1,2030) | 1:143:A:ILE:HG21 | 1:143:A:ILE:HD11 | 1        | 0.27          |
| (1,2030) | 1:143:A:ILE:HG21 | 1:143:A:ILE:HD12 | 1        | 0.27          |
| (1,2030) | 1:143:A:ILE:HG21 | 1:143:A:ILE:HD13 | 1        | 0.27          |
| (1,2030) | 1:143:A:ILE:HG22 | 1:143:A:ILE:HD11 | 1        | 0.27          |
| (1,2030) | 1:143:A:ILE:HG22 | 1:143:A:ILE:HD12 | 1        | 0.27          |
| (1,2030) | 1:143:A:ILE:HG22 | 1:143:A:ILE:HD13 | 1        | 0.27          |
| (1,2030) | 1:143:A:ILE:HG23 | 1:143:A:ILE:HD11 | 1        | 0.27          |
| (1,2030) | 1:143:A:ILE:HG23 | 1:143:A:ILE:HD12 | 1        | 0.27          |
| (1,2030) | 1:143:A:ILE:HG23 | 1:143:A:ILE:HD13 | 1        | 0.27          |
| (1,2021) | 1:143:A:ILE:HA   | 1:143:A:ILE:HD11 | 2        | 0.27          |
| (1,2021) | 1:143:A:ILE:HA   | 1:143:A:ILE:HD12 | 2        | 0.27          |
| (1,2021) | 1:143:A:ILE:HA   | 1:143:A:ILE:HD13 | 2        | 0.27          |
| (1,2003) | 1:142:A:ILE:HA   | 1:142:A:ILE:HG21 | 8        | 0.27          |
| (1,2003) | 1:142:A:ILE:HA   | 1:142:A:ILE:HG22 | 8        | 0.27          |
| (1,2003) | 1:142:A:ILE:HA   | 1:142:A:ILE:HG23 | 8        | 0.27          |
| (1,1941) | 1:135:A:VAL:HG21 | 1:135:A:VAL:H    | 7        | 0.27          |
| (1,1941) | 1:135:A:VAL:HG22 | 1:135:A:VAL:H    | 7        | 0.27          |
| (1,1941) | 1:135:A:VAL:HG23 | 1:135:A:VAL:H    | 7        | 0.27          |
| (1,1859) | 1:133:A:ILE:HD11 | 1:144:A:VAL:HB   | 2        | 0.27          |
| (1,1859) | 1:133:A:ILE:HD12 | 1:144:A:VAL:HB   | 2        | 0.27          |
| (1,1859) | 1:133:A:ILE:HD13 | 1:144:A:VAL:HB   | 2        | 0.27          |
| (1,1767) | 1:120:A:VAL:HG11 | 1:121:A:LEU:H    | 1        | 0.27          |
| (1,1767) | 1:120:A:VAL:HG12 | 1:121:A:LEU:H    | 1        | 0.27          |
| (1,1767) | 1:120:A:VAL:HG13 | 1:121:A:LEU:H    | 1        | 0.27          |
| (1,1767) | 1:120:A:VAL:HG11 | 1:121:A:LEU:H    | 2        | 0.27          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1767) | 1:120:A:VAL:HG12 | 1:121:A:LEU:H    | 2        | 0.27          |
| (1,1767) | 1:120:A:VAL:HG13 | 1:121:A:LEU:H    | 2        | 0.27          |
| (1,1767) | 1:120:A:VAL:HG11 | 1:121:A:LEU:H    | 9        | 0.27          |
| (1,1767) | 1:120:A:VAL:HG12 | 1:121:A:LEU:H    | 9        | 0.27          |
| (1,1767) | 1:120:A:VAL:HG13 | 1:121:A:LEU:H    | 9        | 0.27          |
| (1,1546) | 1:102:A:ILE:HG21 | 1:108:A:SER:HA   | 2        | 0.27          |
| (1,1546) | 1:102:A:ILE:HG22 | 1:108:A:SER:HA   | 2        | 0.27          |
| (1,1546) | 1:102:A:ILE:HG23 | 1:108:A:SER:HA   | 2        | 0.27          |
| (1,1474) | 1:95:A:PHE:HB2   | 1:95:A:PHE:H     | 6        | 0.27          |
| (1,1474) | 1:95:A:PHE:HB3   | 1:95:A:PHE:H     | 6        | 0.27          |
| (1,1445) | 1:90:A:THR:HA    | 1:90:A:THR:HG21  | 3        | 0.27          |
| (1,1445) | 1:90:A:THR:HA    | 1:90:A:THR:HG22  | 3        | 0.27          |
| (1,1445) | 1:90:A:THR:HA    | 1:90:A:THR:HG23  | 3        | 0.27          |
| (1,1342) | 1:85:A:TYR:HE1   | 1:143:A:ILE:HG21 | 7        | 0.27          |
| (1,1342) | 1:85:A:TYR:HE1   | 1:143:A:ILE:HG22 | 7        | 0.27          |
| (1,1342) | 1:85:A:TYR:HE1   | 1:143:A:ILE:HG23 | 7        | 0.27          |
| (1,1342) | 1:85:A:TYR:HE2   | 1:143:A:ILE:HG21 | 7        | 0.27          |
| (1,1342) | 1:85:A:TYR:HE2   | 1:143:A:ILE:HG22 | 7        | 0.27          |
| (1,1342) | 1:85:A:TYR:HE2   | 1:143:A:ILE:HG23 | 7        | 0.27          |
| (1,1298) | 1:83:A:SER:HA    | 1:154:A:LEU:HD21 | 1        | 0.27          |
| (1,1298) | 1:83:A:SER:HA    | 1:154:A:LEU:HD22 | 1        | 0.27          |
| (1,1298) | 1:83:A:SER:HA    | 1:154:A:LEU:HD23 | 1        | 0.27          |
| (1,1298) | 1:83:A:SER:HA    | 1:154:A:LEU:HD21 | 10       | 0.27          |
| (1,1298) | 1:83:A:SER:HA    | 1:154:A:LEU:HD22 | 10       | 0.27          |
| (1,1298) | 1:83:A:SER:HA    | 1:154:A:LEU:HD23 | 10       | 0.27          |
| (1,1216) | 1:81:A:ILE:HD11  | 1:100:A:ALA:H    | 3        | 0.27          |
| (1,1216) | 1:81:A:ILE:HD12  | 1:100:A:ALA:H    | 3        | 0.27          |
| (1,1216) | 1:81:A:ILE:HD13  | 1:100:A:ALA:H    | 3        | 0.27          |
| (1,1189) | 1:80:A:GLN:HG2   | 1:98:A:THR:HG21  | 10       | 0.27          |
| (1,1189) | 1:80:A:GLN:HG2   | 1:98:A:THR:HG22  | 10       | 0.27          |
| (1,1189) | 1:80:A:GLN:HG2   | 1:98:A:THR:HG23  | 10       | 0.27          |
| (1,1189) | 1:80:A:GLN:HG3   | 1:98:A:THR:HG21  | 10       | 0.27          |
| (1,1189) | 1:80:A:GLN:HG3   | 1:98:A:THR:HG22  | 10       | 0.27          |
| (1,1189) | 1:80:A:GLN:HG3   | 1:98:A:THR:HG23  | 10       | 0.27          |
| (1,1173) | 1:79:A:ILE:H     | 1:158:A:ALA:HA   | 3        | 0.27          |
| (1,1173) | 1:79:A:ILE:H     | 1:158:A:ALA:HA   | 8        | 0.27          |
| (1,1173) | 1:79:A:ILE:H     | 1:158:A:ALA:HA   | 10       | 0.27          |
| (1,1162) | 1:79:A:ILE:HG13  | 1:80:A:GLN:H     | 2        | 0.27          |
| (1,1013) | 1:74:A:PHE:HB2   | 1:163:A:LYS:H    | 8        | 0.27          |
| (1,873)  | 1:67:A:ALA:HB1   | 1:68:A:GLU:H     | 7        | 0.27          |
| (1,873)  | 1:67:A:ALA:HB2   | 1:68:A:GLU:H     | 7        | 0.27          |
| (1,873)  | 1:67:A:ALA:HB3   | 1:68:A:GLU:H     | 7        | 0.27          |

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| Key     | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,779) | 1:64:A:LEU:HD11 | 1:64:A:LEU:HD21  | 4        | 0.27          |
| (1,779) | 1:64:A:LEU:HD11 | 1:64:A:LEU:HD22  | 4        | 0.27          |
| (1,779) | 1:64:A:LEU:HD11 | 1:64:A:LEU:HD23  | 4        | 0.27          |
| (1,779) | 1:64:A:LEU:HD12 | 1:64:A:LEU:HD21  | 4        | 0.27          |
| (1,779) | 1:64:A:LEU:HD12 | 1:64:A:LEU:HD22  | 4        | 0.27          |
| (1,779) | 1:64:A:LEU:HD12 | 1:64:A:LEU:HD23  | 4        | 0.27          |
| (1,779) | 1:64:A:LEU:HD13 | 1:64:A:LEU:HD21  | 4        | 0.27          |
| (1,779) | 1:64:A:LEU:HD13 | 1:64:A:LEU:HD22  | 4        | 0.27          |
| (1,779) | 1:64:A:LEU:HD13 | 1:64:A:LEU:HD23  | 4        | 0.27          |
| (1,755) | 1:63:A:THR:HG21 | 1:108:A:SER:HA   | 9        | 0.27          |
| (1,755) | 1:63:A:THR:HG22 | 1:108:A:SER:HA   | 9        | 0.27          |
| (1,755) | 1:63:A:THR:HG23 | 1:108:A:SER:HA   | 9        | 0.27          |
| (1,679) | 1:60:A:LEU:HD11 | 1:177:A:PHE:HD1  | 7        | 0.27          |
| (1,679) | 1:60:A:LEU:HD11 | 1:177:A:PHE:HD2  | 7        | 0.27          |
| (1,679) | 1:60:A:LEU:HD12 | 1:177:A:PHE:HD1  | 7        | 0.27          |
| (1,679) | 1:60:A:LEU:HD12 | 1:177:A:PHE:HD2  | 7        | 0.27          |
| (1,679) | 1:60:A:LEU:HD13 | 1:177:A:PHE:HD1  | 7        | 0.27          |
| (1,679) | 1:60:A:LEU:HD13 | 1:177:A:PHE:HD2  | 7        | 0.27          |
| (1,610) | 1:55:A:VAL:HA   | 1:55:A:VAL:HG11  | 9        | 0.27          |
| (1,610) | 1:55:A:VAL:HA   | 1:55:A:VAL:HG12  | 9        | 0.27          |
| (1,610) | 1:55:A:VAL:HA   | 1:55:A:VAL:HG13  | 9        | 0.27          |
| (1,556) | 1:50:A:TRP:HD1  | 1:151:A:VAL:HG21 | 3        | 0.27          |
| (1,556) | 1:50:A:TRP:HD1  | 1:151:A:VAL:HG22 | 3        | 0.27          |
| (1,556) | 1:50:A:TRP:HD1  | 1:151:A:VAL:HG23 | 3        | 0.27          |
| (1,556) | 1:50:A:TRP:HD1  | 1:151:A:VAL:HG21 | 9        | 0.27          |
| (1,556) | 1:50:A:TRP:HD1  | 1:151:A:VAL:HG22 | 9        | 0.27          |
| (1,556) | 1:50:A:TRP:HD1  | 1:151:A:VAL:HG23 | 9        | 0.27          |
| (1,268) | 1:34:A:PRO:HD3  | 1:35:A:ALA:H     | 2        | 0.27          |
| (1,268) | 1:34:A:PRO:HD3  | 1:35:A:ALA:H     | 4        | 0.27          |
| (1,257) | 1:33:A:THR:HB   | 1:33:A:THR:HG21  | 1        | 0.27          |
| (1,257) | 1:33:A:THR:HB   | 1:33:A:THR:HG22  | 1        | 0.27          |
| (1,257) | 1:33:A:THR:HB   | 1:33:A:THR:HG23  | 1        | 0.27          |
| (1,257) | 1:33:A:THR:HB   | 1:33:A:THR:HG21  | 9        | 0.27          |
| (1,257) | 1:33:A:THR:HB   | 1:33:A:THR:HG22  | 9        | 0.27          |
| (1,257) | 1:33:A:THR:HB   | 1:33:A:THR:HG23  | 9        | 0.27          |
| (1,257) | 1:33:A:THR:HB   | 1:33:A:THR:HG21  | 10       | 0.27          |
| (1,257) | 1:33:A:THR:HB   | 1:33:A:THR:HG22  | 10       | 0.27          |
| (1,257) | 1:33:A:THR:HB   | 1:33:A:THR:HG23  | 10       | 0.27          |
| (1,170) | 1:29:A:LEU:HD21 | 1:175:A:PHE:HD1  | 10       | 0.27          |
| (1,170) | 1:29:A:LEU:HD21 | 1:175:A:PHE:HD2  | 10       | 0.27          |
| (1,170) | 1:29:A:LEU:HD22 | 1:175:A:PHE:HD1  | 10       | 0.27          |
| (1,170) | 1:29:A:LEU:HD22 | 1:175:A:PHE:HD2  | 10       | 0.27          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,170)  | 1:29:A:LEU:HD23  | 1:175:A:PHE:HD1  | 10       | 0.27          |
| (1,170)  | 1:29:A:LEU:HD23  | 1:175:A:PHE:HD2  | 10       | 0.27          |
| (2,735)  | 1:158:A:ALA:H    | 1:160:A:TYR:HE1  | 1        | 0.26          |
| (2,735)  | 1:158:A:ALA:H    | 1:160:A:TYR:HE2  | 1        | 0.26          |
| (2,735)  | 1:158:A:ALA:H    | 1:160:A:TYR:HE1  | 5        | 0.26          |
| (2,735)  | 1:158:A:ALA:H    | 1:160:A:TYR:HE2  | 5        | 0.26          |
| (2,731)  | 1:155:A:ASN:H    | 1:156:A:PHE:HD1  | 3        | 0.26          |
| (2,731)  | 1:155:A:ASN:H    | 1:156:A:PHE:HD2  | 3        | 0.26          |
| (2,709)  | 1:133:A:ILE:HD11 | 1:147:A:GLU:H    | 6        | 0.26          |
| (2,709)  | 1:133:A:ILE:HD12 | 1:147:A:GLU:H    | 6        | 0.26          |
| (2,709)  | 1:133:A:ILE:HD13 | 1:147:A:GLU:H    | 6        | 0.26          |
| (2,635)  | 1:122:A:TYR:HD1  | 1:126:A:THR:H    | 2        | 0.26          |
| (2,635)  | 1:122:A:TYR:HD2  | 1:126:A:THR:H    | 2        | 0.26          |
| (2,632)  | 1:122:A:TYR:HD1  | 1:125:A:LYS:H    | 1        | 0.26          |
| (2,632)  | 1:122:A:TYR:HD2  | 1:125:A:LYS:H    | 1        | 0.26          |
| (2,592)  | 1:114:A:ASP:HB3  | 1:116:A:GLU:HG2  | 1        | 0.26          |
| (2,592)  | 1:114:A:ASP:HB3  | 1:116:A:GLU:HG3  | 1        | 0.26          |
| (2,522)  | 1:85:A:TYR:HD1   | 1:134:A:TRP:HA   | 10       | 0.26          |
| (2,522)  | 1:85:A:TYR:HD2   | 1:134:A:TRP:HA   | 10       | 0.26          |
| (2,481)  | 1:80:A:GLN:HE22  | 1:98:A:THR:HG21  | 5        | 0.26          |
| (2,481)  | 1:80:A:GLN:HE22  | 1:98:A:THR:HG22  | 5        | 0.26          |
| (2,481)  | 1:80:A:GLN:HE22  | 1:98:A:THR:HG23  | 5        | 0.26          |
| (2,481)  | 1:80:A:GLN:HE22  | 1:98:A:THR:HG21  | 9        | 0.26          |
| (2,481)  | 1:80:A:GLN:HE22  | 1:98:A:THR:HG22  | 9        | 0.26          |
| (2,481)  | 1:80:A:GLN:HE22  | 1:98:A:THR:HG23  | 9        | 0.26          |
| (2,194)  | 1:38:A:ALA:HB1   | 1:39:A:GLN:HE21  | 1        | 0.26          |
| (2,194)  | 1:38:A:ALA:HB2   | 1:39:A:GLN:HE21  | 1        | 0.26          |
| (2,194)  | 1:38:A:ALA:HB3   | 1:39:A:GLN:HE21  | 1        | 0.26          |
| (1,2354) | 1:173:A:VAL:HG11 | 1:175:A:PHE:HE1  | 2        | 0.26          |
| (1,2354) | 1:173:A:VAL:HG11 | 1:175:A:PHE:HE2  | 2        | 0.26          |
| (1,2354) | 1:173:A:VAL:HG12 | 1:175:A:PHE:HE1  | 2        | 0.26          |
| (1,2354) | 1:173:A:VAL:HG12 | 1:175:A:PHE:HE2  | 2        | 0.26          |
| (1,2354) | 1:173:A:VAL:HG13 | 1:175:A:PHE:HE1  | 2        | 0.26          |
| (1,2354) | 1:173:A:VAL:HG13 | 1:175:A:PHE:HE2  | 2        | 0.26          |
| (1,2177) | 1:157:A:LYS:H    | 1:158:A:ALA:HA   | 2        | 0.26          |
| (1,2177) | 1:157:A:LYS:H    | 1:158:A:ALA:HA   | 5        | 0.26          |
| (1,2066) | 1:148:A:THR:HA   | 1:149:A:LYS:H    | 6        | 0.26          |
| (1,2066) | 1:148:A:THR:HA   | 1:149:A:LYS:H    | 7        | 0.26          |
| (1,2021) | 1:143:A:ILE:HA   | 1:143:A:ILE:HD11 | 1        | 0.26          |
| (1,2021) | 1:143:A:ILE:HA   | 1:143:A:ILE:HD12 | 1        | 0.26          |
| (1,2021) | 1:143:A:ILE:HA   | 1:143:A:ILE:HD13 | 1        | 0.26          |
| (1,2003) | 1:142:A:ILE:HA   | 1:142:A:ILE:HG21 | 2        | 0.26          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2003) | 1:142:A:ILE:HA   | 1:142:A:ILE:HG22 | 2        | 0.26          |
| (1,2003) | 1:142:A:ILE:HA   | 1:142:A:ILE:HG23 | 2        | 0.26          |
| (1,2003) | 1:142:A:ILE:HA   | 1:142:A:ILE:HG21 | 3        | 0.26          |
| (1,2003) | 1:142:A:ILE:HA   | 1:142:A:ILE:HG22 | 3        | 0.26          |
| (1,2003) | 1:142:A:ILE:HA   | 1:142:A:ILE:HG23 | 3        | 0.26          |
| (1,2003) | 1:142:A:ILE:HA   | 1:142:A:ILE:HG21 | 10       | 0.26          |
| (1,2003) | 1:142:A:ILE:HA   | 1:142:A:ILE:HG22 | 10       | 0.26          |
| (1,2003) | 1:142:A:ILE:HA   | 1:142:A:ILE:HG23 | 10       | 0.26          |
| (1,1789) | 1:125:A:LYS:HG2  | 1:125:A:LYS:HE2  | 5        | 0.26          |
| (1,1789) | 1:125:A:LYS:HG2  | 1:125:A:LYS:HE3  | 5        | 0.26          |
| (1,1789) | 1:125:A:LYS:HG3  | 1:125:A:LYS:HE2  | 5        | 0.26          |
| (1,1789) | 1:125:A:LYS:HG3  | 1:125:A:LYS:HE3  | 5        | 0.26          |
| (1,1789) | 1:125:A:LYS:HG2  | 1:125:A:LYS:HE2  | 6        | 0.26          |
| (1,1789) | 1:125:A:LYS:HG2  | 1:125:A:LYS:HE3  | 6        | 0.26          |
| (1,1789) | 1:125:A:LYS:HG3  | 1:125:A:LYS:HE2  | 6        | 0.26          |
| (1,1789) | 1:125:A:LYS:HG3  | 1:125:A:LYS:HE3  | 6        | 0.26          |
| (1,1789) | 1:125:A:LYS:HG2  | 1:125:A:LYS:HE2  | 8        | 0.26          |
| (1,1789) | 1:125:A:LYS:HG2  | 1:125:A:LYS:HE3  | 8        | 0.26          |
| (1,1789) | 1:125:A:LYS:HG3  | 1:125:A:LYS:HE2  | 8        | 0.26          |
| (1,1789) | 1:125:A:LYS:HG3  | 1:125:A:LYS:HE3  | 8        | 0.26          |
| (1,1769) | 1:120:A:VAL:HG21 | 1:120:A:VAL:H    | 2        | 0.26          |
| (1,1769) | 1:120:A:VAL:HG22 | 1:120:A:VAL:H    | 2        | 0.26          |
| (1,1769) | 1:120:A:VAL:HG23 | 1:120:A:VAL:H    | 2        | 0.26          |
| (1,1723) | 1:116:A:GLU:HG2  | 1:116:A:GLU:H    | 10       | 0.26          |
| (1,1723) | 1:116:A:GLU:HG3  | 1:116:A:GLU:H    | 10       | 0.26          |
| (1,1537) | 1:102:A:ILE:HD11 | 1:107:A:PRO:HA   | 10       | 0.26          |
| (1,1537) | 1:102:A:ILE:HD12 | 1:107:A:PRO:HA   | 10       | 0.26          |
| (1,1537) | 1:102:A:ILE:HD13 | 1:107:A:PRO:HA   | 10       | 0.26          |
| (1,1522) | 1:100:A:ALA:H    | 1:111:A:ILE:HD11 | 5        | 0.26          |
| (1,1522) | 1:100:A:ALA:H    | 1:111:A:ILE:HD12 | 5        | 0.26          |
| (1,1522) | 1:100:A:ALA:H    | 1:111:A:ILE:HD13 | 5        | 0.26          |
| (1,1445) | 1:90:A:THR:HA    | 1:90:A:THR:HG21  | 1        | 0.26          |
| (1,1445) | 1:90:A:THR:HA    | 1:90:A:THR:HG22  | 1        | 0.26          |
| (1,1445) | 1:90:A:THR:HA    | 1:90:A:THR:HG23  | 1        | 0.26          |
| (1,1445) | 1:90:A:THR:HA    | 1:90:A:THR:HG21  | 10       | 0.26          |
| (1,1445) | 1:90:A:THR:HA    | 1:90:A:THR:HG22  | 10       | 0.26          |
| (1,1445) | 1:90:A:THR:HA    | 1:90:A:THR:HG23  | 10       | 0.26          |
| (1,1399) | 1:87:A:THR:HG21  | 1:87:A:THR:H     | 10       | 0.26          |
| (1,1399) | 1:87:A:THR:HG22  | 1:87:A:THR:H     | 10       | 0.26          |
| (1,1399) | 1:87:A:THR:HG23  | 1:87:A:THR:H     | 10       | 0.26          |
| (1,1338) | 1:85:A:TYR:HD1   | 1:86:A:GLU:H     | 3        | 0.26          |
| (1,1338) | 1:85:A:TYR:HD2   | 1:86:A:GLU:H     | 3        | 0.26          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1180) | 1:80:A:GLN:HA   | 1:101:A:VAL:H    | 10       | 0.26          |
| (1,1173) | 1:79:A:ILE:H    | 1:158:A:ALA:HA   | 4        | 0.26          |
| (1,1173) | 1:79:A:ILE:H    | 1:158:A:ALA:HA   | 7        | 0.26          |
| (1,1165) | 1:79:A:ILE:HG12 | 1:79:A:ILE:H     | 10       | 0.26          |
| (1,1114) | 1:78:A:GLN:HA   | 1:159:A:PHE:HB3  | 7        | 0.26          |
| (1,873)  | 1:67:A:ALA:HB1  | 1:68:A:GLU:H     | 1        | 0.26          |
| (1,873)  | 1:67:A:ALA:HB2  | 1:68:A:GLU:H     | 1        | 0.26          |
| (1,873)  | 1:67:A:ALA:HB3  | 1:68:A:GLU:H     | 1        | 0.26          |
| (1,724)  | 1:62:A:VAL:HG11 | 1:63:A:THR:H     | 3        | 0.26          |
| (1,724)  | 1:62:A:VAL:HG12 | 1:63:A:THR:H     | 3        | 0.26          |
| (1,724)  | 1:62:A:VAL:HG13 | 1:63:A:THR:H     | 3        | 0.26          |
| (1,709)  | 1:62:A:VAL:HA   | 1:62:A:VAL:HG11  | 4        | 0.26          |
| (1,709)  | 1:62:A:VAL:HA   | 1:62:A:VAL:HG12  | 4        | 0.26          |
| (1,709)  | 1:62:A:VAL:HA   | 1:62:A:VAL:HG13  | 4        | 0.26          |
| (1,709)  | 1:62:A:VAL:HA   | 1:62:A:VAL:HG11  | 9        | 0.26          |
| (1,709)  | 1:62:A:VAL:HA   | 1:62:A:VAL:HG12  | 9        | 0.26          |
| (1,709)  | 1:62:A:VAL:HA   | 1:62:A:VAL:HG13  | 9        | 0.26          |
| (1,623)  | 1:55:A:VAL:H    | 1:115:A:LYS:HA   | 6        | 0.26          |
| (1,610)  | 1:55:A:VAL:HA   | 1:55:A:VAL:HG11  | 10       | 0.26          |
| (1,610)  | 1:55:A:VAL:HA   | 1:55:A:VAL:HG12  | 10       | 0.26          |
| (1,610)  | 1:55:A:VAL:HA   | 1:55:A:VAL:HG13  | 10       | 0.26          |
| (1,556)  | 1:50:A:TRP:HD1  | 1:151:A:VAL:HG21 | 4        | 0.26          |
| (1,556)  | 1:50:A:TRP:HD1  | 1:151:A:VAL:HG22 | 4        | 0.26          |
| (1,556)  | 1:50:A:TRP:HD1  | 1:151:A:VAL:HG23 | 4        | 0.26          |
| (1,436)  | 1:46:A:TYR:HB2  | 1:153:A:ILE:HG21 | 1        | 0.26          |
| (1,436)  | 1:46:A:TYR:HB2  | 1:153:A:ILE:HG22 | 1        | 0.26          |
| (1,436)  | 1:46:A:TYR:HB2  | 1:153:A:ILE:HG23 | 1        | 0.26          |
| (1,299)  | 1:39:A:GLN:HA   | 1:39:A:GLN:H     | 10       | 0.26          |
| (1,292)  | 1:37:A:GLY:HA2  | 1:37:A:GLY:H     | 10       | 0.26          |
| (1,232)  | 1:32:A:ILE:HG21 | 1:32:A:ILE:HD11  | 8        | 0.26          |
| (1,232)  | 1:32:A:ILE:HG21 | 1:32:A:ILE:HD12  | 8        | 0.26          |
| (1,232)  | 1:32:A:ILE:HG21 | 1:32:A:ILE:HD13  | 8        | 0.26          |
| (1,232)  | 1:32:A:ILE:HG22 | 1:32:A:ILE:HD11  | 8        | 0.26          |
| (1,232)  | 1:32:A:ILE:HG22 | 1:32:A:ILE:HD12  | 8        | 0.26          |
| (1,232)  | 1:32:A:ILE:HG22 | 1:32:A:ILE:HD13  | 8        | 0.26          |
| (1,232)  | 1:32:A:ILE:HG23 | 1:32:A:ILE:HD11  | 8        | 0.26          |
| (1,232)  | 1:32:A:ILE:HG23 | 1:32:A:ILE:HD12  | 8        | 0.26          |
| (1,232)  | 1:32:A:ILE:HG23 | 1:32:A:ILE:HD13  | 8        | 0.26          |
| (1,109)  | 1:26:A:GLU:H    | 1:47:A:ALA:HA    | 1        | 0.26          |
| (1,109)  | 1:26:A:GLU:H    | 1:47:A:ALA:HA    | 4        | 0.26          |
| (3,13)   | 1:181:A:GLN:HA  | 1:181:A:GLN:HB2  | 5        | 0.25          |
| (3,4)    | 1:57:A:ASP:HA   | 1:114:A:ASP:HA   | 7        | 0.25          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,768)  | 1:173:A:VAL:HB   | 1:175:A:PHE:HE1  | 8        | 0.25          |
| (2,768)  | 1:173:A:VAL:HB   | 1:175:A:PHE:HE2  | 8        | 0.25          |
| (2,673)  | 1:127:A:GLY:H    | 1:128:A:TYR:HD1  | 6        | 0.25          |
| (2,673)  | 1:127:A:GLY:H    | 1:128:A:TYR:HD2  | 6        | 0.25          |
| (2,614)  | 1:118:A:ILE:HG21 | 1:151:A:VAL:HA   | 7        | 0.25          |
| (2,614)  | 1:118:A:ILE:HG22 | 1:151:A:VAL:HA   | 7        | 0.25          |
| (2,614)  | 1:118:A:ILE:HG23 | 1:151:A:VAL:HA   | 7        | 0.25          |
| (2,552)  | 1:87:A:THR:H     | 1:92:A:LEU:HB2   | 2        | 0.25          |
| (2,468)  | 1:79:A:ILE:HG21  | 1:156:A:PHE:HE1  | 5        | 0.25          |
| (2,468)  | 1:79:A:ILE:HG21  | 1:156:A:PHE:HE2  | 5        | 0.25          |
| (2,468)  | 1:79:A:ILE:HG22  | 1:156:A:PHE:HE1  | 5        | 0.25          |
| (2,468)  | 1:79:A:ILE:HG22  | 1:156:A:PHE:HE2  | 5        | 0.25          |
| (2,468)  | 1:79:A:ILE:HG23  | 1:156:A:PHE:HE1  | 5        | 0.25          |
| (2,468)  | 1:79:A:ILE:HG23  | 1:156:A:PHE:HE2  | 5        | 0.25          |
| (2,383)  | 1:70:A:LEU:HA    | 1:74:A:PHE:HD1   | 10       | 0.25          |
| (2,383)  | 1:70:A:LEU:HA    | 1:74:A:PHE:HD2   | 10       | 0.25          |
| (2,4)    | 1:15:A:THR:HG21  | 1:16:A:ALA:H     | 7        | 0.25          |
| (2,4)    | 1:15:A:THR:HG22  | 1:16:A:ALA:H     | 7        | 0.25          |
| (2,4)    | 1:15:A:THR:HG23  | 1:16:A:ALA:H     | 7        | 0.25          |
| (1,2425) | 1:177:A:PHE:HD1  | 1:177:A:PHE:H    | 4        | 0.25          |
| (1,2425) | 1:177:A:PHE:HD2  | 1:177:A:PHE:H    | 4        | 0.25          |
| (1,2370) | 1:174:A:ILE:HG21 | 1:175:A:PHE:HA   | 3        | 0.25          |
| (1,2370) | 1:174:A:ILE:HG22 | 1:175:A:PHE:HA   | 3        | 0.25          |
| (1,2370) | 1:174:A:ILE:HG23 | 1:175:A:PHE:HA   | 3        | 0.25          |
| (1,2370) | 1:174:A:ILE:HG21 | 1:175:A:PHE:HA   | 5        | 0.25          |
| (1,2370) | 1:174:A:ILE:HG22 | 1:175:A:PHE:HA   | 5        | 0.25          |
| (1,2370) | 1:174:A:ILE:HG23 | 1:175:A:PHE:HA   | 5        | 0.25          |
| (1,2327) | 1:171:A:LEU:HG   | 1:171:A:LEU:H    | 8        | 0.25          |
| (1,2327) | 1:171:A:LEU:HG   | 1:171:A:LEU:H    | 10       | 0.25          |
| (1,2177) | 1:157:A:LYS:H    | 1:158:A:ALA:HA   | 3        | 0.25          |
| (1,2177) | 1:157:A:LYS:H    | 1:158:A:ALA:HA   | 7        | 0.25          |
| (1,2066) | 1:148:A:THR:HA   | 1:149:A:LYS:H    | 1        | 0.25          |
| (1,2066) | 1:148:A:THR:HA   | 1:149:A:LYS:H    | 4        | 0.25          |
| (1,2066) | 1:148:A:THR:HA   | 1:149:A:LYS:H    | 5        | 0.25          |
| (1,2038) | 1:144:A:VAL:HG21 | 1:144:A:VAL:H    | 9        | 0.25          |
| (1,2038) | 1:144:A:VAL:HG22 | 1:144:A:VAL:H    | 9        | 0.25          |
| (1,2038) | 1:144:A:VAL:HG23 | 1:144:A:VAL:H    | 9        | 0.25          |
| (1,2021) | 1:143:A:ILE:HA   | 1:143:A:ILE:HD11 | 10       | 0.25          |
| (1,2021) | 1:143:A:ILE:HA   | 1:143:A:ILE:HD12 | 10       | 0.25          |
| (1,2021) | 1:143:A:ILE:HA   | 1:143:A:ILE:HD13 | 10       | 0.25          |
| (1,2010) | 1:142:A:ILE:HD11 | 1:145:A:TYR:HD1  | 7        | 0.25          |
| (1,2010) | 1:142:A:ILE:HD11 | 1:145:A:TYR:HD2  | 7        | 0.25          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2010) | 1:142:A:ILE:HD12 | 1:145:A:TYR:HD1  | 7        | 0.25          |
| (1,2010) | 1:142:A:ILE:HD12 | 1:145:A:TYR:HD2  | 7        | 0.25          |
| (1,2010) | 1:142:A:ILE:HD13 | 1:145:A:TYR:HD1  | 7        | 0.25          |
| (1,2010) | 1:142:A:ILE:HD13 | 1:145:A:TYR:HD2  | 7        | 0.25          |
| (1,1803) | 1:129:A:THR:HA   | 1:129:A:THR:HG21 | 9        | 0.25          |
| (1,1803) | 1:129:A:THR:HA   | 1:129:A:THR:HG22 | 9        | 0.25          |
| (1,1803) | 1:129:A:THR:HA   | 1:129:A:THR:HG23 | 9        | 0.25          |
| (1,1793) | 1:128:A:TYR:HA   | 1:128:A:TYR:HB3  | 3        | 0.25          |
| (1,1770) | 1:120:A:VAL:HG21 | 1:121:A:LEU:H    | 10       | 0.25          |
| (1,1770) | 1:120:A:VAL:HG22 | 1:121:A:LEU:H    | 10       | 0.25          |
| (1,1770) | 1:120:A:VAL:HG23 | 1:121:A:LEU:H    | 10       | 0.25          |
| (1,1768) | 1:120:A:VAL:HG11 | 1:122:A:TYR:HE1  | 4        | 0.25          |
| (1,1768) | 1:120:A:VAL:HG11 | 1:122:A:TYR:HE2  | 4        | 0.25          |
| (1,1768) | 1:120:A:VAL:HG12 | 1:122:A:TYR:HE1  | 4        | 0.25          |
| (1,1768) | 1:120:A:VAL:HG12 | 1:122:A:TYR:HE2  | 4        | 0.25          |
| (1,1768) | 1:120:A:VAL:HG13 | 1:122:A:TYR:HE1  | 4        | 0.25          |
| (1,1768) | 1:120:A:VAL:HG13 | 1:122:A:TYR:HE2  | 4        | 0.25          |
| (1,1767) | 1:120:A:VAL:HG11 | 1:121:A:LEU:H    | 5        | 0.25          |
| (1,1767) | 1:120:A:VAL:HG12 | 1:121:A:LEU:H    | 5        | 0.25          |
| (1,1767) | 1:120:A:VAL:HG13 | 1:121:A:LEU:H    | 5        | 0.25          |
| (1,1474) | 1:95:A:PHE:HB2   | 1:95:A:PHE:H     | 3        | 0.25          |
| (1,1474) | 1:95:A:PHE:HB3   | 1:95:A:PHE:H     | 3        | 0.25          |
| (1,1445) | 1:90:A:THR:HA    | 1:90:A:THR:HG21  | 4        | 0.25          |
| (1,1445) | 1:90:A:THR:HA    | 1:90:A:THR:HG22  | 4        | 0.25          |
| (1,1445) | 1:90:A:THR:HA    | 1:90:A:THR:HG23  | 4        | 0.25          |
| (1,1445) | 1:90:A:THR:HA    | 1:90:A:THR:HG21  | 5        | 0.25          |
| (1,1445) | 1:90:A:THR:HA    | 1:90:A:THR:HG22  | 5        | 0.25          |
| (1,1445) | 1:90:A:THR:HA    | 1:90:A:THR:HG23  | 5        | 0.25          |
| (1,1445) | 1:90:A:THR:HA    | 1:90:A:THR:HG21  | 6        | 0.25          |
| (1,1445) | 1:90:A:THR:HA    | 1:90:A:THR:HG22  | 6        | 0.25          |
| (1,1445) | 1:90:A:THR:HA    | 1:90:A:THR:HG23  | 6        | 0.25          |
| (1,1445) | 1:90:A:THR:HA    | 1:90:A:THR:HG21  | 8        | 0.25          |
| (1,1445) | 1:90:A:THR:HA    | 1:90:A:THR:HG22  | 8        | 0.25          |
| (1,1445) | 1:90:A:THR:HA    | 1:90:A:THR:HG23  | 8        | 0.25          |
| (1,1343) | 1:85:A:TYR:HE1   | 1:152:A:ALA:HA   | 2        | 0.25          |
| (1,1343) | 1:85:A:TYR:HE2   | 1:152:A:ALA:HA   | 2        | 0.25          |
| (1,1298) | 1:83:A:SER:HA    | 1:154:A:LEU:HD21 | 5        | 0.25          |
| (1,1298) | 1:83:A:SER:HA    | 1:154:A:LEU:HD22 | 5        | 0.25          |
| (1,1298) | 1:83:A:SER:HA    | 1:154:A:LEU:HD23 | 5        | 0.25          |
| (1,1252) | 1:82:A:THR:HA    | 1:82:A:THR:HG21  | 7        | 0.25          |
| (1,1252) | 1:82:A:THR:HA    | 1:82:A:THR:HG22  | 7        | 0.25          |
| (1,1252) | 1:82:A:THR:HA    | 1:82:A:THR:HG23  | 7        | 0.25          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1242) | 1:81:A:ILE:HG21 | 1:156:A:PHE:HE1 | 2        | 0.25          |
| (1,1242) | 1:81:A:ILE:HG21 | 1:156:A:PHE:HE2 | 2        | 0.25          |
| (1,1242) | 1:81:A:ILE:HG22 | 1:156:A:PHE:HE1 | 2        | 0.25          |
| (1,1242) | 1:81:A:ILE:HG22 | 1:156:A:PHE:HE2 | 2        | 0.25          |
| (1,1242) | 1:81:A:ILE:HG23 | 1:156:A:PHE:HE1 | 2        | 0.25          |
| (1,1242) | 1:81:A:ILE:HG23 | 1:156:A:PHE:HE2 | 2        | 0.25          |
| (1,1189) | 1:80:A:GLN:HG2  | 1:98:A:THR:HG21 | 4        | 0.25          |
| (1,1189) | 1:80:A:GLN:HG2  | 1:98:A:THR:HG22 | 4        | 0.25          |
| (1,1189) | 1:80:A:GLN:HG2  | 1:98:A:THR:HG23 | 4        | 0.25          |
| (1,1189) | 1:80:A:GLN:HG3  | 1:98:A:THR:HG21 | 4        | 0.25          |
| (1,1189) | 1:80:A:GLN:HG3  | 1:98:A:THR:HG22 | 4        | 0.25          |
| (1,1189) | 1:80:A:GLN:HG3  | 1:98:A:THR:HG23 | 4        | 0.25          |
| (1,1180) | 1:80:A:GLN:HA   | 1:101:A:VAL:H   | 6        | 0.25          |
| (1,1173) | 1:79:A:ILE:H    | 1:158:A:ALA:HA  | 9        | 0.25          |
| (1,1114) | 1:78:A:GLN:HA   | 1:159:A:PHE:HB3 | 3        | 0.25          |
| (1,1032) | 1:74:A:PHE:HE1  | 1:168:A:PHE:HZ  | 6        | 0.25          |
| (1,1032) | 1:74:A:PHE:HE2  | 1:168:A:PHE:HZ  | 6        | 0.25          |
| (1,1013) | 1:74:A:PHE:HB2  | 1:163:A:LYS:H   | 2        | 0.25          |
| (1,924)  | 1:70:A:LEU:HD11 | 1:74:A:PHE:HD1  | 1        | 0.25          |
| (1,924)  | 1:70:A:LEU:HD11 | 1:74:A:PHE:HD2  | 1        | 0.25          |
| (1,924)  | 1:70:A:LEU:HD12 | 1:74:A:PHE:HD1  | 1        | 0.25          |
| (1,924)  | 1:70:A:LEU:HD12 | 1:74:A:PHE:HD2  | 1        | 0.25          |
| (1,924)  | 1:70:A:LEU:HD13 | 1:74:A:PHE:HD1  | 1        | 0.25          |
| (1,924)  | 1:70:A:LEU:HD13 | 1:74:A:PHE:HD2  | 1        | 0.25          |
| (1,779)  | 1:64:A:LEU:HD11 | 1:64:A:LEU:HD21 | 3        | 0.25          |
| (1,779)  | 1:64:A:LEU:HD11 | 1:64:A:LEU:HD22 | 3        | 0.25          |
| (1,779)  | 1:64:A:LEU:HD11 | 1:64:A:LEU:HD23 | 3        | 0.25          |
| (1,779)  | 1:64:A:LEU:HD12 | 1:64:A:LEU:HD21 | 3        | 0.25          |
| (1,779)  | 1:64:A:LEU:HD12 | 1:64:A:LEU:HD22 | 3        | 0.25          |
| (1,779)  | 1:64:A:LEU:HD12 | 1:64:A:LEU:HD23 | 3        | 0.25          |
| (1,779)  | 1:64:A:LEU:HD13 | 1:64:A:LEU:HD21 | 3        | 0.25          |
| (1,779)  | 1:64:A:LEU:HD13 | 1:64:A:LEU:HD22 | 3        | 0.25          |
| (1,779)  | 1:64:A:LEU:HD13 | 1:64:A:LEU:HD23 | 3        | 0.25          |
| (1,709)  | 1:62:A:VAL:HA   | 1:62:A:VAL:HG11 | 1        | 0.25          |
| (1,709)  | 1:62:A:VAL:HA   | 1:62:A:VAL:HG12 | 1        | 0.25          |
| (1,709)  | 1:62:A:VAL:HA   | 1:62:A:VAL:HG13 | 1        | 0.25          |
| (1,709)  | 1:62:A:VAL:HA   | 1:62:A:VAL:HG11 | 5        | 0.25          |
| (1,709)  | 1:62:A:VAL:HA   | 1:62:A:VAL:HG12 | 5        | 0.25          |
| (1,709)  | 1:62:A:VAL:HA   | 1:62:A:VAL:HG13 | 5        | 0.25          |
| (1,709)  | 1:62:A:VAL:HA   | 1:62:A:VAL:HG11 | 7        | 0.25          |
| (1,709)  | 1:62:A:VAL:HA   | 1:62:A:VAL:HG12 | 7        | 0.25          |
| (1,709)  | 1:62:A:VAL:HA   | 1:62:A:VAL:HG13 | 7        | 0.25          |

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| Key     | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,621) | 1:55:A:VAL:H    | 1:55:A:VAL:HG21  | 3        | 0.25          |
| (1,621) | 1:55:A:VAL:H    | 1:55:A:VAL:HG22  | 3        | 0.25          |
| (1,621) | 1:55:A:VAL:H    | 1:55:A:VAL:HG23  | 3        | 0.25          |
| (1,621) | 1:55:A:VAL:H    | 1:55:A:VAL:HG21  | 6        | 0.25          |
| (1,621) | 1:55:A:VAL:H    | 1:55:A:VAL:HG22  | 6        | 0.25          |
| (1,621) | 1:55:A:VAL:H    | 1:55:A:VAL:HG23  | 6        | 0.25          |
| (1,621) | 1:55:A:VAL:H    | 1:55:A:VAL:HG21  | 9        | 0.25          |
| (1,621) | 1:55:A:VAL:H    | 1:55:A:VAL:HG22  | 9        | 0.25          |
| (1,621) | 1:55:A:VAL:H    | 1:55:A:VAL:HG23  | 9        | 0.25          |
| (1,621) | 1:55:A:VAL:H    | 1:55:A:VAL:HG21  | 10       | 0.25          |
| (1,621) | 1:55:A:VAL:H    | 1:55:A:VAL:HG22  | 10       | 0.25          |
| (1,621) | 1:55:A:VAL:H    | 1:55:A:VAL:HG23  | 10       | 0.25          |
| (1,556) | 1:50:A:TRP:HD1  | 1:151:A:VAL:HG21 | 1        | 0.25          |
| (1,556) | 1:50:A:TRP:HD1  | 1:151:A:VAL:HG22 | 1        | 0.25          |
| (1,556) | 1:50:A:TRP:HD1  | 1:151:A:VAL:HG23 | 1        | 0.25          |
| (1,543) | 1:50:A:TRP:HA   | 1:151:A:VAL:HA   | 4        | 0.25          |
| (1,543) | 1:50:A:TRP:HA   | 1:151:A:VAL:HA   | 7        | 0.25          |
| (1,268) | 1:34:A:PRO:HD3  | 1:35:A:ALA:H     | 8        | 0.25          |
| (1,232) | 1:32:A:ILE:HG21 | 1:32:A:ILE:HD11  | 3        | 0.25          |
| (1,232) | 1:32:A:ILE:HG21 | 1:32:A:ILE:HD12  | 3        | 0.25          |
| (1,232) | 1:32:A:ILE:HG21 | 1:32:A:ILE:HD13  | 3        | 0.25          |
| (1,232) | 1:32:A:ILE:HG22 | 1:32:A:ILE:HD11  | 3        | 0.25          |
| (1,232) | 1:32:A:ILE:HG22 | 1:32:A:ILE:HD12  | 3        | 0.25          |
| (1,232) | 1:32:A:ILE:HG22 | 1:32:A:ILE:HD13  | 3        | 0.25          |
| (1,232) | 1:32:A:ILE:HG23 | 1:32:A:ILE:HD11  | 3        | 0.25          |
| (1,232) | 1:32:A:ILE:HG23 | 1:32:A:ILE:HD12  | 3        | 0.25          |
| (1,232) | 1:32:A:ILE:HG23 | 1:32:A:ILE:HD13  | 3        | 0.25          |
| (1,212) | 1:32:A:ILE:HB   | 1:32:A:ILE:HD11  | 10       | 0.25          |
| (1,212) | 1:32:A:ILE:HB   | 1:32:A:ILE:HD12  | 10       | 0.25          |
| (1,212) | 1:32:A:ILE:HB   | 1:32:A:ILE:HD13  | 10       | 0.25          |
| (1,170) | 1:29:A:LEU:HD21 | 1:175:A:PHE:HD1  | 3        | 0.25          |
| (1,170) | 1:29:A:LEU:HD21 | 1:175:A:PHE:HD2  | 3        | 0.25          |
| (1,170) | 1:29:A:LEU:HD22 | 1:175:A:PHE:HD1  | 3        | 0.25          |
| (1,170) | 1:29:A:LEU:HD22 | 1:175:A:PHE:HD2  | 3        | 0.25          |
| (1,170) | 1:29:A:LEU:HD23 | 1:175:A:PHE:HD1  | 3        | 0.25          |
| (1,170) | 1:29:A:LEU:HD23 | 1:175:A:PHE:HD2  | 3        | 0.25          |
| (1,126) | 1:27:A:SER:HB2  | 1:177:A:PHE:HE1  | 7        | 0.25          |
| (1,126) | 1:27:A:SER:HB2  | 1:177:A:PHE:HE2  | 7        | 0.25          |
| (1,126) | 1:27:A:SER:HB3  | 1:177:A:PHE:HE1  | 7        | 0.25          |
| (1,126) | 1:27:A:SER:HB3  | 1:177:A:PHE:HE2  | 7        | 0.25          |
| (1,86)  | 1:25:A:VAL:HG21 | 1:49:A:VAL:HG21  | 7        | 0.25          |
| (1,86)  | 1:25:A:VAL:HG21 | 1:49:A:VAL:HG22  | 7        | 0.25          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,86)   | 1:25:A:VAL:HG21  | 1:49:A:VAL:HG23  | 7        | 0.25          |
| (1,86)   | 1:25:A:VAL:HG22  | 1:49:A:VAL:HG21  | 7        | 0.25          |
| (1,86)   | 1:25:A:VAL:HG22  | 1:49:A:VAL:HG22  | 7        | 0.25          |
| (1,86)   | 1:25:A:VAL:HG22  | 1:49:A:VAL:HG23  | 7        | 0.25          |
| (1,86)   | 1:25:A:VAL:HG23  | 1:49:A:VAL:HG21  | 7        | 0.25          |
| (1,86)   | 1:25:A:VAL:HG23  | 1:49:A:VAL:HG22  | 7        | 0.25          |
| (1,86)   | 1:25:A:VAL:HG23  | 1:49:A:VAL:HG23  | 7        | 0.25          |
| (3,4)    | 1:57:A:ASP:HA    | 1:114:A:ASP:HA   | 9        | 0.24          |
| (2,689)  | 1:131:A:THR:HA   | 1:145:A:TYR:HD1  | 3        | 0.24          |
| (2,689)  | 1:131:A:THR:HA   | 1:145:A:TYR:HD2  | 3        | 0.24          |
| (2,673)  | 1:127:A:GLY:H    | 1:128:A:TYR:HD1  | 5        | 0.24          |
| (2,673)  | 1:127:A:GLY:H    | 1:128:A:TYR:HD2  | 5        | 0.24          |
| (2,632)  | 1:122:A:TYR:HD1  | 1:125:A:LYS:H    | 5        | 0.24          |
| (2,632)  | 1:122:A:TYR:HD2  | 1:125:A:LYS:H    | 5        | 0.24          |
| (2,628)  | 1:122:A:TYR:HB3  | 1:123:A:PRO:HD2  | 4        | 0.24          |
| (2,628)  | 1:122:A:TYR:HB3  | 1:123:A:PRO:HD2  | 8        | 0.24          |
| (2,253)  | 1:47:A:ALA:H     | 1:48:A:ILE:HD11  | 5        | 0.24          |
| (2,253)  | 1:47:A:ALA:H     | 1:48:A:ILE:HD12  | 5        | 0.24          |
| (2,253)  | 1:47:A:ALA:H     | 1:48:A:ILE:HD13  | 5        | 0.24          |
| (2,194)  | 1:38:A:ALA:HB1   | 1:39:A:GLN:HE21  | 7        | 0.24          |
| (2,194)  | 1:38:A:ALA:HB2   | 1:39:A:GLN:HE21  | 7        | 0.24          |
| (2,194)  | 1:38:A:ALA:HB3   | 1:39:A:GLN:HE21  | 7        | 0.24          |
| (2,178)  | 1:36:A:ALA:H     | 1:37:A:GLY:H     | 8        | 0.24          |
| (1,2177) | 1:157:A:LYS:H    | 1:158:A:ALA:HA   | 10       | 0.24          |
| (1,2089) | 1:152:A:ALA:HB1  | 1:152:A:ALA:H    | 5        | 0.24          |
| (1,2089) | 1:152:A:ALA:HB2  | 1:152:A:ALA:H    | 5        | 0.24          |
| (1,2089) | 1:152:A:ALA:HB3  | 1:152:A:ALA:H    | 5        | 0.24          |
| (1,2089) | 1:152:A:ALA:HB1  | 1:152:A:ALA:H    | 7        | 0.24          |
| (1,2089) | 1:152:A:ALA:HB2  | 1:152:A:ALA:H    | 7        | 0.24          |
| (1,2089) | 1:152:A:ALA:HB3  | 1:152:A:ALA:H    | 7        | 0.24          |
| (1,2066) | 1:148:A:THR:HA   | 1:149:A:LYS:H    | 2        | 0.24          |
| (1,2066) | 1:148:A:THR:HA   | 1:149:A:LYS:H    | 3        | 0.24          |
| (1,2066) | 1:148:A:THR:HA   | 1:149:A:LYS:H    | 8        | 0.24          |
| (1,2030) | 1:143:A:ILE:HG21 | 1:143:A:ILE:HD11 | 6        | 0.24          |
| (1,2030) | 1:143:A:ILE:HG21 | 1:143:A:ILE:HD12 | 6        | 0.24          |
| (1,2030) | 1:143:A:ILE:HG21 | 1:143:A:ILE:HD13 | 6        | 0.24          |
| (1,2030) | 1:143:A:ILE:HG22 | 1:143:A:ILE:HD11 | 6        | 0.24          |
| (1,2030) | 1:143:A:ILE:HG22 | 1:143:A:ILE:HD12 | 6        | 0.24          |
| (1,2030) | 1:143:A:ILE:HG22 | 1:143:A:ILE:HD13 | 6        | 0.24          |
| (1,2030) | 1:143:A:ILE:HG23 | 1:143:A:ILE:HD11 | 6        | 0.24          |
| (1,2030) | 1:143:A:ILE:HG23 | 1:143:A:ILE:HD12 | 6        | 0.24          |
| (1,2030) | 1:143:A:ILE:HG23 | 1:143:A:ILE:HD13 | 6        | 0.24          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2030) | 1:143:A:ILE:HG21 | 1:143:A:ILE:HD11 | 7        | 0.24          |
| (1,2030) | 1:143:A:ILE:HG21 | 1:143:A:ILE:HD12 | 7        | 0.24          |
| (1,2030) | 1:143:A:ILE:HG21 | 1:143:A:ILE:HD13 | 7        | 0.24          |
| (1,2030) | 1:143:A:ILE:HG22 | 1:143:A:ILE:HD11 | 7        | 0.24          |
| (1,2030) | 1:143:A:ILE:HG22 | 1:143:A:ILE:HD12 | 7        | 0.24          |
| (1,2030) | 1:143:A:ILE:HG22 | 1:143:A:ILE:HD13 | 7        | 0.24          |
| (1,2030) | 1:143:A:ILE:HG23 | 1:143:A:ILE:HD11 | 7        | 0.24          |
| (1,2030) | 1:143:A:ILE:HG23 | 1:143:A:ILE:HD12 | 7        | 0.24          |
| (1,2030) | 1:143:A:ILE:HG23 | 1:143:A:ILE:HD13 | 7        | 0.24          |
| (1,2021) | 1:143:A:ILE:HA   | 1:143:A:ILE:HD11 | 7        | 0.24          |
| (1,2021) | 1:143:A:ILE:HA   | 1:143:A:ILE:HD12 | 7        | 0.24          |
| (1,2021) | 1:143:A:ILE:HA   | 1:143:A:ILE:HD13 | 7        | 0.24          |
| (1,1923) | 1:134:A:TRP:HE1  | 1:139:A:PRO:HD2  | 7        | 0.24          |
| (1,1852) | 1:133:A:ILE:HA   | 1:133:A:ILE:HG21 | 8        | 0.24          |
| (1,1852) | 1:133:A:ILE:HA   | 1:133:A:ILE:HG22 | 8        | 0.24          |
| (1,1852) | 1:133:A:ILE:HA   | 1:133:A:ILE:HG23 | 8        | 0.24          |
| (1,1803) | 1:129:A:THR:HA   | 1:129:A:THR:HG21 | 1        | 0.24          |
| (1,1803) | 1:129:A:THR:HA   | 1:129:A:THR:HG22 | 1        | 0.24          |
| (1,1803) | 1:129:A:THR:HA   | 1:129:A:THR:HG23 | 1        | 0.24          |
| (1,1803) | 1:129:A:THR:HA   | 1:129:A:THR:HG21 | 2        | 0.24          |
| (1,1803) | 1:129:A:THR:HA   | 1:129:A:THR:HG22 | 2        | 0.24          |
| (1,1803) | 1:129:A:THR:HA   | 1:129:A:THR:HG23 | 2        | 0.24          |
| (1,1800) | 1:128:A:TYR:HD1  | 1:129:A:THR:HG21 | 4        | 0.24          |
| (1,1800) | 1:128:A:TYR:HD1  | 1:129:A:THR:HG22 | 4        | 0.24          |
| (1,1800) | 1:128:A:TYR:HD1  | 1:129:A:THR:HG23 | 4        | 0.24          |
| (1,1800) | 1:128:A:TYR:HD2  | 1:129:A:THR:HG21 | 4        | 0.24          |
| (1,1800) | 1:128:A:TYR:HD2  | 1:129:A:THR:HG22 | 4        | 0.24          |
| (1,1800) | 1:128:A:TYR:HD2  | 1:129:A:THR:HG23 | 4        | 0.24          |
| (1,1769) | 1:120:A:VAL:HG21 | 1:120:A:VAL:H    | 6        | 0.24          |
| (1,1769) | 1:120:A:VAL:HG22 | 1:120:A:VAL:H    | 6        | 0.24          |
| (1,1769) | 1:120:A:VAL:HG23 | 1:120:A:VAL:H    | 6        | 0.24          |
| (1,1706) | 1:115:A:LYS:HG2  | 1:115:A:LYS:H    | 2        | 0.24          |
| (1,1706) | 1:115:A:LYS:HG3  | 1:115:A:LYS:H    | 2        | 0.24          |
| (1,1635) | 1:111:A:ILE:HB   | 1:111:A:ILE:H    | 8        | 0.24          |
| (1,1445) | 1:90:A:THR:HA    | 1:90:A:THR:HG21  | 9        | 0.24          |
| (1,1445) | 1:90:A:THR:HA    | 1:90:A:THR:HG22  | 9        | 0.24          |
| (1,1445) | 1:90:A:THR:HA    | 1:90:A:THR:HG23  | 9        | 0.24          |
| (1,1252) | 1:82:A:THR:HA    | 1:82:A:THR:HG21  | 10       | 0.24          |
| (1,1252) | 1:82:A:THR:HA    | 1:82:A:THR:HG22  | 10       | 0.24          |
| (1,1252) | 1:82:A:THR:HA    | 1:82:A:THR:HG23  | 10       | 0.24          |
| (1,1165) | 1:79:A:ILE:HG12  | 1:79:A:ILE:H     | 3        | 0.24          |
| (1,1165) | 1:79:A:ILE:HG12  | 1:79:A:ILE:H     | 8        | 0.24          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1114) | 1:78:A:GLN:HA   | 1:159:A:PHE:HB3 | 4        | 0.24          |
| (1,1013) | 1:74:A:PHE:HB2  | 1:163:A:LYS:H   | 1        | 0.24          |
| (1,1013) | 1:74:A:PHE:HB2  | 1:163:A:LYS:H   | 3        | 0.24          |
| (1,941)  | 1:71:A:LYS:HA   | 1:74:A:PHE:HD1  | 5        | 0.24          |
| (1,941)  | 1:71:A:LYS:HA   | 1:74:A:PHE:HD2  | 5        | 0.24          |
| (1,886)  | 1:68:A:GLU:HA   | 1:71:A:LYS:HD2  | 5        | 0.24          |
| (1,886)  | 1:68:A:GLU:HA   | 1:71:A:LYS:HD3  | 5        | 0.24          |
| (1,873)  | 1:67:A:ALA:HB1  | 1:68:A:GLU:H    | 3        | 0.24          |
| (1,873)  | 1:67:A:ALA:HB2  | 1:68:A:GLU:H    | 3        | 0.24          |
| (1,873)  | 1:67:A:ALA:HB3  | 1:68:A:GLU:H    | 3        | 0.24          |
| (1,837)  | 1:66:A:ASN:HB2  | 1:66:A:ASN:HD22 | 8        | 0.24          |
| (1,833)  | 1:66:A:ASN:HB3  | 1:66:A:ASN:HD22 | 9        | 0.24          |
| (1,779)  | 1:64:A:LEU:HD11 | 1:64:A:LEU:HD21 | 5        | 0.24          |
| (1,779)  | 1:64:A:LEU:HD11 | 1:64:A:LEU:HD22 | 5        | 0.24          |
| (1,779)  | 1:64:A:LEU:HD11 | 1:64:A:LEU:HD23 | 5        | 0.24          |
| (1,779)  | 1:64:A:LEU:HD12 | 1:64:A:LEU:HD21 | 5        | 0.24          |
| (1,779)  | 1:64:A:LEU:HD12 | 1:64:A:LEU:HD22 | 5        | 0.24          |
| (1,779)  | 1:64:A:LEU:HD12 | 1:64:A:LEU:HD23 | 5        | 0.24          |
| (1,779)  | 1:64:A:LEU:HD13 | 1:64:A:LEU:HD21 | 5        | 0.24          |
| (1,779)  | 1:64:A:LEU:HD13 | 1:64:A:LEU:HD22 | 5        | 0.24          |
| (1,779)  | 1:64:A:LEU:HD13 | 1:64:A:LEU:HD23 | 5        | 0.24          |
| (1,779)  | 1:64:A:LEU:HD11 | 1:64:A:LEU:HD21 | 8        | 0.24          |
| (1,779)  | 1:64:A:LEU:HD11 | 1:64:A:LEU:HD22 | 8        | 0.24          |
| (1,779)  | 1:64:A:LEU:HD11 | 1:64:A:LEU:HD23 | 8        | 0.24          |
| (1,779)  | 1:64:A:LEU:HD12 | 1:64:A:LEU:HD21 | 8        | 0.24          |
| (1,779)  | 1:64:A:LEU:HD12 | 1:64:A:LEU:HD22 | 8        | 0.24          |
| (1,779)  | 1:64:A:LEU:HD12 | 1:64:A:LEU:HD23 | 8        | 0.24          |
| (1,779)  | 1:64:A:LEU:HD13 | 1:64:A:LEU:HD21 | 8        | 0.24          |
| (1,779)  | 1:64:A:LEU:HD13 | 1:64:A:LEU:HD22 | 8        | 0.24          |
| (1,779)  | 1:64:A:LEU:HD13 | 1:64:A:LEU:HD23 | 8        | 0.24          |
| (1,728)  | 1:62:A:VAL:HG21 | 1:62:A:VAL:H    | 3        | 0.24          |
| (1,728)  | 1:62:A:VAL:HG22 | 1:62:A:VAL:H    | 3        | 0.24          |
| (1,728)  | 1:62:A:VAL:HG23 | 1:62:A:VAL:H    | 3        | 0.24          |
| (1,727)  | 1:62:A:VAL:HG11 | 1:177:A:PHE:HE1 | 3        | 0.24          |
| (1,727)  | 1:62:A:VAL:HG11 | 1:177:A:PHE:HE2 | 3        | 0.24          |
| (1,727)  | 1:62:A:VAL:HG12 | 1:177:A:PHE:HE1 | 3        | 0.24          |
| (1,727)  | 1:62:A:VAL:HG12 | 1:177:A:PHE:HE2 | 3        | 0.24          |
| (1,727)  | 1:62:A:VAL:HG13 | 1:177:A:PHE:HE1 | 3        | 0.24          |
| (1,727)  | 1:62:A:VAL:HG13 | 1:177:A:PHE:HE2 | 3        | 0.24          |
| (1,709)  | 1:62:A:VAL:HA   | 1:62:A:VAL:HG11 | 8        | 0.24          |
| (1,709)  | 1:62:A:VAL:HA   | 1:62:A:VAL:HG12 | 8        | 0.24          |
| (1,709)  | 1:62:A:VAL:HA   | 1:62:A:VAL:HG13 | 8        | 0.24          |

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| Key     | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,684) | 1:60:A:LEU:H    | 1:61:A:LYS:H     | 5        | 0.24          |
| (1,627) | 1:56:A:ASN:HB2  | 1:56:A:ASN:HD21  | 2        | 0.24          |
| (1,627) | 1:56:A:ASN:HB3  | 1:56:A:ASN:HD21  | 2        | 0.24          |
| (1,627) | 1:56:A:ASN:HB2  | 1:56:A:ASN:HD21  | 7        | 0.24          |
| (1,627) | 1:56:A:ASN:HB3  | 1:56:A:ASN:HD21  | 7        | 0.24          |
| (1,582) | 1:51:A:ILE:HG21 | 1:55:A:VAL:H     | 8        | 0.24          |
| (1,582) | 1:51:A:ILE:HG22 | 1:55:A:VAL:H     | 8        | 0.24          |
| (1,582) | 1:51:A:ILE:HG23 | 1:55:A:VAL:H     | 8        | 0.24          |
| (1,475) | 1:48:A:ILE:HA   | 1:151:A:VAL:HG21 | 5        | 0.24          |
| (1,475) | 1:48:A:ILE:HA   | 1:151:A:VAL:HG22 | 5        | 0.24          |
| (1,475) | 1:48:A:ILE:HA   | 1:151:A:VAL:HG23 | 5        | 0.24          |
| (1,427) | 1:46:A:TYR:HA   | 1:156:A:PHE:HE1  | 4        | 0.24          |
| (1,427) | 1:46:A:TYR:HA   | 1:156:A:PHE:HE2  | 4        | 0.24          |
| (1,392) | 1:44:A:ILE:HG21 | 1:158:A:ALA:H    | 10       | 0.24          |
| (1,392) | 1:44:A:ILE:HG22 | 1:158:A:ALA:H    | 10       | 0.24          |
| (1,392) | 1:44:A:ILE:HG23 | 1:158:A:ALA:H    | 10       | 0.24          |
| (1,240) | 1:32:A:ILE:HG21 | 1:74:A:PHE:HE1   | 2        | 0.24          |
| (1,240) | 1:32:A:ILE:HG21 | 1:74:A:PHE:HE2   | 2        | 0.24          |
| (1,240) | 1:32:A:ILE:HG22 | 1:74:A:PHE:HE1   | 2        | 0.24          |
| (1,240) | 1:32:A:ILE:HG22 | 1:74:A:PHE:HE2   | 2        | 0.24          |
| (1,240) | 1:32:A:ILE:HG23 | 1:74:A:PHE:HE1   | 2        | 0.24          |
| (1,240) | 1:32:A:ILE:HG23 | 1:74:A:PHE:HE2   | 2        | 0.24          |
| (1,232) | 1:32:A:ILE:HG21 | 1:32:A:ILE:HD11  | 4        | 0.24          |
| (1,232) | 1:32:A:ILE:HG21 | 1:32:A:ILE:HD12  | 4        | 0.24          |
| (1,232) | 1:32:A:ILE:HG21 | 1:32:A:ILE:HD13  | 4        | 0.24          |
| (1,232) | 1:32:A:ILE:HG22 | 1:32:A:ILE:HD11  | 4        | 0.24          |
| (1,232) | 1:32:A:ILE:HG22 | 1:32:A:ILE:HD12  | 4        | 0.24          |
| (1,232) | 1:32:A:ILE:HG22 | 1:32:A:ILE:HD13  | 4        | 0.24          |
| (1,232) | 1:32:A:ILE:HG23 | 1:32:A:ILE:HD11  | 4        | 0.24          |
| (1,232) | 1:32:A:ILE:HG23 | 1:32:A:ILE:HD12  | 4        | 0.24          |
| (1,232) | 1:32:A:ILE:HG23 | 1:32:A:ILE:HD13  | 4        | 0.24          |
| (1,170) | 1:29:A:LEU:HD21 | 1:175:A:PHE:HD1  | 2        | 0.24          |
| (1,170) | 1:29:A:LEU:HD21 | 1:175:A:PHE:HD2  | 2        | 0.24          |
| (1,170) | 1:29:A:LEU:HD22 | 1:175:A:PHE:HD1  | 2        | 0.24          |
| (1,170) | 1:29:A:LEU:HD22 | 1:175:A:PHE:HD2  | 2        | 0.24          |
| (1,170) | 1:29:A:LEU:HD23 | 1:175:A:PHE:HD1  | 2        | 0.24          |
| (1,170) | 1:29:A:LEU:HD23 | 1:175:A:PHE:HD2  | 2        | 0.24          |
| (1,170) | 1:29:A:LEU:HD21 | 1:175:A:PHE:HD1  | 4        | 0.24          |
| (1,170) | 1:29:A:LEU:HD21 | 1:175:A:PHE:HD2  | 4        | 0.24          |
| (1,170) | 1:29:A:LEU:HD22 | 1:175:A:PHE:HD1  | 4        | 0.24          |
| (1,170) | 1:29:A:LEU:HD22 | 1:175:A:PHE:HD2  | 4        | 0.24          |
| (1,170) | 1:29:A:LEU:HD23 | 1:175:A:PHE:HD1  | 4        | 0.24          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,170)  | 1:29:A:LEU:HD23  | 1:175:A:PHE:HD2  | 4        | 0.24          |
| (1,109)  | 1:26:A:GLU:H     | 1:47:A:ALA:HA    | 6        | 0.24          |
| (1,109)  | 1:26:A:GLU:H     | 1:47:A:ALA:HA    | 8        | 0.24          |
| (1,25)   | 1:23:A:ILE:HA    | 1:23:A:ILE:HG21  | 5        | 0.24          |
| (1,25)   | 1:23:A:ILE:HA    | 1:23:A:ILE:HG22  | 5        | 0.24          |
| (1,25)   | 1:23:A:ILE:HA    | 1:23:A:ILE:HG23  | 5        | 0.24          |
| (3,12)   | 1:181:A:GLN:HA   | 1:181:A:GLN:HB3  | 7        | 0.23          |
| (2,731)  | 1:155:A:ASN:H    | 1:156:A:PHE:HD1  | 5        | 0.23          |
| (2,731)  | 1:155:A:ASN:H    | 1:156:A:PHE:HD2  | 5        | 0.23          |
| (2,729)  | 1:151:A:VAL:H    | 1:153:A:ILE:HD11 | 3        | 0.23          |
| (2,729)  | 1:151:A:VAL:H    | 1:153:A:ILE:HD12 | 3        | 0.23          |
| (2,729)  | 1:151:A:VAL:H    | 1:153:A:ILE:HD13 | 3        | 0.23          |
| (2,628)  | 1:122:A:TYR:HB3  | 1:123:A:PRO:HD2  | 2        | 0.23          |
| (2,547)  | 1:87:A:THR:HG21  | 1:91:A:ALA:H     | 9        | 0.23          |
| (2,547)  | 1:87:A:THR:HG22  | 1:91:A:ALA:H     | 9        | 0.23          |
| (2,547)  | 1:87:A:THR:HG23  | 1:91:A:ALA:H     | 9        | 0.23          |
| (2,227)  | 1:43:A:ASP:HB3   | 1:46:A:TYR:HE1   | 9        | 0.23          |
| (2,227)  | 1:43:A:ASP:HB3   | 1:46:A:TYR:HE2   | 9        | 0.23          |
| (2,174)  | 1:35:A:ALA:HB1   | 1:40:A:GLY:H     | 5        | 0.23          |
| (2,174)  | 1:35:A:ALA:HB2   | 1:40:A:GLY:H     | 5        | 0.23          |
| (2,174)  | 1:35:A:ALA:HB3   | 1:40:A:GLY:H     | 5        | 0.23          |
| (2,4)    | 1:15:A:THR:HG21  | 1:16:A:ALA:H     | 5        | 0.23          |
| (2,4)    | 1:15:A:THR:HG22  | 1:16:A:ALA:H     | 5        | 0.23          |
| (2,4)    | 1:15:A:THR:HG23  | 1:16:A:ALA:H     | 5        | 0.23          |
| (1,2463) | 1:182:A:VAL:HG21 | 1:182:A:VAL:H    | 10       | 0.23          |
| (1,2463) | 1:182:A:VAL:HG22 | 1:182:A:VAL:H    | 10       | 0.23          |
| (1,2463) | 1:182:A:VAL:HG23 | 1:182:A:VAL:H    | 10       | 0.23          |
| (1,2371) | 1:174:A:ILE:HG21 | 1:175:A:PHE:H    | 3        | 0.23          |
| (1,2371) | 1:174:A:ILE:HG22 | 1:175:A:PHE:H    | 3        | 0.23          |
| (1,2371) | 1:174:A:ILE:HG23 | 1:175:A:PHE:H    | 3        | 0.23          |
| (1,2349) | 1:173:A:VAL:HB   | 1:174:A:ILE:H    | 1        | 0.23          |
| (1,2349) | 1:173:A:VAL:HB   | 1:174:A:ILE:H    | 2        | 0.23          |
| (1,2321) | 1:171:A:LEU:HD11 | 1:171:A:LEU:H    | 2        | 0.23          |
| (1,2321) | 1:171:A:LEU:HD12 | 1:171:A:LEU:H    | 2        | 0.23          |
| (1,2321) | 1:171:A:LEU:HD13 | 1:171:A:LEU:H    | 2        | 0.23          |
| (1,2310) | 1:170:A:SER:H    | 1:171:A:LEU:HD11 | 2        | 0.23          |
| (1,2310) | 1:170:A:SER:H    | 1:171:A:LEU:HD12 | 2        | 0.23          |
| (1,2310) | 1:170:A:SER:H    | 1:171:A:LEU:HD13 | 2        | 0.23          |
| (1,2093) | 1:153:A:ILE:HA   | 1:153:A:ILE:HG21 | 10       | 0.23          |
| (1,2093) | 1:153:A:ILE:HA   | 1:153:A:ILE:HG22 | 10       | 0.23          |
| (1,2093) | 1:153:A:ILE:HA   | 1:153:A:ILE:HG23 | 10       | 0.23          |
| (1,2066) | 1:148:A:THR:HA   | 1:149:A:LYS:H    | 10       | 0.23          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2030) | 1:143:A:ILE:HG21 | 1:143:A:ILE:HD11 | 2        | 0.23          |
| (1,2030) | 1:143:A:ILE:HG21 | 1:143:A:ILE:HD12 | 2        | 0.23          |
| (1,2030) | 1:143:A:ILE:HG21 | 1:143:A:ILE:HD13 | 2        | 0.23          |
| (1,2030) | 1:143:A:ILE:HG22 | 1:143:A:ILE:HD11 | 2        | 0.23          |
| (1,2030) | 1:143:A:ILE:HG22 | 1:143:A:ILE:HD12 | 2        | 0.23          |
| (1,2030) | 1:143:A:ILE:HG22 | 1:143:A:ILE:HD13 | 2        | 0.23          |
| (1,2030) | 1:143:A:ILE:HG23 | 1:143:A:ILE:HD11 | 2        | 0.23          |
| (1,2030) | 1:143:A:ILE:HG23 | 1:143:A:ILE:HD12 | 2        | 0.23          |
| (1,2030) | 1:143:A:ILE:HG23 | 1:143:A:ILE:HD13 | 2        | 0.23          |
| (1,2030) | 1:143:A:ILE:HG21 | 1:143:A:ILE:HD11 | 3        | 0.23          |
| (1,2030) | 1:143:A:ILE:HG21 | 1:143:A:ILE:HD12 | 3        | 0.23          |
| (1,2030) | 1:143:A:ILE:HG21 | 1:143:A:ILE:HD13 | 3        | 0.23          |
| (1,2030) | 1:143:A:ILE:HG22 | 1:143:A:ILE:HD11 | 3        | 0.23          |
| (1,2030) | 1:143:A:ILE:HG22 | 1:143:A:ILE:HD12 | 3        | 0.23          |
| (1,2030) | 1:143:A:ILE:HG22 | 1:143:A:ILE:HD13 | 3        | 0.23          |
| (1,2030) | 1:143:A:ILE:HG23 | 1:143:A:ILE:HD11 | 3        | 0.23          |
| (1,2030) | 1:143:A:ILE:HG23 | 1:143:A:ILE:HD12 | 3        | 0.23          |
| (1,2030) | 1:143:A:ILE:HG23 | 1:143:A:ILE:HD13 | 3        | 0.23          |
| (1,2030) | 1:143:A:ILE:HG21 | 1:143:A:ILE:HD11 | 10       | 0.23          |
| (1,2030) | 1:143:A:ILE:HG21 | 1:143:A:ILE:HD12 | 10       | 0.23          |
| (1,2030) | 1:143:A:ILE:HG21 | 1:143:A:ILE:HD13 | 10       | 0.23          |
| (1,2030) | 1:143:A:ILE:HG22 | 1:143:A:ILE:HD11 | 10       | 0.23          |
| (1,2030) | 1:143:A:ILE:HG22 | 1:143:A:ILE:HD12 | 10       | 0.23          |
| (1,2030) | 1:143:A:ILE:HG22 | 1:143:A:ILE:HD13 | 10       | 0.23          |
| (1,2030) | 1:143:A:ILE:HG23 | 1:143:A:ILE:HD11 | 10       | 0.23          |
| (1,2030) | 1:143:A:ILE:HG23 | 1:143:A:ILE:HD12 | 10       | 0.23          |
| (1,2030) | 1:143:A:ILE:HG23 | 1:143:A:ILE:HD13 | 10       | 0.23          |
| (1,2022) | 1:143:A:ILE:HA   | 1:143:A:ILE:HG21 | 8        | 0.23          |
| (1,2022) | 1:143:A:ILE:HA   | 1:143:A:ILE:HG22 | 8        | 0.23          |
| (1,2022) | 1:143:A:ILE:HA   | 1:143:A:ILE:HG23 | 8        | 0.23          |
| (1,2021) | 1:143:A:ILE:HA   | 1:143:A:ILE:HD11 | 3        | 0.23          |
| (1,2021) | 1:143:A:ILE:HA   | 1:143:A:ILE:HD12 | 3        | 0.23          |
| (1,2021) | 1:143:A:ILE:HA   | 1:143:A:ILE:HD13 | 3        | 0.23          |
| (1,2021) | 1:143:A:ILE:HA   | 1:143:A:ILE:HD11 | 9        | 0.23          |
| (1,2021) | 1:143:A:ILE:HA   | 1:143:A:ILE:HD12 | 9        | 0.23          |
| (1,2021) | 1:143:A:ILE:HA   | 1:143:A:ILE:HD13 | 9        | 0.23          |
| (1,2003) | 1:142:A:ILE:HA   | 1:142:A:ILE:HG21 | 5        | 0.23          |
| (1,2003) | 1:142:A:ILE:HA   | 1:142:A:ILE:HG22 | 5        | 0.23          |
| (1,2003) | 1:142:A:ILE:HA   | 1:142:A:ILE:HG23 | 5        | 0.23          |
| (1,2003) | 1:142:A:ILE:HA   | 1:142:A:ILE:HG21 | 6        | 0.23          |
| (1,2003) | 1:142:A:ILE:HA   | 1:142:A:ILE:HG22 | 6        | 0.23          |
| (1,2003) | 1:142:A:ILE:HA   | 1:142:A:ILE:HG23 | 6        | 0.23          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1978) | 1:139:A:PRO:HA   | 1:142:A:ILE:HD11 | 1        | 0.23          |
| (1,1978) | 1:139:A:PRO:HA   | 1:142:A:ILE:HD12 | 1        | 0.23          |
| (1,1978) | 1:139:A:PRO:HA   | 1:142:A:ILE:HD13 | 1        | 0.23          |
| (1,1852) | 1:133:A:ILE:HA   | 1:133:A:ILE:HG21 | 4        | 0.23          |
| (1,1852) | 1:133:A:ILE:HA   | 1:133:A:ILE:HG22 | 4        | 0.23          |
| (1,1852) | 1:133:A:ILE:HA   | 1:133:A:ILE:HG23 | 4        | 0.23          |
| (1,1852) | 1:133:A:ILE:HA   | 1:133:A:ILE:HG21 | 7        | 0.23          |
| (1,1852) | 1:133:A:ILE:HA   | 1:133:A:ILE:HG22 | 7        | 0.23          |
| (1,1852) | 1:133:A:ILE:HA   | 1:133:A:ILE:HG23 | 7        | 0.23          |
| (1,1818) | 1:131:A:THR:HG21 | 1:131:A:THR:H    | 9        | 0.23          |
| (1,1818) | 1:131:A:THR:HG22 | 1:131:A:THR:H    | 9        | 0.23          |
| (1,1818) | 1:131:A:THR:HG23 | 1:131:A:THR:H    | 9        | 0.23          |
| (1,1769) | 1:120:A:VAL:HG21 | 1:120:A:VAL:H    | 1        | 0.23          |
| (1,1769) | 1:120:A:VAL:HG22 | 1:120:A:VAL:H    | 1        | 0.23          |
| (1,1769) | 1:120:A:VAL:HG23 | 1:120:A:VAL:H    | 1        | 0.23          |
| (1,1769) | 1:120:A:VAL:HG21 | 1:120:A:VAL:H    | 5        | 0.23          |
| (1,1769) | 1:120:A:VAL:HG22 | 1:120:A:VAL:H    | 5        | 0.23          |
| (1,1769) | 1:120:A:VAL:HG23 | 1:120:A:VAL:H    | 5        | 0.23          |
| (1,1653) | 1:113:A:LEU:HA   | 1:113:A:LEU:HD21 | 8        | 0.23          |
| (1,1653) | 1:113:A:LEU:HA   | 1:113:A:LEU:HD22 | 8        | 0.23          |
| (1,1653) | 1:113:A:LEU:HA   | 1:113:A:LEU:HD23 | 8        | 0.23          |
| (1,1653) | 1:113:A:LEU:HA   | 1:113:A:LEU:HD21 | 9        | 0.23          |
| (1,1653) | 1:113:A:LEU:HA   | 1:113:A:LEU:HD22 | 9        | 0.23          |
| (1,1653) | 1:113:A:LEU:HA   | 1:113:A:LEU:HD23 | 9        | 0.23          |
| (1,1640) | 1:111:A:ILE:HG21 | 1:112:A:VAL:H    | 4        | 0.23          |
| (1,1640) | 1:111:A:ILE:HG22 | 1:112:A:VAL:H    | 4        | 0.23          |
| (1,1640) | 1:111:A:ILE:HG23 | 1:112:A:VAL:H    | 4        | 0.23          |
| (1,1399) | 1:87:A:THR:HG21  | 1:87:A:THR:H     | 1        | 0.23          |
| (1,1399) | 1:87:A:THR:HG22  | 1:87:A:THR:H     | 1        | 0.23          |
| (1,1399) | 1:87:A:THR:HG23  | 1:87:A:THR:H     | 1        | 0.23          |
| (1,1252) | 1:82:A:THR:HA    | 1:82:A:THR:HG21  | 5        | 0.23          |
| (1,1252) | 1:82:A:THR:HA    | 1:82:A:THR:HG22  | 5        | 0.23          |
| (1,1252) | 1:82:A:THR:HA    | 1:82:A:THR:HG23  | 5        | 0.23          |
| (1,1236) | 1:81:A:ILE:HG21  | 1:154:A:LEU:HB3  | 1        | 0.23          |
| (1,1236) | 1:81:A:ILE:HG22  | 1:154:A:LEU:HB3  | 1        | 0.23          |
| (1,1236) | 1:81:A:ILE:HG23  | 1:154:A:LEU:HB3  | 1        | 0.23          |
| (1,1180) | 1:80:A:GLN:HA    | 1:101:A:VAL:H    | 7        | 0.23          |
| (1,1173) | 1:79:A:ILE:H     | 1:158:A:ALA:HA   | 5        | 0.23          |
| (1,1165) | 1:79:A:ILE:HG12  | 1:79:A:ILE:H     | 7        | 0.23          |
| (1,1114) | 1:78:A:GLN:HA    | 1:159:A:PHE:HB3  | 6        | 0.23          |
| (1,1114) | 1:78:A:GLN:HA    | 1:159:A:PHE:HB3  | 8        | 0.23          |
| (1,1038) | 1:74:A:PHE:HZ    | 1:171:A:LEU:H    | 8        | 0.23          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1013) | 1:74:A:PHE:HB2  | 1:163:A:LYS:H   | 4        | 0.23          |
| (1,1013) | 1:74:A:PHE:HB2  | 1:163:A:LYS:H   | 5        | 0.23          |
| (1,1013) | 1:74:A:PHE:HB2  | 1:163:A:LYS:H   | 6        | 0.23          |
| (1,1013) | 1:74:A:PHE:HB2  | 1:163:A:LYS:H   | 7        | 0.23          |
| (1,915)  | 1:69:A:GLN:HG3  | 1:70:A:LEU:H    | 6        | 0.23          |
| (1,915)  | 1:69:A:GLN:HG3  | 1:70:A:LEU:H    | 9        | 0.23          |
| (1,911)  | 1:69:A:GLN:HE22 | 1:70:A:LEU:H    | 9        | 0.23          |
| (1,779)  | 1:64:A:LEU:HD11 | 1:64:A:LEU:HD21 | 10       | 0.23          |
| (1,779)  | 1:64:A:LEU:HD11 | 1:64:A:LEU:HD22 | 10       | 0.23          |
| (1,779)  | 1:64:A:LEU:HD11 | 1:64:A:LEU:HD23 | 10       | 0.23          |
| (1,779)  | 1:64:A:LEU:HD12 | 1:64:A:LEU:HD21 | 10       | 0.23          |
| (1,779)  | 1:64:A:LEU:HD12 | 1:64:A:LEU:HD22 | 10       | 0.23          |
| (1,779)  | 1:64:A:LEU:HD12 | 1:64:A:LEU:HD23 | 10       | 0.23          |
| (1,779)  | 1:64:A:LEU:HD13 | 1:64:A:LEU:HD21 | 10       | 0.23          |
| (1,779)  | 1:64:A:LEU:HD13 | 1:64:A:LEU:HD22 | 10       | 0.23          |
| (1,779)  | 1:64:A:LEU:HD13 | 1:64:A:LEU:HD23 | 10       | 0.23          |
| (1,709)  | 1:62:A:VAL:HA   | 1:62:A:VAL:HG11 | 2        | 0.23          |
| (1,709)  | 1:62:A:VAL:HA   | 1:62:A:VAL:HG12 | 2        | 0.23          |
| (1,709)  | 1:62:A:VAL:HA   | 1:62:A:VAL:HG13 | 2        | 0.23          |
| (1,627)  | 1:56:A:ASN:HB2  | 1:56:A:ASN:HD21 | 1        | 0.23          |
| (1,627)  | 1:56:A:ASN:HB3  | 1:56:A:ASN:HD21 | 1        | 0.23          |
| (1,627)  | 1:56:A:ASN:HB2  | 1:56:A:ASN:HD21 | 3        | 0.23          |
| (1,627)  | 1:56:A:ASN:HB3  | 1:56:A:ASN:HD21 | 3        | 0.23          |
| (1,627)  | 1:56:A:ASN:HB2  | 1:56:A:ASN:HD21 | 4        | 0.23          |
| (1,627)  | 1:56:A:ASN:HB3  | 1:56:A:ASN:HD21 | 4        | 0.23          |
| (1,627)  | 1:56:A:ASN:HB2  | 1:56:A:ASN:HD21 | 5        | 0.23          |
| (1,627)  | 1:56:A:ASN:HB3  | 1:56:A:ASN:HD21 | 5        | 0.23          |
| (1,627)  | 1:56:A:ASN:HB2  | 1:56:A:ASN:HD21 | 8        | 0.23          |
| (1,627)  | 1:56:A:ASN:HB3  | 1:56:A:ASN:HD21 | 8        | 0.23          |
| (1,627)  | 1:56:A:ASN:HB2  | 1:56:A:ASN:HD21 | 9        | 0.23          |
| (1,627)  | 1:56:A:ASN:HB3  | 1:56:A:ASN:HD21 | 9        | 0.23          |
| (1,627)  | 1:56:A:ASN:HB2  | 1:56:A:ASN:HD21 | 10       | 0.23          |
| (1,627)  | 1:56:A:ASN:HB3  | 1:56:A:ASN:HD21 | 10       | 0.23          |
| (1,621)  | 1:55:A:VAL:H    | 1:55:A:VAL:HG21 | 5        | 0.23          |
| (1,621)  | 1:55:A:VAL:H    | 1:55:A:VAL:HG22 | 5        | 0.23          |
| (1,621)  | 1:55:A:VAL:H    | 1:55:A:VAL:HG23 | 5        | 0.23          |
| (1,553)  | 1:50:A:TRP:HB2  | 1:52:A:LYS:H    | 5        | 0.23          |
| (1,498)  | 1:48:A:ILE:HG21 | 1:50:A:TRP:HZ2  | 5        | 0.23          |
| (1,498)  | 1:48:A:ILE:HG22 | 1:50:A:TRP:HZ2  | 5        | 0.23          |
| (1,498)  | 1:48:A:ILE:HG23 | 1:50:A:TRP:HZ2  | 5        | 0.23          |
| (1,467)  | 1:47:A:ALA:H    | 1:156:A:PHE:HE1 | 3        | 0.23          |
| (1,467)  | 1:47:A:ALA:H    | 1:156:A:PHE:HE2 | 3        | 0.23          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,455)  | 1:47:A:ALA:HB1   | 1:48:A:ILE:H     | 4        | 0.23          |
| (1,455)  | 1:47:A:ALA:HB2   | 1:48:A:ILE:H     | 4        | 0.23          |
| (1,455)  | 1:47:A:ALA:HB3   | 1:48:A:ILE:H     | 4        | 0.23          |
| (1,389)  | 1:44:A:ILE:HG21  | 1:44:A:ILE:H     | 10       | 0.23          |
| (1,389)  | 1:44:A:ILE:HG22  | 1:44:A:ILE:H     | 10       | 0.23          |
| (1,389)  | 1:44:A:ILE:HG23  | 1:44:A:ILE:H     | 10       | 0.23          |
| (1,246)  | 1:32:A:ILE:HG21  | 1:168:A:PHE:HE1  | 10       | 0.23          |
| (1,246)  | 1:32:A:ILE:HG21  | 1:168:A:PHE:HE2  | 10       | 0.23          |
| (1,246)  | 1:32:A:ILE:HG22  | 1:168:A:PHE:HE1  | 10       | 0.23          |
| (1,246)  | 1:32:A:ILE:HG22  | 1:168:A:PHE:HE2  | 10       | 0.23          |
| (1,246)  | 1:32:A:ILE:HG23  | 1:168:A:PHE:HE1  | 10       | 0.23          |
| (1,246)  | 1:32:A:ILE:HG23  | 1:168:A:PHE:HE2  | 10       | 0.23          |
| (1,109)  | 1:26:A:GLU:H     | 1:47:A:ALA:HA    | 10       | 0.23          |
| (1,25)   | 1:23:A:ILE:HA    | 1:23:A:ILE:HG21  | 10       | 0.23          |
| (1,25)   | 1:23:A:ILE:HA    | 1:23:A:ILE:HG22  | 10       | 0.23          |
| (1,25)   | 1:23:A:ILE:HA    | 1:23:A:ILE:HG23  | 10       | 0.23          |
| (2,732)  | 1:155:A:ASN:H    | 1:156:A:PHE:HE1  | 4        | 0.22          |
| (2,732)  | 1:155:A:ASN:H    | 1:156:A:PHE:HE2  | 4        | 0.22          |
| (2,714)  | 1:141:A:LYS:HD2  | 1:142:A:ILE:H    | 9        | 0.22          |
| (2,714)  | 1:141:A:LYS:HD3  | 1:142:A:ILE:H    | 9        | 0.22          |
| (2,593)  | 1:114:A:ASP:HB2  | 1:116:A:GLU:HG2  | 7        | 0.22          |
| (2,593)  | 1:114:A:ASP:HB2  | 1:116:A:GLU:HG3  | 7        | 0.22          |
| (2,590)  | 1:110:A:VAL:H    | 1:111:A:ILE:HD11 | 1        | 0.22          |
| (2,590)  | 1:110:A:VAL:H    | 1:111:A:ILE:HD12 | 1        | 0.22          |
| (2,590)  | 1:110:A:VAL:H    | 1:111:A:ILE:HD13 | 1        | 0.22          |
| (2,537)  | 1:85:A:TYR:H     | 1:85:A:TYR:HE1   | 2        | 0.22          |
| (2,537)  | 1:85:A:TYR:H     | 1:85:A:TYR:HE2   | 2        | 0.22          |
| (2,525)  | 1:85:A:TYR:HE1   | 1:85:A:TYR:H     | 2        | 0.22          |
| (2,525)  | 1:85:A:TYR:HE2   | 1:85:A:TYR:H     | 2        | 0.22          |
| (2,488)  | 1:80:A:GLN:H     | 1:81:A:ILE:HD11  | 4        | 0.22          |
| (2,488)  | 1:80:A:GLN:H     | 1:81:A:ILE:HD12  | 4        | 0.22          |
| (2,488)  | 1:80:A:GLN:H     | 1:81:A:ILE:HD13  | 4        | 0.22          |
| (1,2448) | 1:179:A:VAL:HG11 | 1:179:A:VAL:H    | 10       | 0.22          |
| (1,2448) | 1:179:A:VAL:HG12 | 1:179:A:VAL:H    | 10       | 0.22          |
| (1,2448) | 1:179:A:VAL:HG13 | 1:179:A:VAL:H    | 10       | 0.22          |
| (1,2425) | 1:177:A:PHE:HD1  | 1:177:A:PHE:H    | 1        | 0.22          |
| (1,2425) | 1:177:A:PHE:HD2  | 1:177:A:PHE:H    | 1        | 0.22          |
| (1,2370) | 1:174:A:ILE:HG21 | 1:175:A:PHE:HA   | 10       | 0.22          |
| (1,2370) | 1:174:A:ILE:HG22 | 1:175:A:PHE:HA   | 10       | 0.22          |
| (1,2370) | 1:174:A:ILE:HG23 | 1:175:A:PHE:HA   | 10       | 0.22          |
| (1,2349) | 1:173:A:VAL:HB   | 1:174:A:ILE:H    | 7        | 0.22          |
| (1,2286) | 1:168:A:PHE:HD1  | 1:168:A:PHE:H    | 8        | 0.22          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2286) | 1:168:A:PHE:HD2  | 1:168:A:PHE:H    | 8        | 0.22          |
| (1,2154) | 1:156:A:PHE:HD1  | 1:156:A:PHE:H    | 9        | 0.22          |
| (1,2154) | 1:156:A:PHE:HD2  | 1:156:A:PHE:H    | 9        | 0.22          |
| (1,2154) | 1:156:A:PHE:HD1  | 1:156:A:PHE:H    | 10       | 0.22          |
| (1,2154) | 1:156:A:PHE:HD2  | 1:156:A:PHE:H    | 10       | 0.22          |
| (1,2093) | 1:153:A:ILE:HA   | 1:153:A:ILE:HG21 | 3        | 0.22          |
| (1,2093) | 1:153:A:ILE:HA   | 1:153:A:ILE:HG22 | 3        | 0.22          |
| (1,2093) | 1:153:A:ILE:HA   | 1:153:A:ILE:HG23 | 3        | 0.22          |
| (1,2093) | 1:153:A:ILE:HA   | 1:153:A:ILE:HG21 | 6        | 0.22          |
| (1,2093) | 1:153:A:ILE:HA   | 1:153:A:ILE:HG22 | 6        | 0.22          |
| (1,2093) | 1:153:A:ILE:HA   | 1:153:A:ILE:HG23 | 6        | 0.22          |
| (1,2022) | 1:143:A:ILE:HA   | 1:143:A:ILE:HG21 | 4        | 0.22          |
| (1,2022) | 1:143:A:ILE:HA   | 1:143:A:ILE:HG22 | 4        | 0.22          |
| (1,2022) | 1:143:A:ILE:HA   | 1:143:A:ILE:HG23 | 4        | 0.22          |
| (1,2013) | 1:142:A:ILE:HG21 | 1:143:A:ILE:H    | 5        | 0.22          |
| (1,2013) | 1:142:A:ILE:HG22 | 1:143:A:ILE:H    | 5        | 0.22          |
| (1,2013) | 1:142:A:ILE:HG23 | 1:143:A:ILE:H    | 5        | 0.22          |
| (1,2003) | 1:142:A:ILE:HA   | 1:142:A:ILE:HG21 | 1        | 0.22          |
| (1,2003) | 1:142:A:ILE:HA   | 1:142:A:ILE:HG22 | 1        | 0.22          |
| (1,2003) | 1:142:A:ILE:HA   | 1:142:A:ILE:HG23 | 1        | 0.22          |
| (1,1852) | 1:133:A:ILE:HA   | 1:133:A:ILE:HG21 | 1        | 0.22          |
| (1,1852) | 1:133:A:ILE:HA   | 1:133:A:ILE:HG22 | 1        | 0.22          |
| (1,1852) | 1:133:A:ILE:HA   | 1:133:A:ILE:HG23 | 1        | 0.22          |
| (1,1852) | 1:133:A:ILE:HA   | 1:133:A:ILE:HG21 | 3        | 0.22          |
| (1,1852) | 1:133:A:ILE:HA   | 1:133:A:ILE:HG22 | 3        | 0.22          |
| (1,1852) | 1:133:A:ILE:HA   | 1:133:A:ILE:HG23 | 3        | 0.22          |
| (1,1852) | 1:133:A:ILE:HA   | 1:133:A:ILE:HG21 | 5        | 0.22          |
| (1,1852) | 1:133:A:ILE:HA   | 1:133:A:ILE:HG22 | 5        | 0.22          |
| (1,1852) | 1:133:A:ILE:HA   | 1:133:A:ILE:HG23 | 5        | 0.22          |
| (1,1852) | 1:133:A:ILE:HA   | 1:133:A:ILE:HG21 | 10       | 0.22          |
| (1,1852) | 1:133:A:ILE:HA   | 1:133:A:ILE:HG22 | 10       | 0.22          |
| (1,1852) | 1:133:A:ILE:HA   | 1:133:A:ILE:HG23 | 10       | 0.22          |
| (1,1845) | 1:132:A:SER:HB2  | 1:145:A:TYR:HD1  | 9        | 0.22          |
| (1,1845) | 1:132:A:SER:HB2  | 1:145:A:TYR:HD2  | 9        | 0.22          |
| (1,1769) | 1:120:A:VAL:HG21 | 1:120:A:VAL:H    | 3        | 0.22          |
| (1,1769) | 1:120:A:VAL:HG22 | 1:120:A:VAL:H    | 3        | 0.22          |
| (1,1769) | 1:120:A:VAL:HG23 | 1:120:A:VAL:H    | 3        | 0.22          |
| (1,1769) | 1:120:A:VAL:HG21 | 1:120:A:VAL:H    | 9        | 0.22          |
| (1,1769) | 1:120:A:VAL:HG22 | 1:120:A:VAL:H    | 9        | 0.22          |
| (1,1769) | 1:120:A:VAL:HG23 | 1:120:A:VAL:H    | 9        | 0.22          |
| (1,1653) | 1:113:A:LEU:HA   | 1:113:A:LEU:HD21 | 3        | 0.22          |
| (1,1653) | 1:113:A:LEU:HA   | 1:113:A:LEU:HD22 | 3        | 0.22          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1653) | 1:113:A:LEU:HA  | 1:113:A:LEU:HD23 | 3        | 0.22          |
| (1,1502) | 1:97:A:GLU:H    | 1:98:A:THR:HA    | 2        | 0.22          |
| (1,1502) | 1:97:A:GLU:H    | 1:98:A:THR:HA    | 5        | 0.22          |
| (1,1502) | 1:97:A:GLU:H    | 1:98:A:THR:HA    | 9        | 0.22          |
| (1,1446) | 1:90:A:THR:HA   | 1:93:A:GLY:H     | 9        | 0.22          |
| (1,1445) | 1:90:A:THR:HA   | 1:90:A:THR:HG21  | 2        | 0.22          |
| (1,1445) | 1:90:A:THR:HA   | 1:90:A:THR:HG22  | 2        | 0.22          |
| (1,1445) | 1:90:A:THR:HA   | 1:90:A:THR:HG23  | 2        | 0.22          |
| (1,1400) | 1:87:A:THR:HG21 | 1:88:A:ASN:HA    | 9        | 0.22          |
| (1,1400) | 1:87:A:THR:HG22 | 1:88:A:ASN:HA    | 9        | 0.22          |
| (1,1400) | 1:87:A:THR:HG23 | 1:88:A:ASN:HA    | 9        | 0.22          |
| (1,1338) | 1:85:A:TYR:HD1  | 1:86:A:GLU:H     | 8        | 0.22          |
| (1,1338) | 1:85:A:TYR:HD2  | 1:86:A:GLU:H     | 8        | 0.22          |
| (1,1298) | 1:83:A:SER:HA   | 1:154:A:LEU:HD21 | 7        | 0.22          |
| (1,1298) | 1:83:A:SER:HA   | 1:154:A:LEU:HD22 | 7        | 0.22          |
| (1,1298) | 1:83:A:SER:HA   | 1:154:A:LEU:HD23 | 7        | 0.22          |
| (1,1216) | 1:81:A:ILE:HD11 | 1:100:A:ALA:H    | 4        | 0.22          |
| (1,1216) | 1:81:A:ILE:HD12 | 1:100:A:ALA:H    | 4        | 0.22          |
| (1,1216) | 1:81:A:ILE:HD13 | 1:100:A:ALA:H    | 4        | 0.22          |
| (1,1185) | 1:80:A:GLN:HB2  | 1:159:A:PHE:HD1  | 7        | 0.22          |
| (1,1185) | 1:80:A:GLN:HB2  | 1:159:A:PHE:HD2  | 7        | 0.22          |
| (1,1185) | 1:80:A:GLN:HB3  | 1:159:A:PHE:HD1  | 7        | 0.22          |
| (1,1185) | 1:80:A:GLN:HB3  | 1:159:A:PHE:HD2  | 7        | 0.22          |
| (1,1173) | 1:79:A:ILE:H    | 1:158:A:ALA:HA   | 2        | 0.22          |
| (1,1173) | 1:79:A:ILE:H    | 1:158:A:ALA:HA   | 6        | 0.22          |
| (1,1116) | 1:78:A:GLN:HB3  | 1:78:A:GLN:H     | 4        | 0.22          |
| (1,1114) | 1:78:A:GLN:HA   | 1:159:A:PHE:HB3  | 10       | 0.22          |
| (1,1109) | 1:78:A:GLN:HA   | 1:78:A:GLN:HG2   | 10       | 0.22          |
| (1,1109) | 1:78:A:GLN:HA   | 1:78:A:GLN:HG3   | 10       | 0.22          |
| (1,1089) | 1:77:A:LEU:HD11 | 1:79:A:ILE:HD11  | 3        | 0.22          |
| (1,1089) | 1:77:A:LEU:HD11 | 1:79:A:ILE:HD12  | 3        | 0.22          |
| (1,1089) | 1:77:A:LEU:HD11 | 1:79:A:ILE:HD13  | 3        | 0.22          |
| (1,1089) | 1:77:A:LEU:HD12 | 1:79:A:ILE:HD11  | 3        | 0.22          |
| (1,1089) | 1:77:A:LEU:HD12 | 1:79:A:ILE:HD12  | 3        | 0.22          |
| (1,1089) | 1:77:A:LEU:HD12 | 1:79:A:ILE:HD13  | 3        | 0.22          |
| (1,1089) | 1:77:A:LEU:HD13 | 1:79:A:ILE:HD11  | 3        | 0.22          |
| (1,1089) | 1:77:A:LEU:HD13 | 1:79:A:ILE:HD12  | 3        | 0.22          |
| (1,1089) | 1:77:A:LEU:HD13 | 1:79:A:ILE:HD13  | 3        | 0.22          |
| (1,1089) | 1:77:A:LEU:HD21 | 1:79:A:ILE:HD11  | 3        | 0.22          |
| (1,1089) | 1:77:A:LEU:HD21 | 1:79:A:ILE:HD12  | 3        | 0.22          |
| (1,1089) | 1:77:A:LEU:HD21 | 1:79:A:ILE:HD13  | 3        | 0.22          |
| (1,1089) | 1:77:A:LEU:HD22 | 1:79:A:ILE:HD11  | 3        | 0.22          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1089) | 1:77:A:LEU:HD22 | 1:79:A:ILE:HD12 | 3        | 0.22          |
| (1,1089) | 1:77:A:LEU:HD22 | 1:79:A:ILE:HD13 | 3        | 0.22          |
| (1,1089) | 1:77:A:LEU:HD23 | 1:79:A:ILE:HD11 | 3        | 0.22          |
| (1,1089) | 1:77:A:LEU:HD23 | 1:79:A:ILE:HD12 | 3        | 0.22          |
| (1,1089) | 1:77:A:LEU:HD23 | 1:79:A:ILE:HD13 | 3        | 0.22          |
| (1,1089) | 1:77:A:LEU:HD11 | 1:79:A:ILE:HD11 | 7        | 0.22          |
| (1,1089) | 1:77:A:LEU:HD11 | 1:79:A:ILE:HD12 | 7        | 0.22          |
| (1,1089) | 1:77:A:LEU:HD11 | 1:79:A:ILE:HD13 | 7        | 0.22          |
| (1,1089) | 1:77:A:LEU:HD12 | 1:79:A:ILE:HD11 | 7        | 0.22          |
| (1,1089) | 1:77:A:LEU:HD12 | 1:79:A:ILE:HD12 | 7        | 0.22          |
| (1,1089) | 1:77:A:LEU:HD12 | 1:79:A:ILE:HD13 | 7        | 0.22          |
| (1,1089) | 1:77:A:LEU:HD13 | 1:79:A:ILE:HD11 | 7        | 0.22          |
| (1,1089) | 1:77:A:LEU:HD13 | 1:79:A:ILE:HD12 | 7        | 0.22          |
| (1,1089) | 1:77:A:LEU:HD13 | 1:79:A:ILE:HD13 | 7        | 0.22          |
| (1,1089) | 1:77:A:LEU:HD21 | 1:79:A:ILE:HD11 | 7        | 0.22          |
| (1,1089) | 1:77:A:LEU:HD21 | 1:79:A:ILE:HD12 | 7        | 0.22          |
| (1,1089) | 1:77:A:LEU:HD21 | 1:79:A:ILE:HD13 | 7        | 0.22          |
| (1,1089) | 1:77:A:LEU:HD22 | 1:79:A:ILE:HD11 | 7        | 0.22          |
| (1,1089) | 1:77:A:LEU:HD22 | 1:79:A:ILE:HD12 | 7        | 0.22          |
| (1,1089) | 1:77:A:LEU:HD22 | 1:79:A:ILE:HD13 | 7        | 0.22          |
| (1,1089) | 1:77:A:LEU:HD23 | 1:79:A:ILE:HD11 | 7        | 0.22          |
| (1,1089) | 1:77:A:LEU:HD23 | 1:79:A:ILE:HD12 | 7        | 0.22          |
| (1,1089) | 1:77:A:LEU:HD23 | 1:79:A:ILE:HD13 | 7        | 0.22          |
| (1,1020) | 1:74:A:PHE:HD1  | 1:162:A:ALA:HA  | 9        | 0.22          |
| (1,1020) | 1:74:A:PHE:HD2  | 1:162:A:ALA:HA  | 9        | 0.22          |
| (1,911)  | 1:69:A:GLN:HE22 | 1:70:A:LEU:H    | 5        | 0.22          |
| (1,909)  | 1:69:A:GLN:HB2  | 1:70:A:LEU:H    | 6        | 0.22          |
| (1,873)  | 1:67:A:ALA:HB1  | 1:68:A:GLU:H    | 5        | 0.22          |
| (1,873)  | 1:67:A:ALA:HB2  | 1:68:A:GLU:H    | 5        | 0.22          |
| (1,873)  | 1:67:A:ALA:HB3  | 1:68:A:GLU:H    | 5        | 0.22          |
| (1,728)  | 1:62:A:VAL:HG21 | 1:62:A:VAL:H    | 5        | 0.22          |
| (1,728)  | 1:62:A:VAL:HG22 | 1:62:A:VAL:H    | 5        | 0.22          |
| (1,728)  | 1:62:A:VAL:HG23 | 1:62:A:VAL:H    | 5        | 0.22          |
| (1,709)  | 1:62:A:VAL:HA   | 1:62:A:VAL:HG11 | 10       | 0.22          |
| (1,709)  | 1:62:A:VAL:HA   | 1:62:A:VAL:HG12 | 10       | 0.22          |
| (1,709)  | 1:62:A:VAL:HA   | 1:62:A:VAL:HG13 | 10       | 0.22          |
| (1,684)  | 1:60:A:LEU:H    | 1:61:A:LYS:H    | 7        | 0.22          |
| (1,623)  | 1:55:A:VAL:H    | 1:115:A:LYS:HA  | 4        | 0.22          |
| (1,621)  | 1:55:A:VAL:H    | 1:55:A:VAL:HG21 | 7        | 0.22          |
| (1,621)  | 1:55:A:VAL:H    | 1:55:A:VAL:HG22 | 7        | 0.22          |
| (1,621)  | 1:55:A:VAL:H    | 1:55:A:VAL:HG23 | 7        | 0.22          |
| (1,568)  | 1:51:A:ILE:HA   | 1:51:A:ILE:HG21 | 1        | 0.22          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,568)  | 1:51:A:ILE:HA    | 1:51:A:ILE:HG22  | 1        | 0.22          |
| (1,568)  | 1:51:A:ILE:HA    | 1:51:A:ILE:HG23  | 1        | 0.22          |
| (1,556)  | 1:50:A:TRP:HD1   | 1:151:A:VAL:HG21 | 8        | 0.22          |
| (1,556)  | 1:50:A:TRP:HD1   | 1:151:A:VAL:HG22 | 8        | 0.22          |
| (1,556)  | 1:50:A:TRP:HD1   | 1:151:A:VAL:HG23 | 8        | 0.22          |
| (1,543)  | 1:50:A:TRP:HA    | 1:151:A:VAL:HA   | 5        | 0.22          |
| (1,495)  | 1:48:A:ILE:HG21  | 1:50:A:TRP:HE1   | 10       | 0.22          |
| (1,495)  | 1:48:A:ILE:HG22  | 1:50:A:TRP:HE1   | 10       | 0.22          |
| (1,495)  | 1:48:A:ILE:HG23  | 1:50:A:TRP:HE1   | 10       | 0.22          |
| (1,467)  | 1:47:A:ALA:H     | 1:156:A:PHE:HE1  | 10       | 0.22          |
| (1,467)  | 1:47:A:ALA:H     | 1:156:A:PHE:HE2  | 10       | 0.22          |
| (1,461)  | 1:47:A:ALA:H     | 1:153:A:ILE:HG21 | 3        | 0.22          |
| (1,461)  | 1:47:A:ALA:H     | 1:153:A:ILE:HG22 | 3        | 0.22          |
| (1,461)  | 1:47:A:ALA:H     | 1:153:A:ILE:HG23 | 3        | 0.22          |
| (1,289)  | 1:37:A:GLY:HA3   | 1:37:A:GLY:H     | 7        | 0.22          |
| (3,4)    | 1:57:A:ASP:HA    | 1:114:A:ASP:HA   | 2        | 0.21          |
| (2,768)  | 1:173:A:VAL:HB   | 1:175:A:PHE:HE1  | 1        | 0.21          |
| (2,768)  | 1:173:A:VAL:HB   | 1:175:A:PHE:HE2  | 1        | 0.21          |
| (2,731)  | 1:155:A:ASN:H    | 1:156:A:PHE:HD1  | 9        | 0.21          |
| (2,731)  | 1:155:A:ASN:H    | 1:156:A:PHE:HD2  | 9        | 0.21          |
| (2,714)  | 1:141:A:LYS:HD2  | 1:142:A:ILE:H    | 3        | 0.21          |
| (2,714)  | 1:141:A:LYS:HD3  | 1:142:A:ILE:H    | 3        | 0.21          |
| (2,632)  | 1:122:A:TYR:HD1  | 1:125:A:LYS:H    | 9        | 0.21          |
| (2,632)  | 1:122:A:TYR:HD2  | 1:125:A:LYS:H    | 9        | 0.21          |
| (2,618)  | 1:119:A:ALA:HB1  | 1:149:A:LYS:H    | 3        | 0.21          |
| (2,618)  | 1:119:A:ALA:HB2  | 1:149:A:LYS:H    | 3        | 0.21          |
| (2,618)  | 1:119:A:ALA:HB3  | 1:149:A:LYS:H    | 3        | 0.21          |
| (2,552)  | 1:87:A:THR:H     | 1:92:A:LEU:HB2   | 9        | 0.21          |
| (2,468)  | 1:79:A:ILE:HG21  | 1:156:A:PHE:HE1  | 3        | 0.21          |
| (2,468)  | 1:79:A:ILE:HG21  | 1:156:A:PHE:HE2  | 3        | 0.21          |
| (2,468)  | 1:79:A:ILE:HG22  | 1:156:A:PHE:HE1  | 3        | 0.21          |
| (2,468)  | 1:79:A:ILE:HG22  | 1:156:A:PHE:HE2  | 3        | 0.21          |
| (2,468)  | 1:79:A:ILE:HG23  | 1:156:A:PHE:HE1  | 3        | 0.21          |
| (2,468)  | 1:79:A:ILE:HG23  | 1:156:A:PHE:HE2  | 3        | 0.21          |
| (2,341)  | 1:59:A:LYS:H     | 1:59:A:LYS:HE2   | 5        | 0.21          |
| (2,341)  | 1:59:A:LYS:H     | 1:59:A:LYS:HE3   | 5        | 0.21          |
| (2,194)  | 1:38:A:ALA:HB1   | 1:39:A:GLN:HE21  | 10       | 0.21          |
| (2,194)  | 1:38:A:ALA:HB2   | 1:39:A:GLN:HE21  | 10       | 0.21          |
| (2,194)  | 1:38:A:ALA:HB3   | 1:39:A:GLN:HE21  | 10       | 0.21          |
| (2,178)  | 1:36:A:ALA:H     | 1:37:A:GLY:H     | 4        | 0.21          |
| (1,2370) | 1:174:A:ILE:HG21 | 1:175:A:PHE:HA   | 8        | 0.21          |
| (1,2370) | 1:174:A:ILE:HG22 | 1:175:A:PHE:HA   | 8        | 0.21          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2370) | 1:174:A:ILE:HG23 | 1:175:A:PHE:HA   | 8        | 0.21          |
| (1,2354) | 1:173:A:VAL:HG11 | 1:175:A:PHE:HE1  | 7        | 0.21          |
| (1,2354) | 1:173:A:VAL:HG11 | 1:175:A:PHE:HE2  | 7        | 0.21          |
| (1,2354) | 1:173:A:VAL:HG12 | 1:175:A:PHE:HE1  | 7        | 0.21          |
| (1,2354) | 1:173:A:VAL:HG12 | 1:175:A:PHE:HE2  | 7        | 0.21          |
| (1,2354) | 1:173:A:VAL:HG13 | 1:175:A:PHE:HE1  | 7        | 0.21          |
| (1,2354) | 1:173:A:VAL:HG13 | 1:175:A:PHE:HE2  | 7        | 0.21          |
| (1,2349) | 1:173:A:VAL:HB   | 1:174:A:ILE:H    | 8        | 0.21          |
| (1,2343) | 1:173:A:VAL:HA   | 1:173:A:VAL:HG21 | 2        | 0.21          |
| (1,2343) | 1:173:A:VAL:HA   | 1:173:A:VAL:HG22 | 2        | 0.21          |
| (1,2343) | 1:173:A:VAL:HA   | 1:173:A:VAL:HG23 | 2        | 0.21          |
| (1,2343) | 1:173:A:VAL:HA   | 1:173:A:VAL:HG21 | 7        | 0.21          |
| (1,2343) | 1:173:A:VAL:HA   | 1:173:A:VAL:HG22 | 7        | 0.21          |
| (1,2343) | 1:173:A:VAL:HA   | 1:173:A:VAL:HG23 | 7        | 0.21          |
| (1,2154) | 1:156:A:PHE:HD1  | 1:156:A:PHE:H    | 2        | 0.21          |
| (1,2154) | 1:156:A:PHE:HD2  | 1:156:A:PHE:H    | 2        | 0.21          |
| (1,2154) | 1:156:A:PHE:HD1  | 1:156:A:PHE:H    | 8        | 0.21          |
| (1,2154) | 1:156:A:PHE:HD2  | 1:156:A:PHE:H    | 8        | 0.21          |
| (1,2030) | 1:143:A:ILE:HG21 | 1:143:A:ILE:HD11 | 9        | 0.21          |
| (1,2030) | 1:143:A:ILE:HG21 | 1:143:A:ILE:HD12 | 9        | 0.21          |
| (1,2030) | 1:143:A:ILE:HG21 | 1:143:A:ILE:HD13 | 9        | 0.21          |
| (1,2030) | 1:143:A:ILE:HG22 | 1:143:A:ILE:HD11 | 9        | 0.21          |
| (1,2030) | 1:143:A:ILE:HG22 | 1:143:A:ILE:HD12 | 9        | 0.21          |
| (1,2030) | 1:143:A:ILE:HG22 | 1:143:A:ILE:HD13 | 9        | 0.21          |
| (1,2030) | 1:143:A:ILE:HG23 | 1:143:A:ILE:HD11 | 9        | 0.21          |
| (1,2030) | 1:143:A:ILE:HG23 | 1:143:A:ILE:HD12 | 9        | 0.21          |
| (1,2030) | 1:143:A:ILE:HG23 | 1:143:A:ILE:HD13 | 9        | 0.21          |
| (1,2021) | 1:143:A:ILE:HA   | 1:143:A:ILE:HD11 | 6        | 0.21          |
| (1,2021) | 1:143:A:ILE:HA   | 1:143:A:ILE:HD12 | 6        | 0.21          |
| (1,2021) | 1:143:A:ILE:HA   | 1:143:A:ILE:HD13 | 6        | 0.21          |
| (1,1892) | 1:134:A:TRP:HB3  | 1:135:A:VAL:H    | 5        | 0.21          |
| (1,1859) | 1:133:A:ILE:HD11 | 1:144:A:VAL:HB   | 6        | 0.21          |
| (1,1859) | 1:133:A:ILE:HD12 | 1:144:A:VAL:HB   | 6        | 0.21          |
| (1,1859) | 1:133:A:ILE:HD13 | 1:144:A:VAL:HB   | 6        | 0.21          |
| (1,1852) | 1:133:A:ILE:HA   | 1:133:A:ILE:HG21 | 9        | 0.21          |
| (1,1852) | 1:133:A:ILE:HA   | 1:133:A:ILE:HG22 | 9        | 0.21          |
| (1,1852) | 1:133:A:ILE:HA   | 1:133:A:ILE:HG23 | 9        | 0.21          |
| (1,1818) | 1:131:A:THR:HG21 | 1:131:A:THR:H    | 1        | 0.21          |
| (1,1818) | 1:131:A:THR:HG22 | 1:131:A:THR:H    | 1        | 0.21          |
| (1,1818) | 1:131:A:THR:HG23 | 1:131:A:THR:H    | 1        | 0.21          |
| (1,1775) | 1:121:A:LEU:HB2  | 1:121:A:LEU:H    | 9        | 0.21          |
| (1,1774) | 1:121:A:LEU:HB3  | 1:121:A:LEU:H    | 6        | 0.21          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1770) | 1:120:A:VAL:HG21 | 1:121:A:LEU:H    | 7        | 0.21          |
| (1,1770) | 1:120:A:VAL:HG22 | 1:121:A:LEU:H    | 7        | 0.21          |
| (1,1770) | 1:120:A:VAL:HG23 | 1:121:A:LEU:H    | 7        | 0.21          |
| (1,1767) | 1:120:A:VAL:HG11 | 1:121:A:LEU:H    | 8        | 0.21          |
| (1,1767) | 1:120:A:VAL:HG12 | 1:121:A:LEU:H    | 8        | 0.21          |
| (1,1767) | 1:120:A:VAL:HG13 | 1:121:A:LEU:H    | 8        | 0.21          |
| (1,1653) | 1:113:A:LEU:HA   | 1:113:A:LEU:HD21 | 2        | 0.21          |
| (1,1653) | 1:113:A:LEU:HA   | 1:113:A:LEU:HD22 | 2        | 0.21          |
| (1,1653) | 1:113:A:LEU:HA   | 1:113:A:LEU:HD23 | 2        | 0.21          |
| (1,1635) | 1:111:A:ILE:HB   | 1:111:A:ILE:H    | 6        | 0.21          |
| (1,1505) | 1:98:A:THR:HA    | 1:100:A:ALA:H    | 3        | 0.21          |
| (1,1502) | 1:97:A:GLU:H     | 1:98:A:THR:HA    | 1        | 0.21          |
| (1,1459) | 1:92:A:LEU:HG    | 1:92:A:LEU:H     | 4        | 0.21          |
| (1,1383) | 1:87:A:THR:HB    | 1:87:A:THR:HG21  | 1        | 0.21          |
| (1,1383) | 1:87:A:THR:HB    | 1:87:A:THR:HG22  | 1        | 0.21          |
| (1,1383) | 1:87:A:THR:HB    | 1:87:A:THR:HG23  | 1        | 0.21          |
| (1,1252) | 1:82:A:THR:HA    | 1:82:A:THR:HG21  | 3        | 0.21          |
| (1,1252) | 1:82:A:THR:HA    | 1:82:A:THR:HG22  | 3        | 0.21          |
| (1,1252) | 1:82:A:THR:HA    | 1:82:A:THR:HG23  | 3        | 0.21          |
| (1,1252) | 1:82:A:THR:HA    | 1:82:A:THR:HG21  | 6        | 0.21          |
| (1,1252) | 1:82:A:THR:HA    | 1:82:A:THR:HG22  | 6        | 0.21          |
| (1,1252) | 1:82:A:THR:HA    | 1:82:A:THR:HG23  | 6        | 0.21          |
| (1,1180) | 1:80:A:GLN:HA    | 1:101:A:VAL:H    | 8        | 0.21          |
| (1,1165) | 1:79:A:ILE:HG12  | 1:79:A:ILE:H     | 1        | 0.21          |
| (1,1165) | 1:79:A:ILE:HG12  | 1:79:A:ILE:H     | 9        | 0.21          |
| (1,1116) | 1:78:A:GLN:HB3   | 1:78:A:GLN:H     | 7        | 0.21          |
| (1,1114) | 1:78:A:GLN:HA    | 1:159:A:PHE:HB3  | 1        | 0.21          |
| (1,1114) | 1:78:A:GLN:HA    | 1:159:A:PHE:HB3  | 5        | 0.21          |
| (1,915)  | 1:69:A:GLN:HG3   | 1:70:A:LEU:H     | 2        | 0.21          |
| (1,912)  | 1:69:A:GLN:HG3   | 1:69:A:GLN:HE21  | 9        | 0.21          |
| (1,873)  | 1:67:A:ALA:HB1   | 1:68:A:GLU:H     | 9        | 0.21          |
| (1,873)  | 1:67:A:ALA:HB2   | 1:68:A:GLU:H     | 9        | 0.21          |
| (1,873)  | 1:67:A:ALA:HB3   | 1:68:A:GLU:H     | 9        | 0.21          |
| (1,779)  | 1:64:A:LEU:HD11  | 1:64:A:LEU:HD21  | 9        | 0.21          |
| (1,779)  | 1:64:A:LEU:HD11  | 1:64:A:LEU:HD22  | 9        | 0.21          |
| (1,779)  | 1:64:A:LEU:HD11  | 1:64:A:LEU:HD23  | 9        | 0.21          |
| (1,779)  | 1:64:A:LEU:HD12  | 1:64:A:LEU:HD21  | 9        | 0.21          |
| (1,779)  | 1:64:A:LEU:HD12  | 1:64:A:LEU:HD22  | 9        | 0.21          |
| (1,779)  | 1:64:A:LEU:HD12  | 1:64:A:LEU:HD23  | 9        | 0.21          |
| (1,779)  | 1:64:A:LEU:HD13  | 1:64:A:LEU:HD21  | 9        | 0.21          |
| (1,779)  | 1:64:A:LEU:HD13  | 1:64:A:LEU:HD22  | 9        | 0.21          |
| (1,779)  | 1:64:A:LEU:HD13  | 1:64:A:LEU:HD23  | 9        | 0.21          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,731) | 1:62:A:VAL:HG21  | 1:177:A:PHE:HD1  | 9        | 0.21          |
| (1,731) | 1:62:A:VAL:HG21  | 1:177:A:PHE:HD2  | 9        | 0.21          |
| (1,731) | 1:62:A:VAL:HG22  | 1:177:A:PHE:HD1  | 9        | 0.21          |
| (1,731) | 1:62:A:VAL:HG22  | 1:177:A:PHE:HD2  | 9        | 0.21          |
| (1,731) | 1:62:A:VAL:HG23  | 1:177:A:PHE:HD1  | 9        | 0.21          |
| (1,731) | 1:62:A:VAL:HG23  | 1:177:A:PHE:HD2  | 9        | 0.21          |
| (1,710) | 1:62:A:VAL:HA    | 1:62:A:VAL:HG21  | 6        | 0.21          |
| (1,710) | 1:62:A:VAL:HA    | 1:62:A:VAL:HG22  | 6        | 0.21          |
| (1,710) | 1:62:A:VAL:HA    | 1:62:A:VAL:HG23  | 6        | 0.21          |
| (1,684) | 1:60:A:LEU:H     | 1:61:A:LYS:H     | 4        | 0.21          |
| (1,684) | 1:60:A:LEU:H     | 1:61:A:LYS:H     | 8        | 0.21          |
| (1,623) | 1:55:A:VAL:H     | 1:115:A:LYS:HA   | 7        | 0.21          |
| (1,556) | 1:50:A:TRP:HD1   | 1:151:A:VAL:HG21 | 2        | 0.21          |
| (1,556) | 1:50:A:TRP:HD1   | 1:151:A:VAL:HG22 | 2        | 0.21          |
| (1,556) | 1:50:A:TRP:HD1   | 1:151:A:VAL:HG23 | 2        | 0.21          |
| (1,296) | 1:38:A:ALA:HB1   | 1:39:A:GLN:H     | 8        | 0.21          |
| (1,296) | 1:38:A:ALA:HB2   | 1:39:A:GLN:H     | 8        | 0.21          |
| (1,296) | 1:38:A:ALA:HB3   | 1:39:A:GLN:H     | 8        | 0.21          |
| (1,268) | 1:34:A:PRO:HD3   | 1:35:A:ALA:H     | 7        | 0.21          |
| (1,209) | 1:32:A:ILE:HA    | 1:32:A:ILE:HG21  | 7        | 0.21          |
| (1,209) | 1:32:A:ILE:HA    | 1:32:A:ILE:HG22  | 7        | 0.21          |
| (1,209) | 1:32:A:ILE:HA    | 1:32:A:ILE:HG23  | 7        | 0.21          |
| (1,139) | 1:28:A:HIS:HD2   | 1:46:A:TYR:HE1   | 9        | 0.21          |
| (1,139) | 1:28:A:HIS:HD2   | 1:46:A:TYR:HE2   | 9        | 0.21          |
| (1,109) | 1:26:A:GLU:H     | 1:47:A:ALA:HA    | 2        | 0.21          |
| (1,109) | 1:26:A:GLU:H     | 1:47:A:ALA:HA    | 5        | 0.21          |
| (1,109) | 1:26:A:GLU:H     | 1:47:A:ALA:HA    | 9        | 0.21          |
| (3,12)  | 1:181:A:GLN:HA   | 1:181:A:GLN:HB3  | 2        | 0.2           |
| (3,12)  | 1:181:A:GLN:HA   | 1:181:A:GLN:HB3  | 4        | 0.2           |
| (3,12)  | 1:181:A:GLN:HA   | 1:181:A:GLN:HB3  | 6        | 0.2           |
| (3,12)  | 1:181:A:GLN:HA   | 1:181:A:GLN:HB3  | 8        | 0.2           |
| (3,12)  | 1:181:A:GLN:HA   | 1:181:A:GLN:HB3  | 9        | 0.2           |
| (3,12)  | 1:181:A:GLN:HA   | 1:181:A:GLN:HB3  | 10       | 0.2           |
| (3,4)   | 1:57:A:ASP:HA    | 1:114:A:ASP:HA   | 4        | 0.2           |
| (3,2)   | 1:33:A:THR:HA    | 1:34:A:PRO:HD3   | 2        | 0.2           |
| (2,756) | 1:167:A:LEU:H    | 1:167:A:LEU:HD21 | 1        | 0.2           |
| (2,756) | 1:167:A:LEU:H    | 1:167:A:LEU:HD22 | 1        | 0.2           |
| (2,756) | 1:167:A:LEU:H    | 1:167:A:LEU:HD23 | 1        | 0.2           |
| (2,756) | 1:167:A:LEU:H    | 1:167:A:LEU:HD21 | 10       | 0.2           |
| (2,756) | 1:167:A:LEU:H    | 1:167:A:LEU:HD22 | 10       | 0.2           |
| (2,756) | 1:167:A:LEU:H    | 1:167:A:LEU:HD23 | 10       | 0.2           |
| (2,754) | 1:167:A:LEU:HD21 | 1:167:A:LEU:H    | 1        | 0.2           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,754)  | 1:167:A:LEU:HD22 | 1:167:A:LEU:H    | 1        | 0.2           |
| (2,754)  | 1:167:A:LEU:HD23 | 1:167:A:LEU:H    | 1        | 0.2           |
| (2,754)  | 1:167:A:LEU:HD21 | 1:167:A:LEU:H    | 10       | 0.2           |
| (2,754)  | 1:167:A:LEU:HD22 | 1:167:A:LEU:H    | 10       | 0.2           |
| (2,754)  | 1:167:A:LEU:HD23 | 1:167:A:LEU:H    | 10       | 0.2           |
| (2,732)  | 1:155:A:ASN:H    | 1:156:A:PHE:HE1  | 9        | 0.2           |
| (2,732)  | 1:155:A:ASN:H    | 1:156:A:PHE:HE2  | 9        | 0.2           |
| (2,729)  | 1:151:A:VAL:H    | 1:153:A:ILE:HD11 | 8        | 0.2           |
| (2,729)  | 1:151:A:VAL:H    | 1:153:A:ILE:HD12 | 8        | 0.2           |
| (2,729)  | 1:151:A:VAL:H    | 1:153:A:ILE:HD13 | 8        | 0.2           |
| (2,726)  | 1:145:A:TYR:HE1  | 1:145:A:TYR:H    | 5        | 0.2           |
| (2,726)  | 1:145:A:TYR:HE2  | 1:145:A:TYR:H    | 5        | 0.2           |
| (2,607)  | 1:115:A:LYS:H    | 1:116:A:GLU:HG2  | 3        | 0.2           |
| (2,607)  | 1:115:A:LYS:H    | 1:116:A:GLU:HG3  | 3        | 0.2           |
| (2,298)  | 1:54:A:GLN:HB3   | 1:54:A:GLN:HE21  | 5        | 0.2           |
| (1,2371) | 1:174:A:ILE:HG21 | 1:175:A:PHE:H    | 10       | 0.2           |
| (1,2371) | 1:174:A:ILE:HG22 | 1:175:A:PHE:H    | 10       | 0.2           |
| (1,2371) | 1:174:A:ILE:HG23 | 1:175:A:PHE:H    | 10       | 0.2           |
| (1,2348) | 1:173:A:VAL:HB   | 1:173:A:VAL:H    | 6        | 0.2           |
| (1,2346) | 1:173:A:VAL:HB   | 1:173:A:VAL:HG11 | 2        | 0.2           |
| (1,2346) | 1:173:A:VAL:HB   | 1:173:A:VAL:HG12 | 2        | 0.2           |
| (1,2346) | 1:173:A:VAL:HB   | 1:173:A:VAL:HG13 | 2        | 0.2           |
| (1,2346) | 1:173:A:VAL:HB   | 1:173:A:VAL:HG11 | 6        | 0.2           |
| (1,2346) | 1:173:A:VAL:HB   | 1:173:A:VAL:HG12 | 6        | 0.2           |
| (1,2346) | 1:173:A:VAL:HB   | 1:173:A:VAL:HG13 | 6        | 0.2           |
| (1,2260) | 1:163:A:LYS:H    | 1:168:A:PHE:HZ   | 1        | 0.2           |
| (1,2028) | 1:143:A:ILE:HD11 | 1:143:A:ILE:H    | 7        | 0.2           |
| (1,2028) | 1:143:A:ILE:HD12 | 1:143:A:ILE:H    | 7        | 0.2           |
| (1,2028) | 1:143:A:ILE:HD13 | 1:143:A:ILE:H    | 7        | 0.2           |
| (1,1892) | 1:134:A:TRP:HB3  | 1:135:A:VAL:H    | 2        | 0.2           |
| (1,1892) | 1:134:A:TRP:HB3  | 1:135:A:VAL:H    | 9        | 0.2           |
| (1,1785) | 1:123:A:PRO:HD3  | 1:123:A:PRO:HD2  | 1        | 0.2           |
| (1,1785) | 1:123:A:PRO:HD3  | 1:123:A:PRO:HD2  | 2        | 0.2           |
| (1,1785) | 1:123:A:PRO:HD3  | 1:123:A:PRO:HD2  | 3        | 0.2           |
| (1,1785) | 1:123:A:PRO:HD3  | 1:123:A:PRO:HD2  | 4        | 0.2           |
| (1,1785) | 1:123:A:PRO:HD3  | 1:123:A:PRO:HD2  | 5        | 0.2           |
| (1,1785) | 1:123:A:PRO:HD3  | 1:123:A:PRO:HD2  | 6        | 0.2           |
| (1,1785) | 1:123:A:PRO:HD3  | 1:123:A:PRO:HD2  | 7        | 0.2           |
| (1,1785) | 1:123:A:PRO:HD3  | 1:123:A:PRO:HD2  | 8        | 0.2           |
| (1,1785) | 1:123:A:PRO:HD3  | 1:123:A:PRO:HD2  | 9        | 0.2           |
| (1,1785) | 1:123:A:PRO:HD3  | 1:123:A:PRO:HD2  | 10       | 0.2           |
| (1,1774) | 1:121:A:LEU:HB3  | 1:121:A:LEU:H    | 3        | 0.2           |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1723) | 1:116:A:GLU:HG2  | 1:116:A:GLU:H   | 2        | 0.2           |
| (1,1723) | 1:116:A:GLU:HG3  | 1:116:A:GLU:H   | 2        | 0.2           |
| (1,1640) | 1:111:A:ILE:HG21 | 1:112:A:VAL:H   | 2        | 0.2           |
| (1,1640) | 1:111:A:ILE:HG22 | 1:112:A:VAL:H   | 2        | 0.2           |
| (1,1640) | 1:111:A:ILE:HG23 | 1:112:A:VAL:H   | 2        | 0.2           |
| (1,1572) | 1:104:A:LEU:HD11 | 1:104:A:LEU:H   | 4        | 0.2           |
| (1,1572) | 1:104:A:LEU:HD12 | 1:104:A:LEU:H   | 4        | 0.2           |
| (1,1572) | 1:104:A:LEU:HD13 | 1:104:A:LEU:H   | 4        | 0.2           |
| (1,1383) | 1:87:A:THR:HB    | 1:87:A:THR:HG21 | 6        | 0.2           |
| (1,1383) | 1:87:A:THR:HB    | 1:87:A:THR:HG22 | 6        | 0.2           |
| (1,1383) | 1:87:A:THR:HB    | 1:87:A:THR:HG23 | 6        | 0.2           |
| (1,1371) | 1:86:A:GLU:H     | 1:134:A:TRP:HE1 | 7        | 0.2           |
| (1,1252) | 1:82:A:THR:HA    | 1:82:A:THR:HG21 | 4        | 0.2           |
| (1,1252) | 1:82:A:THR:HA    | 1:82:A:THR:HG22 | 4        | 0.2           |
| (1,1252) | 1:82:A:THR:HA    | 1:82:A:THR:HG23 | 4        | 0.2           |
| (1,1180) | 1:80:A:GLN:HA    | 1:101:A:VAL:H   | 3        | 0.2           |
| (1,1165) | 1:79:A:ILE:HG12  | 1:79:A:ILE:H    | 4        | 0.2           |
| (1,1116) | 1:78:A:GLN:HB3   | 1:78:A:GLN:H    | 3        | 0.2           |
| (1,1116) | 1:78:A:GLN:HB3   | 1:78:A:GLN:H    | 8        | 0.2           |
| (1,1114) | 1:78:A:GLN:HA    | 1:159:A:PHE:HB3 | 2        | 0.2           |
| (1,1089) | 1:77:A:LEU:HD11  | 1:79:A:ILE:HD11 | 10       | 0.2           |
| (1,1089) | 1:77:A:LEU:HD11  | 1:79:A:ILE:HD12 | 10       | 0.2           |
| (1,1089) | 1:77:A:LEU:HD11  | 1:79:A:ILE:HD13 | 10       | 0.2           |
| (1,1089) | 1:77:A:LEU:HD12  | 1:79:A:ILE:HD11 | 10       | 0.2           |
| (1,1089) | 1:77:A:LEU:HD12  | 1:79:A:ILE:HD12 | 10       | 0.2           |
| (1,1089) | 1:77:A:LEU:HD12  | 1:79:A:ILE:HD13 | 10       | 0.2           |
| (1,1089) | 1:77:A:LEU:HD13  | 1:79:A:ILE:HD11 | 10       | 0.2           |
| (1,1089) | 1:77:A:LEU:HD13  | 1:79:A:ILE:HD12 | 10       | 0.2           |
| (1,1089) | 1:77:A:LEU:HD13  | 1:79:A:ILE:HD13 | 10       | 0.2           |
| (1,1089) | 1:77:A:LEU:HD21  | 1:79:A:ILE:HD11 | 10       | 0.2           |
| (1,1089) | 1:77:A:LEU:HD21  | 1:79:A:ILE:HD12 | 10       | 0.2           |
| (1,1089) | 1:77:A:LEU:HD21  | 1:79:A:ILE:HD13 | 10       | 0.2           |
| (1,1089) | 1:77:A:LEU:HD22  | 1:79:A:ILE:HD11 | 10       | 0.2           |
| (1,1089) | 1:77:A:LEU:HD22  | 1:79:A:ILE:HD12 | 10       | 0.2           |
| (1,1089) | 1:77:A:LEU:HD22  | 1:79:A:ILE:HD13 | 10       | 0.2           |
| (1,1089) | 1:77:A:LEU:HD23  | 1:79:A:ILE:HD11 | 10       | 0.2           |
| (1,1089) | 1:77:A:LEU:HD23  | 1:79:A:ILE:HD12 | 10       | 0.2           |
| (1,1089) | 1:77:A:LEU:HD23  | 1:79:A:ILE:HD13 | 10       | 0.2           |
| (1,1019) | 1:74:A:PHE:HD1   | 1:160:A:TYR:HD1 | 7        | 0.2           |
| (1,1019) | 1:74:A:PHE:HD1   | 1:160:A:TYR:HD2 | 7        | 0.2           |
| (1,1019) | 1:74:A:PHE:HD2   | 1:160:A:TYR:HD1 | 7        | 0.2           |
| (1,1019) | 1:74:A:PHE:HD2   | 1:160:A:TYR:HD2 | 7        | 0.2           |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1013) | 1:74:A:PHE:HB2  | 1:163:A:LYS:H    | 9        | 0.2           |
| (1,941)  | 1:71:A:LYS:HA   | 1:74:A:PHE:HD1   | 1        | 0.2           |
| (1,941)  | 1:71:A:LYS:HA   | 1:74:A:PHE:HD2   | 1        | 0.2           |
| (1,914)  | 1:69:A:GLN:HG3  | 1:69:A:GLN:H     | 1        | 0.2           |
| (1,914)  | 1:69:A:GLN:HG3  | 1:69:A:GLN:H     | 7        | 0.2           |
| (1,909)  | 1:69:A:GLN:HB2  | 1:70:A:LEU:H     | 10       | 0.2           |
| (1,908)  | 1:69:A:GLN:HB3  | 1:70:A:LEU:H     | 8        | 0.2           |
| (1,894)  | 1:68:A:GLU:H    | 1:69:A:GLN:H     | 4        | 0.2           |
| (1,857)  | 1:66:A:ASN:HD22 | 1:174:A:ILE:H    | 7        | 0.2           |
| (1,849)  | 1:66:A:ASN:HD22 | 1:66:A:ASN:H     | 10       | 0.2           |
| (1,779)  | 1:64:A:LEU:HD11 | 1:64:A:LEU:HD21  | 1        | 0.2           |
| (1,779)  | 1:64:A:LEU:HD11 | 1:64:A:LEU:HD22  | 1        | 0.2           |
| (1,779)  | 1:64:A:LEU:HD11 | 1:64:A:LEU:HD23  | 1        | 0.2           |
| (1,779)  | 1:64:A:LEU:HD12 | 1:64:A:LEU:HD21  | 1        | 0.2           |
| (1,779)  | 1:64:A:LEU:HD12 | 1:64:A:LEU:HD22  | 1        | 0.2           |
| (1,779)  | 1:64:A:LEU:HD12 | 1:64:A:LEU:HD23  | 1        | 0.2           |
| (1,779)  | 1:64:A:LEU:HD13 | 1:64:A:LEU:HD21  | 1        | 0.2           |
| (1,779)  | 1:64:A:LEU:HD13 | 1:64:A:LEU:HD22  | 1        | 0.2           |
| (1,779)  | 1:64:A:LEU:HD13 | 1:64:A:LEU:HD23  | 1        | 0.2           |
| (1,709)  | 1:62:A:VAL:HA   | 1:62:A:VAL:HG11  | 6        | 0.2           |
| (1,709)  | 1:62:A:VAL:HA   | 1:62:A:VAL:HG12  | 6        | 0.2           |
| (1,709)  | 1:62:A:VAL:HA   | 1:62:A:VAL:HG13  | 6        | 0.2           |
| (1,684)  | 1:60:A:LEU:H    | 1:61:A:LYS:H     | 6        | 0.2           |
| (1,647)  | 1:58:A:VAL:HB   | 1:58:A:VAL:H     | 5        | 0.2           |
| (1,647)  | 1:58:A:VAL:HB   | 1:58:A:VAL:H     | 6        | 0.2           |
| (1,621)  | 1:55:A:VAL:H    | 1:55:A:VAL:HG21  | 4        | 0.2           |
| (1,621)  | 1:55:A:VAL:H    | 1:55:A:VAL:HG22  | 4        | 0.2           |
| (1,621)  | 1:55:A:VAL:H    | 1:55:A:VAL:HG23  | 4        | 0.2           |
| (1,568)  | 1:51:A:ILE:HA   | 1:51:A:ILE:HG21  | 8        | 0.2           |
| (1,568)  | 1:51:A:ILE:HA   | 1:51:A:ILE:HG22  | 8        | 0.2           |
| (1,568)  | 1:51:A:ILE:HA   | 1:51:A:ILE:HG23  | 8        | 0.2           |
| (1,556)  | 1:50:A:TRP:HD1  | 1:151:A:VAL:HG21 | 5        | 0.2           |
| (1,556)  | 1:50:A:TRP:HD1  | 1:151:A:VAL:HG22 | 5        | 0.2           |
| (1,556)  | 1:50:A:TRP:HD1  | 1:151:A:VAL:HG23 | 5        | 0.2           |
| (1,553)  | 1:50:A:TRP:HB2  | 1:52:A:LYS:H     | 8        | 0.2           |
| (1,553)  | 1:50:A:TRP:HB2  | 1:52:A:LYS:H     | 10       | 0.2           |
| (1,543)  | 1:50:A:TRP:HA   | 1:151:A:VAL:HA   | 9        | 0.2           |
| (1,495)  | 1:48:A:ILE:HG21 | 1:50:A:TRP:HE1   | 2        | 0.2           |
| (1,495)  | 1:48:A:ILE:HG22 | 1:50:A:TRP:HE1   | 2        | 0.2           |
| (1,495)  | 1:48:A:ILE:HG23 | 1:50:A:TRP:HE1   | 2        | 0.2           |
| (1,427)  | 1:46:A:TYR:HA   | 1:156:A:PHE:HE1  | 1        | 0.2           |
| (1,427)  | 1:46:A:TYR:HA   | 1:156:A:PHE:HE2  | 1        | 0.2           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,392)  | 1:44:A:ILE:HG21  | 1:158:A:ALA:H    | 8        | 0.2           |
| (1,392)  | 1:44:A:ILE:HG22  | 1:158:A:ALA:H    | 8        | 0.2           |
| (1,392)  | 1:44:A:ILE:HG23  | 1:158:A:ALA:H    | 8        | 0.2           |
| (1,235)  | 1:32:A:ILE:HG21  | 1:33:A:THR:H     | 1        | 0.2           |
| (1,235)  | 1:32:A:ILE:HG22  | 1:33:A:THR:H     | 1        | 0.2           |
| (1,235)  | 1:32:A:ILE:HG23  | 1:33:A:THR:H     | 1        | 0.2           |
| (1,223)  | 1:32:A:ILE:HD11  | 1:160:A:TYR:HE1  | 1        | 0.2           |
| (1,223)  | 1:32:A:ILE:HD11  | 1:160:A:TYR:HE2  | 1        | 0.2           |
| (1,223)  | 1:32:A:ILE:HD12  | 1:160:A:TYR:HE1  | 1        | 0.2           |
| (1,223)  | 1:32:A:ILE:HD12  | 1:160:A:TYR:HE2  | 1        | 0.2           |
| (1,223)  | 1:32:A:ILE:HD13  | 1:160:A:TYR:HE1  | 1        | 0.2           |
| (1,223)  | 1:32:A:ILE:HD13  | 1:160:A:TYR:HE2  | 1        | 0.2           |
| (1,109)  | 1:26:A:GLU:H     | 1:47:A:ALA:HA    | 3        | 0.2           |
| (1,11)   | 1:20:A:SER:HB2   | 1:21:A:GLU:H     | 7        | 0.2           |
| (1,11)   | 1:20:A:SER:HB3   | 1:21:A:GLU:H     | 7        | 0.2           |
| (3,12)   | 1:181:A:GLN:HA   | 1:181:A:GLN:HB3  | 1        | 0.19          |
| (3,12)   | 1:181:A:GLN:HA   | 1:181:A:GLN:HB3  | 3        | 0.19          |
| (2,714)  | 1:141:A:LYS:HD2  | 1:142:A:ILE:H    | 4        | 0.19          |
| (2,714)  | 1:141:A:LYS:HD3  | 1:142:A:ILE:H    | 4        | 0.19          |
| (2,632)  | 1:122:A:TYR:HD1  | 1:125:A:LYS:H    | 6        | 0.19          |
| (2,632)  | 1:122:A:TYR:HD2  | 1:125:A:LYS:H    | 6        | 0.19          |
| (2,607)  | 1:115:A:LYS:H    | 1:116:A:GLU:HG2  | 7        | 0.19          |
| (2,607)  | 1:115:A:LYS:H    | 1:116:A:GLU:HG3  | 7        | 0.19          |
| (2,534)  | 1:85:A:TYR:HE1   | 1:151:A:VAL:H    | 10       | 0.19          |
| (2,534)  | 1:85:A:TYR:HE2   | 1:151:A:VAL:H    | 10       | 0.19          |
| (2,239)  | 1:46:A:TYR:HB3   | 1:155:A:ASN:HD21 | 7        | 0.19          |
| (2,239)  | 1:46:A:TYR:HB3   | 1:155:A:ASN:HD22 | 7        | 0.19          |
| (2,176)  | 1:35:A:ALA:H     | 1:37:A:GLY:H     | 7        | 0.19          |
| (1,2371) | 1:174:A:ILE:HG21 | 1:175:A:PHE:H    | 2        | 0.19          |
| (1,2371) | 1:174:A:ILE:HG22 | 1:175:A:PHE:H    | 2        | 0.19          |
| (1,2371) | 1:174:A:ILE:HG23 | 1:175:A:PHE:H    | 2        | 0.19          |
| (1,2370) | 1:174:A:ILE:HG21 | 1:175:A:PHE:HA   | 4        | 0.19          |
| (1,2370) | 1:174:A:ILE:HG22 | 1:175:A:PHE:HA   | 4        | 0.19          |
| (1,2370) | 1:174:A:ILE:HG23 | 1:175:A:PHE:HA   | 4        | 0.19          |
| (1,2347) | 1:173:A:VAL:HB   | 1:173:A:VAL:HG21 | 2        | 0.19          |
| (1,2347) | 1:173:A:VAL:HB   | 1:173:A:VAL:HG22 | 2        | 0.19          |
| (1,2347) | 1:173:A:VAL:HB   | 1:173:A:VAL:HG23 | 2        | 0.19          |
| (1,2347) | 1:173:A:VAL:HB   | 1:173:A:VAL:HG21 | 6        | 0.19          |
| (1,2347) | 1:173:A:VAL:HB   | 1:173:A:VAL:HG22 | 6        | 0.19          |
| (1,2347) | 1:173:A:VAL:HB   | 1:173:A:VAL:HG23 | 6        | 0.19          |
| (1,2347) | 1:173:A:VAL:HB   | 1:173:A:VAL:HG21 | 8        | 0.19          |
| (1,2347) | 1:173:A:VAL:HB   | 1:173:A:VAL:HG22 | 8        | 0.19          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2347) | 1:173:A:VAL:HB   | 1:173:A:VAL:HG23 | 8        | 0.19          |
| (1,2346) | 1:173:A:VAL:HB   | 1:173:A:VAL:HG11 | 1        | 0.19          |
| (1,2346) | 1:173:A:VAL:HB   | 1:173:A:VAL:HG12 | 1        | 0.19          |
| (1,2346) | 1:173:A:VAL:HB   | 1:173:A:VAL:HG13 | 1        | 0.19          |
| (1,2346) | 1:173:A:VAL:HB   | 1:173:A:VAL:HG11 | 7        | 0.19          |
| (1,2346) | 1:173:A:VAL:HB   | 1:173:A:VAL:HG12 | 7        | 0.19          |
| (1,2346) | 1:173:A:VAL:HB   | 1:173:A:VAL:HG13 | 7        | 0.19          |
| (1,2343) | 1:173:A:VAL:HA   | 1:173:A:VAL:HG21 | 9        | 0.19          |
| (1,2343) | 1:173:A:VAL:HA   | 1:173:A:VAL:HG22 | 9        | 0.19          |
| (1,2343) | 1:173:A:VAL:HA   | 1:173:A:VAL:HG23 | 9        | 0.19          |
| (1,2303) | 1:170:A:SER:HA   | 1:171:A:LEU:HD11 | 9        | 0.19          |
| (1,2303) | 1:170:A:SER:HA   | 1:171:A:LEU:HD12 | 9        | 0.19          |
| (1,2303) | 1:170:A:SER:HA   | 1:171:A:LEU:HD13 | 9        | 0.19          |
| (1,2139) | 1:155:A:ASN:H    | 1:156:A:PHE:HZ   | 1        | 0.19          |
| (1,2091) | 1:152:A:ALA:H    | 1:153:A:ILE:HD11 | 3        | 0.19          |
| (1,2091) | 1:152:A:ALA:H    | 1:153:A:ILE:HD12 | 3        | 0.19          |
| (1,2091) | 1:152:A:ALA:H    | 1:153:A:ILE:HD13 | 3        | 0.19          |
| (1,2079) | 1:151:A:VAL:HG11 | 1:151:A:VAL:H    | 1        | 0.19          |
| (1,2079) | 1:151:A:VAL:HG12 | 1:151:A:VAL:H    | 1        | 0.19          |
| (1,2079) | 1:151:A:VAL:HG13 | 1:151:A:VAL:H    | 1        | 0.19          |
| (1,2079) | 1:151:A:VAL:HG11 | 1:151:A:VAL:H    | 2        | 0.19          |
| (1,2079) | 1:151:A:VAL:HG12 | 1:151:A:VAL:H    | 2        | 0.19          |
| (1,2079) | 1:151:A:VAL:HG13 | 1:151:A:VAL:H    | 2        | 0.19          |
| (1,2015) | 1:142:A:ILE:HG21 | 1:144:A:VAL:H    | 7        | 0.19          |
| (1,2015) | 1:142:A:ILE:HG22 | 1:144:A:VAL:H    | 7        | 0.19          |
| (1,2015) | 1:142:A:ILE:HG23 | 1:144:A:VAL:H    | 7        | 0.19          |
| (1,1892) | 1:134:A:TRP:HB3  | 1:135:A:VAL:H    | 7        | 0.19          |
| (1,1882) | 1:134:A:TRP:HA   | 1:143:A:ILE:HA   | 4        | 0.19          |
| (1,1882) | 1:134:A:TRP:HA   | 1:143:A:ILE:HA   | 8        | 0.19          |
| (1,1852) | 1:133:A:ILE:HA   | 1:133:A:ILE:HG21 | 2        | 0.19          |
| (1,1852) | 1:133:A:ILE:HA   | 1:133:A:ILE:HG22 | 2        | 0.19          |
| (1,1852) | 1:133:A:ILE:HA   | 1:133:A:ILE:HG23 | 2        | 0.19          |
| (1,1835) | 1:132:A:SER:HA   | 1:145:A:TYR:HB2  | 6        | 0.19          |
| (1,1790) | 1:126:A:THR:HA   | 1:126:A:THR:HG21 | 4        | 0.19          |
| (1,1790) | 1:126:A:THR:HA   | 1:126:A:THR:HG22 | 4        | 0.19          |
| (1,1790) | 1:126:A:THR:HA   | 1:126:A:THR:HG23 | 4        | 0.19          |
| (1,1775) | 1:121:A:LEU:HB2  | 1:121:A:LEU:H    | 2        | 0.19          |
| (1,1774) | 1:121:A:LEU:HB3  | 1:121:A:LEU:H    | 4        | 0.19          |
| (1,1635) | 1:111:A:ILE:HB   | 1:111:A:ILE:H    | 7        | 0.19          |
| (1,1505) | 1:98:A:THR:HA    | 1:100:A:ALA:H    | 6        | 0.19          |
| (1,1505) | 1:98:A:THR:HA    | 1:100:A:ALA:H    | 7        | 0.19          |
| (1,1502) | 1:97:A:GLU:H     | 1:98:A:THR:HA    | 3        | 0.19          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1502) | 1:97:A:GLU:H    | 1:98:A:THR:HA   | 4        | 0.19          |
| (1,1502) | 1:97:A:GLU:H    | 1:98:A:THR:HA   | 6        | 0.19          |
| (1,1502) | 1:97:A:GLU:H    | 1:98:A:THR:HA   | 8        | 0.19          |
| (1,1502) | 1:97:A:GLU:H    | 1:98:A:THR:HA   | 10       | 0.19          |
| (1,1399) | 1:87:A:THR:HG21 | 1:87:A:THR:H    | 8        | 0.19          |
| (1,1399) | 1:87:A:THR:HG22 | 1:87:A:THR:H    | 8        | 0.19          |
| (1,1399) | 1:87:A:THR:HG23 | 1:87:A:THR:H    | 8        | 0.19          |
| (1,1252) | 1:82:A:THR:HA   | 1:82:A:THR:HG21 | 1        | 0.19          |
| (1,1252) | 1:82:A:THR:HA   | 1:82:A:THR:HG22 | 1        | 0.19          |
| (1,1252) | 1:82:A:THR:HA   | 1:82:A:THR:HG23 | 1        | 0.19          |
| (1,1233) | 1:81:A:ILE:HG21 | 1:100:A:ALA:HB1 | 2        | 0.19          |
| (1,1233) | 1:81:A:ILE:HG21 | 1:100:A:ALA:HB2 | 2        | 0.19          |
| (1,1233) | 1:81:A:ILE:HG21 | 1:100:A:ALA:HB3 | 2        | 0.19          |
| (1,1233) | 1:81:A:ILE:HG22 | 1:100:A:ALA:HB1 | 2        | 0.19          |
| (1,1233) | 1:81:A:ILE:HG22 | 1:100:A:ALA:HB2 | 2        | 0.19          |
| (1,1233) | 1:81:A:ILE:HG22 | 1:100:A:ALA:HB3 | 2        | 0.19          |
| (1,1233) | 1:81:A:ILE:HG23 | 1:100:A:ALA:HB1 | 2        | 0.19          |
| (1,1233) | 1:81:A:ILE:HG23 | 1:100:A:ALA:HB2 | 2        | 0.19          |
| (1,1233) | 1:81:A:ILE:HG23 | 1:100:A:ALA:HB3 | 2        | 0.19          |
| (1,1173) | 1:79:A:ILE:H    | 1:158:A:ALA:HA  | 1        | 0.19          |
| (1,1169) | 1:79:A:ILE:HG21 | 1:79:A:ILE:HD11 | 7        | 0.19          |
| (1,1169) | 1:79:A:ILE:HG21 | 1:79:A:ILE:HD12 | 7        | 0.19          |
| (1,1169) | 1:79:A:ILE:HG21 | 1:79:A:ILE:HD13 | 7        | 0.19          |
| (1,1169) | 1:79:A:ILE:HG22 | 1:79:A:ILE:HD11 | 7        | 0.19          |
| (1,1169) | 1:79:A:ILE:HG22 | 1:79:A:ILE:HD12 | 7        | 0.19          |
| (1,1169) | 1:79:A:ILE:HG22 | 1:79:A:ILE:HD13 | 7        | 0.19          |
| (1,1169) | 1:79:A:ILE:HG23 | 1:79:A:ILE:HD11 | 7        | 0.19          |
| (1,1169) | 1:79:A:ILE:HG23 | 1:79:A:ILE:HD12 | 7        | 0.19          |
| (1,1169) | 1:79:A:ILE:HG23 | 1:79:A:ILE:HD13 | 7        | 0.19          |
| (1,1165) | 1:79:A:ILE:HG12 | 1:79:A:ILE:H    | 2        | 0.19          |
| (1,1165) | 1:79:A:ILE:HG12 | 1:79:A:ILE:H    | 6        | 0.19          |
| (1,1116) | 1:78:A:GLN:HB3  | 1:78:A:GLN:H    | 5        | 0.19          |
| (1,1116) | 1:78:A:GLN:HB3  | 1:78:A:GLN:H    | 6        | 0.19          |
| (1,1116) | 1:78:A:GLN:HB3  | 1:78:A:GLN:H    | 9        | 0.19          |
| (1,1116) | 1:78:A:GLN:HB3  | 1:78:A:GLN:H    | 10       | 0.19          |
| (1,1095) | 1:77:A:LEU:HD11 | 1:159:A:PHE:H   | 6        | 0.19          |
| (1,1095) | 1:77:A:LEU:HD12 | 1:159:A:PHE:H   | 6        | 0.19          |
| (1,1095) | 1:77:A:LEU:HD13 | 1:159:A:PHE:H   | 6        | 0.19          |
| (1,1095) | 1:77:A:LEU:HD21 | 1:159:A:PHE:H   | 6        | 0.19          |
| (1,1095) | 1:77:A:LEU:HD22 | 1:159:A:PHE:H   | 6        | 0.19          |
| (1,1095) | 1:77:A:LEU:HD23 | 1:159:A:PHE:H   | 6        | 0.19          |
| (1,1089) | 1:77:A:LEU:HD11 | 1:79:A:ILE:HD11 | 1        | 0.19          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1089) | 1:77:A:LEU:HD11 | 1:79:A:ILE:HD12  | 1        | 0.19          |
| (1,1089) | 1:77:A:LEU:HD11 | 1:79:A:ILE:HD13  | 1        | 0.19          |
| (1,1089) | 1:77:A:LEU:HD12 | 1:79:A:ILE:HD11  | 1        | 0.19          |
| (1,1089) | 1:77:A:LEU:HD12 | 1:79:A:ILE:HD12  | 1        | 0.19          |
| (1,1089) | 1:77:A:LEU:HD12 | 1:79:A:ILE:HD13  | 1        | 0.19          |
| (1,1089) | 1:77:A:LEU:HD13 | 1:79:A:ILE:HD11  | 1        | 0.19          |
| (1,1089) | 1:77:A:LEU:HD13 | 1:79:A:ILE:HD12  | 1        | 0.19          |
| (1,1089) | 1:77:A:LEU:HD13 | 1:79:A:ILE:HD13  | 1        | 0.19          |
| (1,1089) | 1:77:A:LEU:HD21 | 1:79:A:ILE:HD11  | 1        | 0.19          |
| (1,1089) | 1:77:A:LEU:HD21 | 1:79:A:ILE:HD12  | 1        | 0.19          |
| (1,1089) | 1:77:A:LEU:HD21 | 1:79:A:ILE:HD13  | 1        | 0.19          |
| (1,1089) | 1:77:A:LEU:HD22 | 1:79:A:ILE:HD11  | 1        | 0.19          |
| (1,1089) | 1:77:A:LEU:HD22 | 1:79:A:ILE:HD12  | 1        | 0.19          |
| (1,1089) | 1:77:A:LEU:HD22 | 1:79:A:ILE:HD13  | 1        | 0.19          |
| (1,1089) | 1:77:A:LEU:HD23 | 1:79:A:ILE:HD11  | 1        | 0.19          |
| (1,1089) | 1:77:A:LEU:HD23 | 1:79:A:ILE:HD12  | 1        | 0.19          |
| (1,1089) | 1:77:A:LEU:HD23 | 1:79:A:ILE:HD13  | 1        | 0.19          |
| (1,1089) | 1:77:A:LEU:HD11 | 1:79:A:ILE:HD11  | 2        | 0.19          |
| (1,1089) | 1:77:A:LEU:HD11 | 1:79:A:ILE:HD12  | 2        | 0.19          |
| (1,1089) | 1:77:A:LEU:HD11 | 1:79:A:ILE:HD13  | 2        | 0.19          |
| (1,1089) | 1:77:A:LEU:HD12 | 1:79:A:ILE:HD11  | 2        | 0.19          |
| (1,1089) | 1:77:A:LEU:HD12 | 1:79:A:ILE:HD12  | 2        | 0.19          |
| (1,1089) | 1:77:A:LEU:HD12 | 1:79:A:ILE:HD13  | 2        | 0.19          |
| (1,1089) | 1:77:A:LEU:HD13 | 1:79:A:ILE:HD11  | 2        | 0.19          |
| (1,1089) | 1:77:A:LEU:HD13 | 1:79:A:ILE:HD12  | 2        | 0.19          |
| (1,1089) | 1:77:A:LEU:HD13 | 1:79:A:ILE:HD13  | 2        | 0.19          |
| (1,1089) | 1:77:A:LEU:HD21 | 1:79:A:ILE:HD11  | 2        | 0.19          |
| (1,1089) | 1:77:A:LEU:HD21 | 1:79:A:ILE:HD12  | 2        | 0.19          |
| (1,1089) | 1:77:A:LEU:HD21 | 1:79:A:ILE:HD13  | 2        | 0.19          |
| (1,1089) | 1:77:A:LEU:HD22 | 1:79:A:ILE:HD11  | 2        | 0.19          |
| (1,1089) | 1:77:A:LEU:HD22 | 1:79:A:ILE:HD12  | 2        | 0.19          |
| (1,1089) | 1:77:A:LEU:HD22 | 1:79:A:ILE:HD13  | 2        | 0.19          |
| (1,1089) | 1:77:A:LEU:HD23 | 1:79:A:ILE:HD11  | 2        | 0.19          |
| (1,1089) | 1:77:A:LEU:HD23 | 1:79:A:ILE:HD12  | 2        | 0.19          |
| (1,1089) | 1:77:A:LEU:HD23 | 1:79:A:ILE:HD13  | 2        | 0.19          |
| (1,1075) | 1:76:A:TYR:H    | 1:162:A:ALA:HA   | 8        | 0.19          |
| (1,1075) | 1:76:A:TYR:H    | 1:162:A:ALA:HA   | 9        | 0.19          |
| (1,992)  | 1:73:A:TYR:HE1  | 1:171:A:LEU:HD21 | 9        | 0.19          |
| (1,992)  | 1:73:A:TYR:HE1  | 1:171:A:LEU:HD22 | 9        | 0.19          |
| (1,992)  | 1:73:A:TYR:HE1  | 1:171:A:LEU:HD23 | 9        | 0.19          |
| (1,992)  | 1:73:A:TYR:HE2  | 1:171:A:LEU:HD21 | 9        | 0.19          |
| (1,992)  | 1:73:A:TYR:HE2  | 1:171:A:LEU:HD22 | 9        | 0.19          |

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| Key     | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,992) | 1:73:A:TYR:HE2  | 1:171:A:LEU:HD23 | 9        | 0.19          |
| (1,989) | 1:73:A:TYR:HD1  | 1:74:A:PHE:HE1   | 2        | 0.19          |
| (1,989) | 1:73:A:TYR:HD1  | 1:74:A:PHE:HE2   | 2        | 0.19          |
| (1,989) | 1:73:A:TYR:HD2  | 1:74:A:PHE:HE1   | 2        | 0.19          |
| (1,989) | 1:73:A:TYR:HD2  | 1:74:A:PHE:HE2   | 2        | 0.19          |
| (1,915) | 1:69:A:GLN:HG3  | 1:70:A:LEU:H     | 8        | 0.19          |
| (1,837) | 1:66:A:ASN:HB2  | 1:66:A:ASN:HD22  | 5        | 0.19          |
| (1,779) | 1:64:A:LEU:HD11 | 1:64:A:LEU:HD21  | 7        | 0.19          |
| (1,779) | 1:64:A:LEU:HD11 | 1:64:A:LEU:HD22  | 7        | 0.19          |
| (1,779) | 1:64:A:LEU:HD11 | 1:64:A:LEU:HD23  | 7        | 0.19          |
| (1,779) | 1:64:A:LEU:HD12 | 1:64:A:LEU:HD21  | 7        | 0.19          |
| (1,779) | 1:64:A:LEU:HD12 | 1:64:A:LEU:HD22  | 7        | 0.19          |
| (1,779) | 1:64:A:LEU:HD12 | 1:64:A:LEU:HD23  | 7        | 0.19          |
| (1,779) | 1:64:A:LEU:HD13 | 1:64:A:LEU:HD21  | 7        | 0.19          |
| (1,779) | 1:64:A:LEU:HD13 | 1:64:A:LEU:HD22  | 7        | 0.19          |
| (1,779) | 1:64:A:LEU:HD13 | 1:64:A:LEU:HD23  | 7        | 0.19          |
| (1,745) | 1:63:A:THR:HB   | 1:63:A:THR:HG21  | 10       | 0.19          |
| (1,745) | 1:63:A:THR:HB   | 1:63:A:THR:HG22  | 10       | 0.19          |
| (1,745) | 1:63:A:THR:HB   | 1:63:A:THR:HG23  | 10       | 0.19          |
| (1,710) | 1:62:A:VAL:HA   | 1:62:A:VAL:HG21  | 8        | 0.19          |
| (1,710) | 1:62:A:VAL:HA   | 1:62:A:VAL:HG22  | 8        | 0.19          |
| (1,710) | 1:62:A:VAL:HA   | 1:62:A:VAL:HG23  | 8        | 0.19          |
| (1,647) | 1:58:A:VAL:HB   | 1:58:A:VAL:H     | 3        | 0.19          |
| (1,623) | 1:55:A:VAL:H    | 1:115:A:LYS:HA   | 10       | 0.19          |
| (1,598) | 1:53:A:ASP:H    | 1:54:A:GLN:H     | 5        | 0.19          |
| (1,568) | 1:51:A:ILE:HA   | 1:51:A:ILE:HG21  | 2        | 0.19          |
| (1,568) | 1:51:A:ILE:HA   | 1:51:A:ILE:HG22  | 2        | 0.19          |
| (1,568) | 1:51:A:ILE:HA   | 1:51:A:ILE:HG23  | 2        | 0.19          |
| (1,553) | 1:50:A:TRP:HB2  | 1:52:A:LYS:H     | 1        | 0.19          |
| (1,543) | 1:50:A:TRP:HA   | 1:151:A:VAL:HA   | 1        | 0.19          |
| (1,543) | 1:50:A:TRP:HA   | 1:151:A:VAL:HA   | 2        | 0.19          |
| (1,543) | 1:50:A:TRP:HA   | 1:151:A:VAL:HA   | 3        | 0.19          |
| (1,543) | 1:50:A:TRP:HA   | 1:151:A:VAL:HA   | 8        | 0.19          |
| (1,467) | 1:47:A:ALA:H    | 1:156:A:PHE:HE1  | 6        | 0.19          |
| (1,467) | 1:47:A:ALA:H    | 1:156:A:PHE:HE2  | 6        | 0.19          |
| (1,445) | 1:46:A:TYR:HE1  | 1:141:A:LYS:HE3  | 4        | 0.19          |
| (1,445) | 1:46:A:TYR:HE2  | 1:141:A:LYS:HE3  | 4        | 0.19          |
| (1,292) | 1:37:A:GLY:HA2  | 1:37:A:GLY:H     | 4        | 0.19          |
| (1,260) | 1:33:A:THR:HG21 | 1:34:A:PRO:HD3   | 4        | 0.19          |
| (1,260) | 1:33:A:THR:HG22 | 1:34:A:PRO:HD3   | 4        | 0.19          |
| (1,260) | 1:33:A:THR:HG23 | 1:34:A:PRO:HD3   | 4        | 0.19          |
| (1,235) | 1:32:A:ILE:HG21 | 1:33:A:THR:H     | 5        | 0.19          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,235)  | 1:32:A:ILE:HG22 | 1:33:A:THR:H     | 5        | 0.19          |
| (1,235)  | 1:32:A:ILE:HG23 | 1:33:A:THR:H     | 5        | 0.19          |
| (1,235)  | 1:32:A:ILE:HG21 | 1:33:A:THR:H     | 6        | 0.19          |
| (1,235)  | 1:32:A:ILE:HG22 | 1:33:A:THR:H     | 6        | 0.19          |
| (1,235)  | 1:32:A:ILE:HG23 | 1:33:A:THR:H     | 6        | 0.19          |
| (1,209)  | 1:32:A:ILE:HA   | 1:32:A:ILE:HG21  | 3        | 0.19          |
| (1,209)  | 1:32:A:ILE:HA   | 1:32:A:ILE:HG22  | 3        | 0.19          |
| (1,209)  | 1:32:A:ILE:HA   | 1:32:A:ILE:HG23  | 3        | 0.19          |
| (1,109)  | 1:26:A:GLU:H    | 1:47:A:ALA:HA    | 7        | 0.19          |
| (1,92)   | 1:25:A:VAL:H    | 1:50:A:TRP:HE1   | 1        | 0.19          |
| (1,92)   | 1:25:A:VAL:H    | 1:50:A:TRP:HE1   | 7        | 0.19          |
| (1,77)   | 1:25:A:VAL:HG11 | 1:25:A:VAL:H     | 6        | 0.19          |
| (1,77)   | 1:25:A:VAL:HG12 | 1:25:A:VAL:H     | 6        | 0.19          |
| (1,77)   | 1:25:A:VAL:HG13 | 1:25:A:VAL:H     | 6        | 0.19          |
| (3,13)   | 1:181:A:GLN:HA  | 1:181:A:GLN:HB2  | 1        | 0.18          |
| (3,13)   | 1:181:A:GLN:HA  | 1:181:A:GLN:HB2  | 2        | 0.18          |
| (3,13)   | 1:181:A:GLN:HA  | 1:181:A:GLN:HB2  | 3        | 0.18          |
| (3,13)   | 1:181:A:GLN:HA  | 1:181:A:GLN:HB2  | 4        | 0.18          |
| (3,13)   | 1:181:A:GLN:HA  | 1:181:A:GLN:HB2  | 8        | 0.18          |
| (3,13)   | 1:181:A:GLN:HA  | 1:181:A:GLN:HB2  | 9        | 0.18          |
| (3,13)   | 1:181:A:GLN:HA  | 1:181:A:GLN:HB2  | 10       | 0.18          |
| (2,760)  | 1:168:A:PHE:HE1 | 1:171:A:LEU:HG   | 1        | 0.18          |
| (2,760)  | 1:168:A:PHE:HE2 | 1:171:A:LEU:HG   | 1        | 0.18          |
| (2,740)  | 1:162:A:ALA:HA  | 1:168:A:PHE:HE1  | 1        | 0.18          |
| (2,740)  | 1:162:A:ALA:HA  | 1:168:A:PHE:HE2  | 1        | 0.18          |
| (2,723)  | 1:145:A:TYR:HA  | 1:147:A:GLU:HG2  | 6        | 0.18          |
| (2,723)  | 1:145:A:TYR:HA  | 1:147:A:GLU:HG3  | 6        | 0.18          |
| (2,425)  | 1:74:A:PHE:HZ   | 1:160:A:TYR:HE1  | 5        | 0.18          |
| (2,425)  | 1:74:A:PHE:HZ   | 1:160:A:TYR:HE2  | 5        | 0.18          |
| (2,352)  | 1:63:A:THR:H    | 1:175:A:PHE:HE1  | 6        | 0.18          |
| (2,352)  | 1:63:A:THR:H    | 1:175:A:PHE:HE2  | 6        | 0.18          |
| (2,194)  | 1:38:A:ALA:HB1  | 1:39:A:GLN:HE21  | 8        | 0.18          |
| (2,194)  | 1:38:A:ALA:HB2  | 1:39:A:GLN:HE21  | 8        | 0.18          |
| (2,194)  | 1:38:A:ALA:HB3  | 1:39:A:GLN:HE21  | 8        | 0.18          |
| (1,2349) | 1:173:A:VAL:HB  | 1:174:A:ILE:H    | 5        | 0.18          |
| (1,2347) | 1:173:A:VAL:HB  | 1:173:A:VAL:HG21 | 1        | 0.18          |
| (1,2347) | 1:173:A:VAL:HB  | 1:173:A:VAL:HG22 | 1        | 0.18          |
| (1,2347) | 1:173:A:VAL:HB  | 1:173:A:VAL:HG23 | 1        | 0.18          |
| (1,2347) | 1:173:A:VAL:HB  | 1:173:A:VAL:HG21 | 3        | 0.18          |
| (1,2347) | 1:173:A:VAL:HB  | 1:173:A:VAL:HG22 | 3        | 0.18          |
| (1,2347) | 1:173:A:VAL:HB  | 1:173:A:VAL:HG23 | 3        | 0.18          |
| (1,2347) | 1:173:A:VAL:HB  | 1:173:A:VAL:HG21 | 4        | 0.18          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2347) | 1:173:A:VAL:HB   | 1:173:A:VAL:HG22 | 4        | 0.18          |
| (1,2347) | 1:173:A:VAL:HB   | 1:173:A:VAL:HG23 | 4        | 0.18          |
| (1,2347) | 1:173:A:VAL:HB   | 1:173:A:VAL:HG21 | 5        | 0.18          |
| (1,2347) | 1:173:A:VAL:HB   | 1:173:A:VAL:HG22 | 5        | 0.18          |
| (1,2347) | 1:173:A:VAL:HB   | 1:173:A:VAL:HG23 | 5        | 0.18          |
| (1,2347) | 1:173:A:VAL:HB   | 1:173:A:VAL:HG21 | 7        | 0.18          |
| (1,2347) | 1:173:A:VAL:HB   | 1:173:A:VAL:HG22 | 7        | 0.18          |
| (1,2347) | 1:173:A:VAL:HB   | 1:173:A:VAL:HG23 | 7        | 0.18          |
| (1,2347) | 1:173:A:VAL:HB   | 1:173:A:VAL:HG21 | 10       | 0.18          |
| (1,2347) | 1:173:A:VAL:HB   | 1:173:A:VAL:HG22 | 10       | 0.18          |
| (1,2347) | 1:173:A:VAL:HB   | 1:173:A:VAL:HG23 | 10       | 0.18          |
| (1,2346) | 1:173:A:VAL:HB   | 1:173:A:VAL:HG11 | 3        | 0.18          |
| (1,2346) | 1:173:A:VAL:HB   | 1:173:A:VAL:HG12 | 3        | 0.18          |
| (1,2346) | 1:173:A:VAL:HB   | 1:173:A:VAL:HG13 | 3        | 0.18          |
| (1,2346) | 1:173:A:VAL:HB   | 1:173:A:VAL:HG11 | 4        | 0.18          |
| (1,2346) | 1:173:A:VAL:HB   | 1:173:A:VAL:HG12 | 4        | 0.18          |
| (1,2346) | 1:173:A:VAL:HB   | 1:173:A:VAL:HG13 | 4        | 0.18          |
| (1,2346) | 1:173:A:VAL:HB   | 1:173:A:VAL:HG11 | 5        | 0.18          |
| (1,2346) | 1:173:A:VAL:HB   | 1:173:A:VAL:HG12 | 5        | 0.18          |
| (1,2346) | 1:173:A:VAL:HB   | 1:173:A:VAL:HG13 | 5        | 0.18          |
| (1,2346) | 1:173:A:VAL:HB   | 1:173:A:VAL:HG11 | 8        | 0.18          |
| (1,2346) | 1:173:A:VAL:HB   | 1:173:A:VAL:HG12 | 8        | 0.18          |
| (1,2346) | 1:173:A:VAL:HB   | 1:173:A:VAL:HG13 | 8        | 0.18          |
| (1,2346) | 1:173:A:VAL:HB   | 1:173:A:VAL:HG11 | 10       | 0.18          |
| (1,2346) | 1:173:A:VAL:HB   | 1:173:A:VAL:HG12 | 10       | 0.18          |
| (1,2346) | 1:173:A:VAL:HB   | 1:173:A:VAL:HG13 | 10       | 0.18          |
| (1,2343) | 1:173:A:VAL:HA   | 1:173:A:VAL:HG21 | 1        | 0.18          |
| (1,2343) | 1:173:A:VAL:HA   | 1:173:A:VAL:HG22 | 1        | 0.18          |
| (1,2343) | 1:173:A:VAL:HA   | 1:173:A:VAL:HG23 | 1        | 0.18          |
| (1,2313) | 1:171:A:LEU:HA   | 1:171:A:LEU:HD11 | 9        | 0.18          |
| (1,2313) | 1:171:A:LEU:HA   | 1:171:A:LEU:HD12 | 9        | 0.18          |
| (1,2313) | 1:171:A:LEU:HA   | 1:171:A:LEU:HD13 | 9        | 0.18          |
| (1,2303) | 1:170:A:SER:HA   | 1:171:A:LEU:HD11 | 2        | 0.18          |
| (1,2303) | 1:170:A:SER:HA   | 1:171:A:LEU:HD12 | 2        | 0.18          |
| (1,2303) | 1:170:A:SER:HA   | 1:171:A:LEU:HD13 | 2        | 0.18          |
| (1,2272) | 1:166:A:MET:HB2  | 1:167:A:LEU:H    | 10       | 0.18          |
| (1,2106) | 1:153:A:ILE:HG21 | 1:155:A:ASN:HD21 | 4        | 0.18          |
| (1,2106) | 1:153:A:ILE:HG21 | 1:155:A:ASN:HD22 | 4        | 0.18          |
| (1,2106) | 1:153:A:ILE:HG22 | 1:155:A:ASN:HD21 | 4        | 0.18          |
| (1,2106) | 1:153:A:ILE:HG22 | 1:155:A:ASN:HD22 | 4        | 0.18          |
| (1,2106) | 1:153:A:ILE:HG23 | 1:155:A:ASN:HD21 | 4        | 0.18          |
| (1,2106) | 1:153:A:ILE:HG23 | 1:155:A:ASN:HD22 | 4        | 0.18          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1892) | 1:134:A:TRP:HB3 | 1:135:A:VAL:H    | 3        | 0.18          |
| (1,1892) | 1:134:A:TRP:HB3 | 1:135:A:VAL:H    | 10       | 0.18          |
| (1,1852) | 1:133:A:ILE:HA  | 1:133:A:ILE:HG21 | 6        | 0.18          |
| (1,1852) | 1:133:A:ILE:HA  | 1:133:A:ILE:HG22 | 6        | 0.18          |
| (1,1852) | 1:133:A:ILE:HA  | 1:133:A:ILE:HG23 | 6        | 0.18          |
| (1,1774) | 1:121:A:LEU:HB3 | 1:121:A:LEU:H    | 1        | 0.18          |
| (1,1757) | 1:119:A:ALA:HB1 | 1:133:A:ILE:HD11 | 5        | 0.18          |
| (1,1757) | 1:119:A:ALA:HB1 | 1:133:A:ILE:HD12 | 5        | 0.18          |
| (1,1757) | 1:119:A:ALA:HB1 | 1:133:A:ILE:HD13 | 5        | 0.18          |
| (1,1757) | 1:119:A:ALA:HB2 | 1:133:A:ILE:HD11 | 5        | 0.18          |
| (1,1757) | 1:119:A:ALA:HB2 | 1:133:A:ILE:HD12 | 5        | 0.18          |
| (1,1757) | 1:119:A:ALA:HB2 | 1:133:A:ILE:HD13 | 5        | 0.18          |
| (1,1757) | 1:119:A:ALA:HB3 | 1:133:A:ILE:HD11 | 5        | 0.18          |
| (1,1757) | 1:119:A:ALA:HB3 | 1:133:A:ILE:HD12 | 5        | 0.18          |
| (1,1757) | 1:119:A:ALA:HB3 | 1:133:A:ILE:HD13 | 5        | 0.18          |
| (1,1502) | 1:97:A:GLU:H    | 1:98:A:THR:HA    | 7        | 0.18          |
| (1,1483) | 1:95:A:PHE:HE1  | 1:116:A:GLU:HB3  | 8        | 0.18          |
| (1,1483) | 1:95:A:PHE:HE2  | 1:116:A:GLU:HB3  | 8        | 0.18          |
| (1,1383) | 1:87:A:THR:HB   | 1:87:A:THR:HG21  | 3        | 0.18          |
| (1,1383) | 1:87:A:THR:HB   | 1:87:A:THR:HG22  | 3        | 0.18          |
| (1,1383) | 1:87:A:THR:HB   | 1:87:A:THR:HG23  | 3        | 0.18          |
| (1,1383) | 1:87:A:THR:HB   | 1:87:A:THR:HG21  | 9        | 0.18          |
| (1,1383) | 1:87:A:THR:HB   | 1:87:A:THR:HG22  | 9        | 0.18          |
| (1,1383) | 1:87:A:THR:HB   | 1:87:A:THR:HG23  | 9        | 0.18          |
| (1,1369) | 1:86:A:GLU:H    | 1:133:A:ILE:HG21 | 4        | 0.18          |
| (1,1369) | 1:86:A:GLU:H    | 1:133:A:ILE:HG22 | 4        | 0.18          |
| (1,1369) | 1:86:A:GLU:H    | 1:133:A:ILE:HG23 | 4        | 0.18          |
| (1,1298) | 1:83:A:SER:HA   | 1:154:A:LEU:HD21 | 3        | 0.18          |
| (1,1298) | 1:83:A:SER:HA   | 1:154:A:LEU:HD22 | 3        | 0.18          |
| (1,1298) | 1:83:A:SER:HA   | 1:154:A:LEU:HD23 | 3        | 0.18          |
| (1,1298) | 1:83:A:SER:HA   | 1:154:A:LEU:HD21 | 8        | 0.18          |
| (1,1298) | 1:83:A:SER:HA   | 1:154:A:LEU:HD22 | 8        | 0.18          |
| (1,1298) | 1:83:A:SER:HA   | 1:154:A:LEU:HD23 | 8        | 0.18          |
| (1,1252) | 1:82:A:THR:HA   | 1:82:A:THR:HG21  | 8        | 0.18          |
| (1,1252) | 1:82:A:THR:HA   | 1:82:A:THR:HG22  | 8        | 0.18          |
| (1,1252) | 1:82:A:THR:HA   | 1:82:A:THR:HG23  | 8        | 0.18          |
| (1,1180) | 1:80:A:GLN:HA   | 1:101:A:VAL:H    | 5        | 0.18          |
| (1,1165) | 1:79:A:ILE:HG12 | 1:79:A:ILE:H     | 5        | 0.18          |
| (1,1128) | 1:78:A:GLN:H    | 1:158:A:ALA:HA   | 8        | 0.18          |
| (1,1128) | 1:78:A:GLN:H    | 1:158:A:ALA:HA   | 10       | 0.18          |
| (1,1116) | 1:78:A:GLN:HB3  | 1:78:A:GLN:H     | 2        | 0.18          |
| (1,1114) | 1:78:A:GLN:HA   | 1:159:A:PHE:HB3  | 9        | 0.18          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1030) | 1:74:A:PHE:HE1  | 1:162:A:ALA:HB1  | 2        | 0.18          |
| (1,1030) | 1:74:A:PHE:HE1  | 1:162:A:ALA:HB2  | 2        | 0.18          |
| (1,1030) | 1:74:A:PHE:HE1  | 1:162:A:ALA:HB3  | 2        | 0.18          |
| (1,1030) | 1:74:A:PHE:HE2  | 1:162:A:ALA:HB1  | 2        | 0.18          |
| (1,1030) | 1:74:A:PHE:HE2  | 1:162:A:ALA:HB2  | 2        | 0.18          |
| (1,1030) | 1:74:A:PHE:HE2  | 1:162:A:ALA:HB3  | 2        | 0.18          |
| (1,1006) | 1:74:A:PHE:HA   | 1:163:A:LYS:H    | 3        | 0.18          |
| (1,1006) | 1:74:A:PHE:HA   | 1:163:A:LYS:H    | 5        | 0.18          |
| (1,1006) | 1:74:A:PHE:HA   | 1:163:A:LYS:H    | 7        | 0.18          |
| (1,1006) | 1:74:A:PHE:HA   | 1:163:A:LYS:H    | 8        | 0.18          |
| (1,922)  | 1:70:A:LEU:HD11 | 1:70:A:LEU:H     | 7        | 0.18          |
| (1,922)  | 1:70:A:LEU:HD12 | 1:70:A:LEU:H     | 7        | 0.18          |
| (1,922)  | 1:70:A:LEU:HD13 | 1:70:A:LEU:H     | 7        | 0.18          |
| (1,914)  | 1:69:A:GLN:HG3  | 1:69:A:GLN:H     | 8        | 0.18          |
| (1,901)  | 1:69:A:GLN:HA   | 1:69:A:GLN:HG2   | 4        | 0.18          |
| (1,854)  | 1:66:A:ASN:HD22 | 1:172:A:PRO:HD3  | 9        | 0.18          |
| (1,849)  | 1:66:A:ASN:HD22 | 1:66:A:ASN:H     | 4        | 0.18          |
| (1,849)  | 1:66:A:ASN:HD22 | 1:66:A:ASN:H     | 5        | 0.18          |
| (1,849)  | 1:66:A:ASN:HD22 | 1:66:A:ASN:H     | 8        | 0.18          |
| (1,845)  | 1:66:A:ASN:HD21 | 1:173:A:VAL:HA   | 4        | 0.18          |
| (1,845)  | 1:66:A:ASN:HD21 | 1:173:A:VAL:HA   | 5        | 0.18          |
| (1,845)  | 1:66:A:ASN:HD21 | 1:173:A:VAL:HA   | 8        | 0.18          |
| (1,837)  | 1:66:A:ASN:HB2  | 1:66:A:ASN:HD22  | 3        | 0.18          |
| (1,837)  | 1:66:A:ASN:HB2  | 1:66:A:ASN:HD22  | 4        | 0.18          |
| (1,745)  | 1:63:A:THR:HB   | 1:63:A:THR:HG21  | 4        | 0.18          |
| (1,745)  | 1:63:A:THR:HB   | 1:63:A:THR:HG22  | 4        | 0.18          |
| (1,745)  | 1:63:A:THR:HB   | 1:63:A:THR:HG23  | 4        | 0.18          |
| (1,710)  | 1:62:A:VAL:HA   | 1:62:A:VAL:HG21  | 4        | 0.18          |
| (1,710)  | 1:62:A:VAL:HA   | 1:62:A:VAL:HG22  | 4        | 0.18          |
| (1,710)  | 1:62:A:VAL:HA   | 1:62:A:VAL:HG23  | 4        | 0.18          |
| (1,623)  | 1:55:A:VAL:H    | 1:115:A:LYS:HA   | 3        | 0.18          |
| (1,623)  | 1:55:A:VAL:H    | 1:115:A:LYS:HA   | 9        | 0.18          |
| (1,554)  | 1:50:A:TRP:HD1  | 1:50:A:TRP:H     | 4        | 0.18          |
| (1,553)  | 1:50:A:TRP:HB2  | 1:52:A:LYS:H     | 2        | 0.18          |
| (1,553)  | 1:50:A:TRP:HB2  | 1:52:A:LYS:H     | 9        | 0.18          |
| (1,545)  | 1:50:A:TRP:HA   | 1:151:A:VAL:HG21 | 6        | 0.18          |
| (1,545)  | 1:50:A:TRP:HA   | 1:151:A:VAL:HG22 | 6        | 0.18          |
| (1,545)  | 1:50:A:TRP:HA   | 1:151:A:VAL:HG23 | 6        | 0.18          |
| (1,541)  | 1:50:A:TRP:HA   | 1:51:A:ILE:HB    | 6        | 0.18          |
| (1,498)  | 1:48:A:ILE:HG21 | 1:50:A:TRP:HZ2   | 10       | 0.18          |
| (1,498)  | 1:48:A:ILE:HG22 | 1:50:A:TRP:HZ2   | 10       | 0.18          |
| (1,498)  | 1:48:A:ILE:HG23 | 1:50:A:TRP:HZ2   | 10       | 0.18          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,287)  | 1:36:A:ALA:HB1   | 1:36:A:ALA:H    | 10       | 0.18          |
| (1,287)  | 1:36:A:ALA:HB2   | 1:36:A:ALA:H    | 10       | 0.18          |
| (1,287)  | 1:36:A:ALA:HB3   | 1:36:A:ALA:H    | 10       | 0.18          |
| (1,256)  | 1:33:A:THR:HA    | 1:168:A:PHE:HZ  | 2        | 0.18          |
| (1,235)  | 1:32:A:ILE:HG21  | 1:33:A:THR:H    | 8        | 0.18          |
| (1,235)  | 1:32:A:ILE:HG22  | 1:33:A:THR:H    | 8        | 0.18          |
| (1,235)  | 1:32:A:ILE:HG23  | 1:33:A:THR:H    | 8        | 0.18          |
| (1,235)  | 1:32:A:ILE:HG21  | 1:33:A:THR:H    | 9        | 0.18          |
| (1,235)  | 1:32:A:ILE:HG22  | 1:33:A:THR:H    | 9        | 0.18          |
| (1,235)  | 1:32:A:ILE:HG23  | 1:33:A:THR:H    | 9        | 0.18          |
| (1,190)  | 1:31:A:SER:HA    | 1:32:A:ILE:HD11 | 5        | 0.18          |
| (1,190)  | 1:31:A:SER:HA    | 1:32:A:ILE:HD12 | 5        | 0.18          |
| (1,190)  | 1:31:A:SER:HA    | 1:32:A:ILE:HD13 | 5        | 0.18          |
| (1,92)   | 1:25:A:VAL:H     | 1:50:A:TRP:HE1  | 3        | 0.18          |
| (1,92)   | 1:25:A:VAL:H     | 1:50:A:TRP:HE1  | 4        | 0.18          |
| (1,92)   | 1:25:A:VAL:H     | 1:50:A:TRP:HE1  | 5        | 0.18          |
| (1,92)   | 1:25:A:VAL:H     | 1:50:A:TRP:HE1  | 8        | 0.18          |
| (1,51)   | 1:24:A:ASP:HB2   | 1:25:A:VAL:H    | 6        | 0.18          |
| (1,48)   | 1:24:A:ASP:HB3   | 1:50:A:TRP:HD1  | 6        | 0.18          |
| (1,48)   | 1:24:A:ASP:HB3   | 1:50:A:TRP:HD1  | 10       | 0.18          |
| (1,46)   | 1:24:A:ASP:HB3   | 1:50:A:TRP:HB3  | 6        | 0.18          |
| (3,13)   | 1:181:A:GLN:HA   | 1:181:A:GLN:HB2 | 6        | 0.17          |
| (3,4)    | 1:57:A:ASP:HA    | 1:114:A:ASP:HA  | 10       | 0.17          |
| (2,721)  | 1:144:A:VAL:HA   | 1:145:A:TYR:HD1 | 5        | 0.17          |
| (2,721)  | 1:144:A:VAL:HA   | 1:145:A:TYR:HD2 | 5        | 0.17          |
| (2,714)  | 1:141:A:LYS:HD2  | 1:142:A:ILE:H   | 8        | 0.17          |
| (2,714)  | 1:141:A:LYS:HD3  | 1:142:A:ILE:H   | 8        | 0.17          |
| (2,618)  | 1:119:A:ALA:HB1  | 1:149:A:LYS:H   | 10       | 0.17          |
| (2,618)  | 1:119:A:ALA:HB2  | 1:149:A:LYS:H   | 10       | 0.17          |
| (2,618)  | 1:119:A:ALA:HB3  | 1:149:A:LYS:H   | 10       | 0.17          |
| (2,534)  | 1:85:A:TYR:HE1   | 1:151:A:VAL:H   | 6        | 0.17          |
| (2,534)  | 1:85:A:TYR:HE2   | 1:151:A:VAL:H   | 6        | 0.17          |
| (2,481)  | 1:80:A:GLN:HE22  | 1:98:A:THR:HG21 | 7        | 0.17          |
| (2,481)  | 1:80:A:GLN:HE22  | 1:98:A:THR:HG22 | 7        | 0.17          |
| (2,481)  | 1:80:A:GLN:HE22  | 1:98:A:THR:HG23 | 7        | 0.17          |
| (2,425)  | 1:74:A:PHE:HZ    | 1:160:A:TYR:HE1 | 4        | 0.17          |
| (2,425)  | 1:74:A:PHE:HZ    | 1:160:A:TYR:HE2 | 4        | 0.17          |
| (2,339)  | 1:59:A:LYS:HE2   | 1:111:A:ILE:H   | 10       | 0.17          |
| (2,339)  | 1:59:A:LYS:HE3   | 1:111:A:ILE:H   | 10       | 0.17          |
| (1,2463) | 1:182:A:VAL:HG21 | 1:182:A:VAL:H   | 3        | 0.17          |
| (1,2463) | 1:182:A:VAL:HG22 | 1:182:A:VAL:H   | 3        | 0.17          |
| (1,2463) | 1:182:A:VAL:HG23 | 1:182:A:VAL:H   | 3        | 0.17          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2455) | 1:182:A:VAL:HA   | 1:182:A:VAL:HB   | 1        | 0.17          |
| (1,2455) | 1:182:A:VAL:HA   | 1:182:A:VAL:HB   | 6        | 0.17          |
| (1,2455) | 1:182:A:VAL:HA   | 1:182:A:VAL:HB   | 8        | 0.17          |
| (1,2455) | 1:182:A:VAL:HA   | 1:182:A:VAL:HB   | 9        | 0.17          |
| (1,2370) | 1:174:A:ILE:HG21 | 1:175:A:PHE:HA   | 7        | 0.17          |
| (1,2370) | 1:174:A:ILE:HG22 | 1:175:A:PHE:HA   | 7        | 0.17          |
| (1,2370) | 1:174:A:ILE:HG23 | 1:175:A:PHE:HA   | 7        | 0.17          |
| (1,2349) | 1:173:A:VAL:HB   | 1:174:A:ILE:H    | 4        | 0.17          |
| (1,2349) | 1:173:A:VAL:HB   | 1:174:A:ILE:H    | 10       | 0.17          |
| (1,2347) | 1:173:A:VAL:HB   | 1:173:A:VAL:HG21 | 9        | 0.17          |
| (1,2347) | 1:173:A:VAL:HB   | 1:173:A:VAL:HG22 | 9        | 0.17          |
| (1,2347) | 1:173:A:VAL:HB   | 1:173:A:VAL:HG23 | 9        | 0.17          |
| (1,2346) | 1:173:A:VAL:HB   | 1:173:A:VAL:HG11 | 9        | 0.17          |
| (1,2346) | 1:173:A:VAL:HB   | 1:173:A:VAL:HG12 | 9        | 0.17          |
| (1,2346) | 1:173:A:VAL:HB   | 1:173:A:VAL:HG13 | 9        | 0.17          |
| (1,2316) | 1:171:A:LEU:HA   | 1:172:A:PRO:HD3  | 3        | 0.17          |
| (1,2276) | 1:167:A:LEU:H    | 1:168:A:PHE:H    | 2        | 0.17          |
| (1,2272) | 1:166:A:MET:HB2  | 1:167:A:LEU:H    | 1        | 0.17          |
| (1,2270) | 1:166:A:MET:HA   | 1:167:A:LEU:H    | 9        | 0.17          |
| (1,2207) | 1:159:A:PHE:HB2  | 1:159:A:PHE:H    | 3        | 0.17          |
| (1,2207) | 1:159:A:PHE:HB2  | 1:159:A:PHE:H    | 8        | 0.17          |
| (1,2207) | 1:159:A:PHE:HB2  | 1:159:A:PHE:H    | 10       | 0.17          |
| (1,2176) | 1:157:A:LYS:HE2  | 1:159:A:PHE:HE1  | 8        | 0.17          |
| (1,2176) | 1:157:A:LYS:HE2  | 1:159:A:PHE:HE2  | 8        | 0.17          |
| (1,2176) | 1:157:A:LYS:HE3  | 1:159:A:PHE:HE1  | 8        | 0.17          |
| (1,2176) | 1:157:A:LYS:HE3  | 1:159:A:PHE:HE2  | 8        | 0.17          |
| (1,1984) | 1:139:A:PRO:HD3  | 1:141:A:LYS:H    | 7        | 0.17          |
| (1,1892) | 1:134:A:TRP:HB3  | 1:135:A:VAL:H    | 4        | 0.17          |
| (1,1892) | 1:134:A:TRP:HB3  | 1:135:A:VAL:H    | 6        | 0.17          |
| (1,1892) | 1:134:A:TRP:HB3  | 1:135:A:VAL:H    | 8        | 0.17          |
| (1,1882) | 1:134:A:TRP:HA   | 1:143:A:ILE:HA   | 5        | 0.17          |
| (1,1706) | 1:115:A:LYS:HG2  | 1:115:A:LYS:H    | 6        | 0.17          |
| (1,1706) | 1:115:A:LYS:HG3  | 1:115:A:LYS:H    | 6        | 0.17          |
| (1,1677) | 1:114:A:ASP:HA   | 1:118:A:ILE:H    | 9        | 0.17          |
| (1,1572) | 1:104:A:LEU:HD11 | 1:104:A:LEU:H    | 8        | 0.17          |
| (1,1572) | 1:104:A:LEU:HD12 | 1:104:A:LEU:H    | 8        | 0.17          |
| (1,1572) | 1:104:A:LEU:HD13 | 1:104:A:LEU:H    | 8        | 0.17          |
| (1,1522) | 1:100:A:ALA:H    | 1:111:A:ILE:HD11 | 1        | 0.17          |
| (1,1522) | 1:100:A:ALA:H    | 1:111:A:ILE:HD12 | 1        | 0.17          |
| (1,1522) | 1:100:A:ALA:H    | 1:111:A:ILE:HD13 | 1        | 0.17          |
| (1,1383) | 1:87:A:THR:HB    | 1:87:A:THR:HG21  | 2        | 0.17          |
| (1,1383) | 1:87:A:THR:HB    | 1:87:A:THR:HG22  | 2        | 0.17          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1383) | 1:87:A:THR:HB   | 1:87:A:THR:HG23  | 2        | 0.17          |
| (1,1383) | 1:87:A:THR:HB   | 1:87:A:THR:HG21  | 4        | 0.17          |
| (1,1383) | 1:87:A:THR:HB   | 1:87:A:THR:HG22  | 4        | 0.17          |
| (1,1383) | 1:87:A:THR:HB   | 1:87:A:THR:HG23  | 4        | 0.17          |
| (1,1383) | 1:87:A:THR:HB   | 1:87:A:THR:HG21  | 7        | 0.17          |
| (1,1383) | 1:87:A:THR:HB   | 1:87:A:THR:HG22  | 7        | 0.17          |
| (1,1383) | 1:87:A:THR:HB   | 1:87:A:THR:HG23  | 7        | 0.17          |
| (1,1383) | 1:87:A:THR:HB   | 1:87:A:THR:HG21  | 8        | 0.17          |
| (1,1383) | 1:87:A:THR:HB   | 1:87:A:THR:HG22  | 8        | 0.17          |
| (1,1383) | 1:87:A:THR:HB   | 1:87:A:THR:HG23  | 8        | 0.17          |
| (1,1383) | 1:87:A:THR:HB   | 1:87:A:THR:HG21  | 10       | 0.17          |
| (1,1383) | 1:87:A:THR:HB   | 1:87:A:THR:HG22  | 10       | 0.17          |
| (1,1383) | 1:87:A:THR:HB   | 1:87:A:THR:HG23  | 10       | 0.17          |
| (1,1371) | 1:86:A:GLU:H    | 1:134:A:TRP:HE1  | 9        | 0.17          |
| (1,1342) | 1:85:A:TYR:HE1  | 1:143:A:ILE:HG21 | 1        | 0.17          |
| (1,1342) | 1:85:A:TYR:HE1  | 1:143:A:ILE:HG22 | 1        | 0.17          |
| (1,1342) | 1:85:A:TYR:HE1  | 1:143:A:ILE:HG23 | 1        | 0.17          |
| (1,1342) | 1:85:A:TYR:HE2  | 1:143:A:ILE:HG21 | 1        | 0.17          |
| (1,1342) | 1:85:A:TYR:HE2  | 1:143:A:ILE:HG22 | 1        | 0.17          |
| (1,1342) | 1:85:A:TYR:HE2  | 1:143:A:ILE:HG23 | 1        | 0.17          |
| (1,1261) | 1:82:A:THR:HB   | 1:82:A:THR:HG21  | 2        | 0.17          |
| (1,1261) | 1:82:A:THR:HB   | 1:82:A:THR:HG22  | 2        | 0.17          |
| (1,1261) | 1:82:A:THR:HB   | 1:82:A:THR:HG23  | 2        | 0.17          |
| (1,1261) | 1:82:A:THR:HB   | 1:82:A:THR:HG21  | 4        | 0.17          |
| (1,1261) | 1:82:A:THR:HB   | 1:82:A:THR:HG22  | 4        | 0.17          |
| (1,1261) | 1:82:A:THR:HB   | 1:82:A:THR:HG23  | 4        | 0.17          |
| (1,1261) | 1:82:A:THR:HB   | 1:82:A:THR:HG21  | 9        | 0.17          |
| (1,1261) | 1:82:A:THR:HB   | 1:82:A:THR:HG22  | 9        | 0.17          |
| (1,1261) | 1:82:A:THR:HB   | 1:82:A:THR:HG23  | 9        | 0.17          |
| (1,1261) | 1:82:A:THR:HB   | 1:82:A:THR:HG21  | 10       | 0.17          |
| (1,1261) | 1:82:A:THR:HB   | 1:82:A:THR:HG22  | 10       | 0.17          |
| (1,1261) | 1:82:A:THR:HB   | 1:82:A:THR:HG23  | 10       | 0.17          |
| (1,1250) | 1:81:A:ILE:H    | 1:156:A:PHE:HA   | 2        | 0.17          |
| (1,1241) | 1:81:A:ILE:HG21 | 1:156:A:PHE:HD1  | 10       | 0.17          |
| (1,1241) | 1:81:A:ILE:HG21 | 1:156:A:PHE:HD2  | 10       | 0.17          |
| (1,1241) | 1:81:A:ILE:HG22 | 1:156:A:PHE:HD1  | 10       | 0.17          |
| (1,1241) | 1:81:A:ILE:HG22 | 1:156:A:PHE:HD2  | 10       | 0.17          |
| (1,1241) | 1:81:A:ILE:HG23 | 1:156:A:PHE:HD1  | 10       | 0.17          |
| (1,1241) | 1:81:A:ILE:HG23 | 1:156:A:PHE:HD2  | 10       | 0.17          |
| (1,1169) | 1:79:A:ILE:HG21 | 1:79:A:ILE:HD11  | 6        | 0.17          |
| (1,1169) | 1:79:A:ILE:HG21 | 1:79:A:ILE:HD12  | 6        | 0.17          |
| (1,1169) | 1:79:A:ILE:HG21 | 1:79:A:ILE:HD13  | 6        | 0.17          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1169) | 1:79:A:ILE:HG22 | 1:79:A:ILE:HD11 | 6        | 0.17          |
| (1,1169) | 1:79:A:ILE:HG22 | 1:79:A:ILE:HD12 | 6        | 0.17          |
| (1,1169) | 1:79:A:ILE:HG22 | 1:79:A:ILE:HD13 | 6        | 0.17          |
| (1,1169) | 1:79:A:ILE:HG23 | 1:79:A:ILE:HD11 | 6        | 0.17          |
| (1,1169) | 1:79:A:ILE:HG23 | 1:79:A:ILE:HD12 | 6        | 0.17          |
| (1,1169) | 1:79:A:ILE:HG23 | 1:79:A:ILE:HD13 | 6        | 0.17          |
| (1,1128) | 1:78:A:GLN:H    | 1:158:A:ALA:HA  | 4        | 0.17          |
| (1,1116) | 1:78:A:GLN:HB3  | 1:78:A:GLN:H    | 1        | 0.17          |
| (1,1075) | 1:76:A:TYR:H    | 1:162:A:ALA:HA  | 1        | 0.17          |
| (1,911)  | 1:69:A:GLN:HE22 | 1:70:A:LEU:H    | 3        | 0.17          |
| (1,911)  | 1:69:A:GLN:HE22 | 1:70:A:LEU:H    | 4        | 0.17          |
| (1,908)  | 1:69:A:GLN:HB3  | 1:70:A:LEU:H    | 2        | 0.17          |
| (1,857)  | 1:66:A:ASN:HD22 | 1:174:A:ILE:H   | 8        | 0.17          |
| (1,849)  | 1:66:A:ASN:HD22 | 1:66:A:ASN:H    | 3        | 0.17          |
| (1,837)  | 1:66:A:ASN:HB2  | 1:66:A:ASN:HD22 | 10       | 0.17          |
| (1,829)  | 1:66:A:ASN:HA   | 1:69:A:GLN:HG2  | 4        | 0.17          |
| (1,779)  | 1:64:A:LEU:HD11 | 1:64:A:LEU:HD21 | 2        | 0.17          |
| (1,779)  | 1:64:A:LEU:HD11 | 1:64:A:LEU:HD22 | 2        | 0.17          |
| (1,779)  | 1:64:A:LEU:HD11 | 1:64:A:LEU:HD23 | 2        | 0.17          |
| (1,779)  | 1:64:A:LEU:HD12 | 1:64:A:LEU:HD21 | 2        | 0.17          |
| (1,779)  | 1:64:A:LEU:HD12 | 1:64:A:LEU:HD22 | 2        | 0.17          |
| (1,779)  | 1:64:A:LEU:HD12 | 1:64:A:LEU:HD23 | 2        | 0.17          |
| (1,779)  | 1:64:A:LEU:HD13 | 1:64:A:LEU:HD21 | 2        | 0.17          |
| (1,779)  | 1:64:A:LEU:HD13 | 1:64:A:LEU:HD22 | 2        | 0.17          |
| (1,779)  | 1:64:A:LEU:HD13 | 1:64:A:LEU:HD23 | 2        | 0.17          |
| (1,761)  | 1:63:A:THR:H    | 1:175:A:PHE:HA  | 6        | 0.17          |
| (1,745)  | 1:63:A:THR:HB   | 1:63:A:THR:HG21 | 1        | 0.17          |
| (1,745)  | 1:63:A:THR:HB   | 1:63:A:THR:HG22 | 1        | 0.17          |
| (1,745)  | 1:63:A:THR:HB   | 1:63:A:THR:HG23 | 1        | 0.17          |
| (1,745)  | 1:63:A:THR:HB   | 1:63:A:THR:HG21 | 2        | 0.17          |
| (1,745)  | 1:63:A:THR:HB   | 1:63:A:THR:HG22 | 2        | 0.17          |
| (1,745)  | 1:63:A:THR:HB   | 1:63:A:THR:HG23 | 2        | 0.17          |
| (1,745)  | 1:63:A:THR:HB   | 1:63:A:THR:HG21 | 3        | 0.17          |
| (1,745)  | 1:63:A:THR:HB   | 1:63:A:THR:HG22 | 3        | 0.17          |
| (1,745)  | 1:63:A:THR:HB   | 1:63:A:THR:HG23 | 3        | 0.17          |
| (1,745)  | 1:63:A:THR:HB   | 1:63:A:THR:HG21 | 5        | 0.17          |
| (1,745)  | 1:63:A:THR:HB   | 1:63:A:THR:HG22 | 5        | 0.17          |
| (1,745)  | 1:63:A:THR:HB   | 1:63:A:THR:HG23 | 5        | 0.17          |
| (1,745)  | 1:63:A:THR:HB   | 1:63:A:THR:HG21 | 6        | 0.17          |
| (1,745)  | 1:63:A:THR:HB   | 1:63:A:THR:HG22 | 6        | 0.17          |
| (1,745)  | 1:63:A:THR:HB   | 1:63:A:THR:HG23 | 6        | 0.17          |
| (1,745)  | 1:63:A:THR:HB   | 1:63:A:THR:HG21 | 7        | 0.17          |

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| Key     | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,745) | 1:63:A:THR:HB   | 1:63:A:THR:HG22  | 7        | 0.17          |
| (1,745) | 1:63:A:THR:HB   | 1:63:A:THR:HG23  | 7        | 0.17          |
| (1,745) | 1:63:A:THR:HB   | 1:63:A:THR:HG21  | 8        | 0.17          |
| (1,745) | 1:63:A:THR:HB   | 1:63:A:THR:HG22  | 8        | 0.17          |
| (1,745) | 1:63:A:THR:HB   | 1:63:A:THR:HG23  | 8        | 0.17          |
| (1,745) | 1:63:A:THR:HB   | 1:63:A:THR:HG21  | 9        | 0.17          |
| (1,745) | 1:63:A:THR:HB   | 1:63:A:THR:HG22  | 9        | 0.17          |
| (1,745) | 1:63:A:THR:HB   | 1:63:A:THR:HG23  | 9        | 0.17          |
| (1,710) | 1:62:A:VAL:HA   | 1:62:A:VAL:HG21  | 7        | 0.17          |
| (1,710) | 1:62:A:VAL:HA   | 1:62:A:VAL:HG22  | 7        | 0.17          |
| (1,710) | 1:62:A:VAL:HA   | 1:62:A:VAL:HG23  | 7        | 0.17          |
| (1,710) | 1:62:A:VAL:HA   | 1:62:A:VAL:HG21  | 10       | 0.17          |
| (1,710) | 1:62:A:VAL:HA   | 1:62:A:VAL:HG22  | 10       | 0.17          |
| (1,710) | 1:62:A:VAL:HA   | 1:62:A:VAL:HG23  | 10       | 0.17          |
| (1,684) | 1:60:A:LEU:H    | 1:61:A:LYS:H     | 1        | 0.17          |
| (1,684) | 1:60:A:LEU:H    | 1:61:A:LYS:H     | 2        | 0.17          |
| (1,684) | 1:60:A:LEU:H    | 1:61:A:LYS:H     | 3        | 0.17          |
| (1,684) | 1:60:A:LEU:H    | 1:61:A:LYS:H     | 9        | 0.17          |
| (1,655) | 1:58:A:VAL:H    | 1:113:A:LEU:HD11 | 7        | 0.17          |
| (1,655) | 1:58:A:VAL:H    | 1:113:A:LEU:HD12 | 7        | 0.17          |
| (1,655) | 1:58:A:VAL:H    | 1:113:A:LEU:HD13 | 7        | 0.17          |
| (1,568) | 1:51:A:ILE:HA   | 1:51:A:ILE:HG21  | 3        | 0.17          |
| (1,568) | 1:51:A:ILE:HA   | 1:51:A:ILE:HG22  | 3        | 0.17          |
| (1,568) | 1:51:A:ILE:HA   | 1:51:A:ILE:HG23  | 3        | 0.17          |
| (1,553) | 1:50:A:TRP:HB2  | 1:52:A:LYS:H     | 3        | 0.17          |
| (1,541) | 1:50:A:TRP:HA   | 1:51:A:ILE:HB    | 4        | 0.17          |
| (1,541) | 1:50:A:TRP:HA   | 1:51:A:ILE:HB    | 7        | 0.17          |
| (1,530) | 1:49:A:VAL:H    | 1:152:A:ALA:HA   | 6        | 0.17          |
| (1,530) | 1:49:A:VAL:H    | 1:152:A:ALA:HA   | 10       | 0.17          |
| (1,496) | 1:48:A:ILE:HG21 | 1:50:A:TRP:HH2   | 6        | 0.17          |
| (1,496) | 1:48:A:ILE:HG22 | 1:50:A:TRP:HH2   | 6        | 0.17          |
| (1,496) | 1:48:A:ILE:HG23 | 1:50:A:TRP:HH2   | 6        | 0.17          |
| (1,470) | 1:48:A:ILE:HA   | 1:48:A:ILE:HG21  | 9        | 0.17          |
| (1,470) | 1:48:A:ILE:HA   | 1:48:A:ILE:HG22  | 9        | 0.17          |
| (1,470) | 1:48:A:ILE:HA   | 1:48:A:ILE:HG23  | 9        | 0.17          |
| (1,427) | 1:46:A:TYR:HA   | 1:156:A:PHE:HE1  | 3        | 0.17          |
| (1,427) | 1:46:A:TYR:HA   | 1:156:A:PHE:HE2  | 3        | 0.17          |
| (1,232) | 1:32:A:ILE:HG21 | 1:32:A:ILE:HD11  | 7        | 0.17          |
| (1,232) | 1:32:A:ILE:HG21 | 1:32:A:ILE:HD12  | 7        | 0.17          |
| (1,232) | 1:32:A:ILE:HG21 | 1:32:A:ILE:HD13  | 7        | 0.17          |
| (1,232) | 1:32:A:ILE:HG22 | 1:32:A:ILE:HD11  | 7        | 0.17          |
| (1,232) | 1:32:A:ILE:HG22 | 1:32:A:ILE:HD12  | 7        | 0.17          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,232) | 1:32:A:ILE:HG22  | 1:32:A:ILE:HD13  | 7        | 0.17          |
| (1,232) | 1:32:A:ILE:HG23  | 1:32:A:ILE:HD11  | 7        | 0.17          |
| (1,232) | 1:32:A:ILE:HG23  | 1:32:A:ILE:HD12  | 7        | 0.17          |
| (1,232) | 1:32:A:ILE:HG23  | 1:32:A:ILE:HD13  | 7        | 0.17          |
| (1,230) | 1:32:A:ILE:HG12  | 1:32:A:ILE:H     | 5        | 0.17          |
| (1,190) | 1:31:A:SER:HA    | 1:32:A:ILE:HD11  | 8        | 0.17          |
| (1,190) | 1:31:A:SER:HA    | 1:32:A:ILE:HD12  | 8        | 0.17          |
| (1,190) | 1:31:A:SER:HA    | 1:32:A:ILE:HD13  | 8        | 0.17          |
| (1,166) | 1:29:A:LEU:HD11  | 1:175:A:PHE:H    | 4        | 0.17          |
| (1,166) | 1:29:A:LEU:HD12  | 1:175:A:PHE:H    | 4        | 0.17          |
| (1,166) | 1:29:A:LEU:HD13  | 1:175:A:PHE:H    | 4        | 0.17          |
| (1,51)  | 1:24:A:ASP:HB2   | 1:25:A:VAL:H     | 2        | 0.17          |
| (1,51)  | 1:24:A:ASP:HB2   | 1:25:A:VAL:H     | 10       | 0.17          |
| (1,46)  | 1:24:A:ASP:HB3   | 1:50:A:TRP:HB3   | 10       | 0.17          |
| (1,25)  | 1:23:A:ILE:HA    | 1:23:A:ILE:HG21  | 3        | 0.17          |
| (1,25)  | 1:23:A:ILE:HA    | 1:23:A:ILE:HG22  | 3        | 0.17          |
| (1,25)  | 1:23:A:ILE:HA    | 1:23:A:ILE:HG23  | 3        | 0.17          |
| (3,4)   | 1:57:A:ASP:HA    | 1:114:A:ASP:HA   | 3        | 0.16          |
| (2,765) | 1:169:A:ASP:H    | 1:171:A:LEU:HD11 | 9        | 0.16          |
| (2,765) | 1:169:A:ASP:H    | 1:171:A:LEU:HD12 | 9        | 0.16          |
| (2,765) | 1:169:A:ASP:H    | 1:171:A:LEU:HD13 | 9        | 0.16          |
| (2,761) | 1:168:A:PHE:H    | 1:169:A:ASP:H    | 10       | 0.16          |
| (2,756) | 1:167:A:LEU:H    | 1:167:A:LEU:HD21 | 4        | 0.16          |
| (2,756) | 1:167:A:LEU:H    | 1:167:A:LEU:HD22 | 4        | 0.16          |
| (2,756) | 1:167:A:LEU:H    | 1:167:A:LEU:HD23 | 4        | 0.16          |
| (2,755) | 1:167:A:LEU:H    | 1:167:A:LEU:HD11 | 3        | 0.16          |
| (2,755) | 1:167:A:LEU:H    | 1:167:A:LEU:HD12 | 3        | 0.16          |
| (2,755) | 1:167:A:LEU:H    | 1:167:A:LEU:HD13 | 3        | 0.16          |
| (2,755) | 1:167:A:LEU:H    | 1:167:A:LEU:HD11 | 5        | 0.16          |
| (2,755) | 1:167:A:LEU:H    | 1:167:A:LEU:HD12 | 5        | 0.16          |
| (2,755) | 1:167:A:LEU:H    | 1:167:A:LEU:HD13 | 5        | 0.16          |
| (2,755) | 1:167:A:LEU:H    | 1:167:A:LEU:HD11 | 6        | 0.16          |
| (2,755) | 1:167:A:LEU:H    | 1:167:A:LEU:HD12 | 6        | 0.16          |
| (2,755) | 1:167:A:LEU:H    | 1:167:A:LEU:HD13 | 6        | 0.16          |
| (2,754) | 1:167:A:LEU:HD21 | 1:167:A:LEU:H    | 4        | 0.16          |
| (2,754) | 1:167:A:LEU:HD22 | 1:167:A:LEU:H    | 4        | 0.16          |
| (2,754) | 1:167:A:LEU:HD23 | 1:167:A:LEU:H    | 4        | 0.16          |
| (2,753) | 1:167:A:LEU:HD11 | 1:167:A:LEU:H    | 3        | 0.16          |
| (2,753) | 1:167:A:LEU:HD12 | 1:167:A:LEU:H    | 3        | 0.16          |
| (2,753) | 1:167:A:LEU:HD13 | 1:167:A:LEU:H    | 3        | 0.16          |
| (2,753) | 1:167:A:LEU:HD11 | 1:167:A:LEU:H    | 5        | 0.16          |
| (2,753) | 1:167:A:LEU:HD12 | 1:167:A:LEU:H    | 5        | 0.16          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,753)  | 1:167:A:LEU:HD13 | 1:167:A:LEU:H    | 5        | 0.16          |
| (2,753)  | 1:167:A:LEU:HD11 | 1:167:A:LEU:H    | 6        | 0.16          |
| (2,753)  | 1:167:A:LEU:HD12 | 1:167:A:LEU:H    | 6        | 0.16          |
| (2,753)  | 1:167:A:LEU:HD13 | 1:167:A:LEU:H    | 6        | 0.16          |
| (2,733)  | 1:157:A:LYS:HE2  | 1:159:A:PHE:HD1  | 5        | 0.16          |
| (2,733)  | 1:157:A:LYS:HE2  | 1:159:A:PHE:HD2  | 5        | 0.16          |
| (2,733)  | 1:157:A:LYS:HE3  | 1:159:A:PHE:HD1  | 5        | 0.16          |
| (2,733)  | 1:157:A:LYS:HE3  | 1:159:A:PHE:HD2  | 5        | 0.16          |
| (1,2316) | 1:171:A:LEU:HA   | 1:172:A:PRO:HD3  | 10       | 0.16          |
| (1,2304) | 1:170:A:SER:HA   | 1:171:A:LEU:HD21 | 2        | 0.16          |
| (1,2304) | 1:170:A:SER:HA   | 1:171:A:LEU:HD22 | 2        | 0.16          |
| (1,2304) | 1:170:A:SER:HA   | 1:171:A:LEU:HD23 | 2        | 0.16          |
| (1,2287) | 1:168:A:PHE:HD1  | 1:169:A:ASP:H    | 1        | 0.16          |
| (1,2287) | 1:168:A:PHE:HD2  | 1:169:A:ASP:H    | 1        | 0.16          |
| (1,2270) | 1:166:A:MET:HA   | 1:167:A:LEU:H    | 3        | 0.16          |
| (1,2270) | 1:166:A:MET:HA   | 1:167:A:LEU:H    | 5        | 0.16          |
| (1,2260) | 1:163:A:LYS:H    | 1:168:A:PHE:HZ   | 6        | 0.16          |
| (1,2207) | 1:159:A:PHE:HB2  | 1:159:A:PHE:H    | 4        | 0.16          |
| (1,2207) | 1:159:A:PHE:HB2  | 1:159:A:PHE:H    | 5        | 0.16          |
| (1,2207) | 1:159:A:PHE:HB2  | 1:159:A:PHE:H    | 7        | 0.16          |
| (1,2139) | 1:155:A:ASN:H    | 1:156:A:PHE:HZ   | 2        | 0.16          |
| (1,2139) | 1:155:A:ASN:H    | 1:156:A:PHE:HZ   | 7        | 0.16          |
| (1,2139) | 1:155:A:ASN:H    | 1:156:A:PHE:HZ   | 9        | 0.16          |
| (1,2106) | 1:153:A:ILE:HG21 | 1:155:A:ASN:HD21 | 10       | 0.16          |
| (1,2106) | 1:153:A:ILE:HG21 | 1:155:A:ASN:HD22 | 10       | 0.16          |
| (1,2106) | 1:153:A:ILE:HG22 | 1:155:A:ASN:HD21 | 10       | 0.16          |
| (1,2106) | 1:153:A:ILE:HG22 | 1:155:A:ASN:HD22 | 10       | 0.16          |
| (1,2106) | 1:153:A:ILE:HG23 | 1:155:A:ASN:HD21 | 10       | 0.16          |
| (1,2106) | 1:153:A:ILE:HG23 | 1:155:A:ASN:HD22 | 10       | 0.16          |
| (1,2079) | 1:151:A:VAL:HG11 | 1:151:A:VAL:H    | 3        | 0.16          |
| (1,2079) | 1:151:A:VAL:HG12 | 1:151:A:VAL:H    | 3        | 0.16          |
| (1,2079) | 1:151:A:VAL:HG13 | 1:151:A:VAL:H    | 3        | 0.16          |
| (1,2079) | 1:151:A:VAL:HG11 | 1:151:A:VAL:H    | 4        | 0.16          |
| (1,2079) | 1:151:A:VAL:HG12 | 1:151:A:VAL:H    | 4        | 0.16          |
| (1,2079) | 1:151:A:VAL:HG13 | 1:151:A:VAL:H    | 4        | 0.16          |
| (1,2079) | 1:151:A:VAL:HG11 | 1:151:A:VAL:H    | 5        | 0.16          |
| (1,2079) | 1:151:A:VAL:HG12 | 1:151:A:VAL:H    | 5        | 0.16          |
| (1,2079) | 1:151:A:VAL:HG13 | 1:151:A:VAL:H    | 5        | 0.16          |
| (1,2079) | 1:151:A:VAL:HG11 | 1:151:A:VAL:H    | 9        | 0.16          |
| (1,2079) | 1:151:A:VAL:HG12 | 1:151:A:VAL:H    | 9        | 0.16          |
| (1,2079) | 1:151:A:VAL:HG13 | 1:151:A:VAL:H    | 9        | 0.16          |
| (1,1894) | 1:134:A:TRP:HB3  | 1:142:A:ILE:HA   | 8        | 0.16          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1774) | 1:121:A:LEU:HB3  | 1:121:A:LEU:H    | 10       | 0.16          |
| (1,1648) | 1:112:A:VAL:HG21 | 1:112:A:VAL:H    | 6        | 0.16          |
| (1,1648) | 1:112:A:VAL:HG22 | 1:112:A:VAL:H    | 6        | 0.16          |
| (1,1648) | 1:112:A:VAL:HG23 | 1:112:A:VAL:H    | 6        | 0.16          |
| (1,1603) | 1:107:A:PRO:HB3  | 1:108:A:SER:HA   | 7        | 0.16          |
| (1,1532) | 1:102:A:ILE:HB   | 1:102:A:ILE:H    | 5        | 0.16          |
| (1,1532) | 1:102:A:ILE:HB   | 1:102:A:ILE:H    | 6        | 0.16          |
| (1,1505) | 1:98:A:THR:HA    | 1:100:A:ALA:H    | 4        | 0.16          |
| (1,1425) | 1:88:A:ASN:HD21  | 1:88:A:ASN:HD22  | 7        | 0.16          |
| (1,1383) | 1:87:A:THR:HB    | 1:87:A:THR:HG21  | 5        | 0.16          |
| (1,1383) | 1:87:A:THR:HB    | 1:87:A:THR:HG22  | 5        | 0.16          |
| (1,1383) | 1:87:A:THR:HB    | 1:87:A:THR:HG23  | 5        | 0.16          |
| (1,1369) | 1:86:A:GLU:H     | 1:133:A:ILE:HG21 | 10       | 0.16          |
| (1,1369) | 1:86:A:GLU:H     | 1:133:A:ILE:HG22 | 10       | 0.16          |
| (1,1369) | 1:86:A:GLU:H     | 1:133:A:ILE:HG23 | 10       | 0.16          |
| (1,1261) | 1:82:A:THR:HB    | 1:82:A:THR:HG21  | 1        | 0.16          |
| (1,1261) | 1:82:A:THR:HB    | 1:82:A:THR:HG22  | 1        | 0.16          |
| (1,1261) | 1:82:A:THR:HB    | 1:82:A:THR:HG23  | 1        | 0.16          |
| (1,1261) | 1:82:A:THR:HB    | 1:82:A:THR:HG21  | 3        | 0.16          |
| (1,1261) | 1:82:A:THR:HB    | 1:82:A:THR:HG22  | 3        | 0.16          |
| (1,1261) | 1:82:A:THR:HB    | 1:82:A:THR:HG23  | 3        | 0.16          |
| (1,1261) | 1:82:A:THR:HB    | 1:82:A:THR:HG21  | 5        | 0.16          |
| (1,1261) | 1:82:A:THR:HB    | 1:82:A:THR:HG22  | 5        | 0.16          |
| (1,1261) | 1:82:A:THR:HB    | 1:82:A:THR:HG23  | 5        | 0.16          |
| (1,1261) | 1:82:A:THR:HB    | 1:82:A:THR:HG21  | 6        | 0.16          |
| (1,1261) | 1:82:A:THR:HB    | 1:82:A:THR:HG22  | 6        | 0.16          |
| (1,1261) | 1:82:A:THR:HB    | 1:82:A:THR:HG23  | 6        | 0.16          |
| (1,1261) | 1:82:A:THR:HB    | 1:82:A:THR:HG21  | 7        | 0.16          |
| (1,1261) | 1:82:A:THR:HB    | 1:82:A:THR:HG22  | 7        | 0.16          |
| (1,1261) | 1:82:A:THR:HB    | 1:82:A:THR:HG23  | 7        | 0.16          |
| (1,1261) | 1:82:A:THR:HB    | 1:82:A:THR:HG21  | 8        | 0.16          |
| (1,1261) | 1:82:A:THR:HB    | 1:82:A:THR:HG22  | 8        | 0.16          |
| (1,1261) | 1:82:A:THR:HB    | 1:82:A:THR:HG23  | 8        | 0.16          |
| (1,1232) | 1:81:A:ILE:HG21  | 1:99:A:LYS:H     | 1        | 0.16          |
| (1,1232) | 1:81:A:ILE:HG22  | 1:99:A:LYS:H     | 1        | 0.16          |
| (1,1232) | 1:81:A:ILE:HG23  | 1:99:A:LYS:H     | 1        | 0.16          |
| (1,1216) | 1:81:A:ILE:HD11  | 1:100:A:ALA:H    | 6        | 0.16          |
| (1,1216) | 1:81:A:ILE:HD12  | 1:100:A:ALA:H    | 6        | 0.16          |
| (1,1216) | 1:81:A:ILE:HD13  | 1:100:A:ALA:H    | 6        | 0.16          |
| (1,1169) | 1:79:A:ILE:HG21  | 1:79:A:ILE:HD11  | 4        | 0.16          |
| (1,1169) | 1:79:A:ILE:HG21  | 1:79:A:ILE:HD12  | 4        | 0.16          |
| (1,1169) | 1:79:A:ILE:HG21  | 1:79:A:ILE:HD13  | 4        | 0.16          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1169) | 1:79:A:ILE:HG22 | 1:79:A:ILE:HD11 | 4        | 0.16          |
| (1,1169) | 1:79:A:ILE:HG22 | 1:79:A:ILE:HD12 | 4        | 0.16          |
| (1,1169) | 1:79:A:ILE:HG22 | 1:79:A:ILE:HD13 | 4        | 0.16          |
| (1,1169) | 1:79:A:ILE:HG23 | 1:79:A:ILE:HD11 | 4        | 0.16          |
| (1,1169) | 1:79:A:ILE:HG23 | 1:79:A:ILE:HD12 | 4        | 0.16          |
| (1,1169) | 1:79:A:ILE:HG23 | 1:79:A:ILE:HD13 | 4        | 0.16          |
| (1,1089) | 1:77:A:LEU:HD11 | 1:79:A:ILE:HD11 | 8        | 0.16          |
| (1,1089) | 1:77:A:LEU:HD11 | 1:79:A:ILE:HD12 | 8        | 0.16          |
| (1,1089) | 1:77:A:LEU:HD11 | 1:79:A:ILE:HD13 | 8        | 0.16          |
| (1,1089) | 1:77:A:LEU:HD12 | 1:79:A:ILE:HD11 | 8        | 0.16          |
| (1,1089) | 1:77:A:LEU:HD12 | 1:79:A:ILE:HD12 | 8        | 0.16          |
| (1,1089) | 1:77:A:LEU:HD12 | 1:79:A:ILE:HD13 | 8        | 0.16          |
| (1,1089) | 1:77:A:LEU:HD13 | 1:79:A:ILE:HD11 | 8        | 0.16          |
| (1,1089) | 1:77:A:LEU:HD13 | 1:79:A:ILE:HD12 | 8        | 0.16          |
| (1,1089) | 1:77:A:LEU:HD13 | 1:79:A:ILE:HD13 | 8        | 0.16          |
| (1,1089) | 1:77:A:LEU:HD21 | 1:79:A:ILE:HD11 | 8        | 0.16          |
| (1,1089) | 1:77:A:LEU:HD21 | 1:79:A:ILE:HD12 | 8        | 0.16          |
| (1,1089) | 1:77:A:LEU:HD21 | 1:79:A:ILE:HD13 | 8        | 0.16          |
| (1,1089) | 1:77:A:LEU:HD22 | 1:79:A:ILE:HD11 | 8        | 0.16          |
| (1,1089) | 1:77:A:LEU:HD22 | 1:79:A:ILE:HD12 | 8        | 0.16          |
| (1,1089) | 1:77:A:LEU:HD22 | 1:79:A:ILE:HD13 | 8        | 0.16          |
| (1,1089) | 1:77:A:LEU:HD23 | 1:79:A:ILE:HD11 | 8        | 0.16          |
| (1,1089) | 1:77:A:LEU:HD23 | 1:79:A:ILE:HD12 | 8        | 0.16          |
| (1,1089) | 1:77:A:LEU:HD23 | 1:79:A:ILE:HD13 | 8        | 0.16          |
| (1,1075) | 1:76:A:TYR:H    | 1:162:A:ALA:HA  | 5        | 0.16          |
| (1,922)  | 1:70:A:LEU:HD11 | 1:70:A:LEU:H    | 9        | 0.16          |
| (1,922)  | 1:70:A:LEU:HD12 | 1:70:A:LEU:H    | 9        | 0.16          |
| (1,922)  | 1:70:A:LEU:HD13 | 1:70:A:LEU:H    | 9        | 0.16          |
| (1,914)  | 1:69:A:GLN:HG3  | 1:69:A:GLN:H    | 3        | 0.16          |
| (1,914)  | 1:69:A:GLN:HG3  | 1:69:A:GLN:H    | 5        | 0.16          |
| (1,908)  | 1:69:A:GLN:HB3  | 1:70:A:LEU:H    | 6        | 0.16          |
| (1,857)  | 1:66:A:ASN:HD22 | 1:174:A:ILE:H   | 1        | 0.16          |
| (1,857)  | 1:66:A:ASN:HD22 | 1:174:A:ILE:H   | 2        | 0.16          |
| (1,845)  | 1:66:A:ASN:HD21 | 1:173:A:VAL:HA  | 3        | 0.16          |
| (1,845)  | 1:66:A:ASN:HD21 | 1:173:A:VAL:HA  | 10       | 0.16          |
| (1,762)  | 1:63:A:THR:H    | 1:175:A:PHE:HD1 | 6        | 0.16          |
| (1,762)  | 1:63:A:THR:H    | 1:175:A:PHE:HD2 | 6        | 0.16          |
| (1,710)  | 1:62:A:VAL:HA   | 1:62:A:VAL:HG21 | 1        | 0.16          |
| (1,710)  | 1:62:A:VAL:HA   | 1:62:A:VAL:HG22 | 1        | 0.16          |
| (1,710)  | 1:62:A:VAL:HA   | 1:62:A:VAL:HG23 | 1        | 0.16          |
| (1,710)  | 1:62:A:VAL:HA   | 1:62:A:VAL:HG21 | 2        | 0.16          |
| (1,710)  | 1:62:A:VAL:HA   | 1:62:A:VAL:HG22 | 2        | 0.16          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,710) | 1:62:A:VAL:HA   | 1:62:A:VAL:HG23 | 2        | 0.16          |
| (1,684) | 1:60:A:LEU:H    | 1:61:A:LYS:H    | 10       | 0.16          |
| (1,632) | 1:56:A:ASN:HD21 | 1:56:A:ASN:HD22 | 1        | 0.16          |
| (1,632) | 1:56:A:ASN:HD21 | 1:56:A:ASN:HD22 | 2        | 0.16          |
| (1,632) | 1:56:A:ASN:HD21 | 1:56:A:ASN:HD22 | 4        | 0.16          |
| (1,632) | 1:56:A:ASN:HD21 | 1:56:A:ASN:HD22 | 6        | 0.16          |
| (1,632) | 1:56:A:ASN:HD21 | 1:56:A:ASN:HD22 | 7        | 0.16          |
| (1,632) | 1:56:A:ASN:HD21 | 1:56:A:ASN:HD22 | 10       | 0.16          |
| (1,627) | 1:56:A:ASN:HB2  | 1:56:A:ASN:HD21 | 6        | 0.16          |
| (1,627) | 1:56:A:ASN:HB3  | 1:56:A:ASN:HD21 | 6        | 0.16          |
| (1,623) | 1:55:A:VAL:H    | 1:115:A:LYS:HA  | 5        | 0.16          |
| (1,568) | 1:51:A:ILE:HA   | 1:51:A:ILE:HG21 | 9        | 0.16          |
| (1,568) | 1:51:A:ILE:HA   | 1:51:A:ILE:HG22 | 9        | 0.16          |
| (1,568) | 1:51:A:ILE:HA   | 1:51:A:ILE:HG23 | 9        | 0.16          |
| (1,568) | 1:51:A:ILE:HA   | 1:51:A:ILE:HG21 | 10       | 0.16          |
| (1,568) | 1:51:A:ILE:HA   | 1:51:A:ILE:HG22 | 10       | 0.16          |
| (1,568) | 1:51:A:ILE:HA   | 1:51:A:ILE:HG23 | 10       | 0.16          |
| (1,554) | 1:50:A:TRP:HD1  | 1:50:A:TRP:H    | 2        | 0.16          |
| (1,554) | 1:50:A:TRP:HD1  | 1:50:A:TRP:H    | 8        | 0.16          |
| (1,470) | 1:48:A:ILE:HA   | 1:48:A:ILE:HG21 | 5        | 0.16          |
| (1,470) | 1:48:A:ILE:HA   | 1:48:A:ILE:HG22 | 5        | 0.16          |
| (1,470) | 1:48:A:ILE:HA   | 1:48:A:ILE:HG23 | 5        | 0.16          |
| (1,470) | 1:48:A:ILE:HA   | 1:48:A:ILE:HG21 | 10       | 0.16          |
| (1,470) | 1:48:A:ILE:HA   | 1:48:A:ILE:HG22 | 10       | 0.16          |
| (1,470) | 1:48:A:ILE:HA   | 1:48:A:ILE:HG23 | 10       | 0.16          |
| (1,467) | 1:47:A:ALA:H    | 1:156:A:PHE:HE1 | 8        | 0.16          |
| (1,467) | 1:47:A:ALA:H    | 1:156:A:PHE:HE2 | 8        | 0.16          |
| (1,455) | 1:47:A:ALA:HB1  | 1:48:A:ILE:H    | 5        | 0.16          |
| (1,455) | 1:47:A:ALA:HB2  | 1:48:A:ILE:H    | 5        | 0.16          |
| (1,455) | 1:47:A:ALA:HB3  | 1:48:A:ILE:H    | 5        | 0.16          |
| (1,455) | 1:47:A:ALA:HB1  | 1:48:A:ILE:H    | 8        | 0.16          |
| (1,455) | 1:47:A:ALA:HB2  | 1:48:A:ILE:H    | 8        | 0.16          |
| (1,455) | 1:47:A:ALA:HB3  | 1:48:A:ILE:H    | 8        | 0.16          |
| (1,426) | 1:46:A:TYR:HA   | 1:156:A:PHE:HA  | 4        | 0.16          |
| (1,389) | 1:44:A:ILE:HG21 | 1:44:A:ILE:H    | 3        | 0.16          |
| (1,389) | 1:44:A:ILE:HG22 | 1:44:A:ILE:H    | 3        | 0.16          |
| (1,389) | 1:44:A:ILE:HG23 | 1:44:A:ILE:H    | 3        | 0.16          |
| (1,389) | 1:44:A:ILE:HG21 | 1:44:A:ILE:H    | 9        | 0.16          |
| (1,389) | 1:44:A:ILE:HG22 | 1:44:A:ILE:H    | 9        | 0.16          |
| (1,389) | 1:44:A:ILE:HG23 | 1:44:A:ILE:H    | 9        | 0.16          |
| (1,339) | 1:41:A:SER:HB2  | 1:159:A:PHE:HD1 | 5        | 0.16          |
| (1,339) | 1:41:A:SER:HB2  | 1:159:A:PHE:HD2 | 5        | 0.16          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,295)  | 1:38:A:ALA:HA    | 1:39:A:GLN:H     | 10       | 0.16          |
| (1,268)  | 1:34:A:PRO:HD3   | 1:35:A:ALA:H     | 5        | 0.16          |
| (1,209)  | 1:32:A:ILE:HA    | 1:32:A:ILE:HG21  | 4        | 0.16          |
| (1,209)  | 1:32:A:ILE:HA    | 1:32:A:ILE:HG22  | 4        | 0.16          |
| (1,209)  | 1:32:A:ILE:HA    | 1:32:A:ILE:HG23  | 4        | 0.16          |
| (1,92)   | 1:25:A:VAL:H     | 1:50:A:TRP:HE1   | 2        | 0.16          |
| (1,92)   | 1:25:A:VAL:H     | 1:50:A:TRP:HE1   | 9        | 0.16          |
| (1,51)   | 1:24:A:ASP:HB2   | 1:25:A:VAL:H     | 1        | 0.16          |
| (3,13)   | 1:181:A:GLN:HA   | 1:181:A:GLN:HB2  | 7        | 0.15          |
| (3,4)    | 1:57:A:ASP:HA    | 1:114:A:ASP:HA   | 1        | 0.15          |
| (3,4)    | 1:57:A:ASP:HA    | 1:114:A:ASP:HA   | 8        | 0.15          |
| (3,2)    | 1:33:A:THR:HA    | 1:34:A:PRO:HD3   | 4        | 0.15          |
| (2,770)  | 1:174:A:ILE:HG21 | 1:176:A:ASN:HA   | 8        | 0.15          |
| (2,770)  | 1:174:A:ILE:HG22 | 1:176:A:ASN:HA   | 8        | 0.15          |
| (2,770)  | 1:174:A:ILE:HG23 | 1:176:A:ASN:HA   | 8        | 0.15          |
| (2,755)  | 1:167:A:LEU:H    | 1:167:A:LEU:HD11 | 9        | 0.15          |
| (2,755)  | 1:167:A:LEU:H    | 1:167:A:LEU:HD12 | 9        | 0.15          |
| (2,755)  | 1:167:A:LEU:H    | 1:167:A:LEU:HD13 | 9        | 0.15          |
| (2,753)  | 1:167:A:LEU:HD11 | 1:167:A:LEU:H    | 9        | 0.15          |
| (2,753)  | 1:167:A:LEU:HD12 | 1:167:A:LEU:H    | 9        | 0.15          |
| (2,753)  | 1:167:A:LEU:HD13 | 1:167:A:LEU:H    | 9        | 0.15          |
| (2,744)  | 1:163:A:LYS:HG3  | 1:166:A:MET:H    | 9        | 0.15          |
| (2,628)  | 1:122:A:TYR:HB3  | 1:123:A:PRO:HD2  | 5        | 0.15          |
| (2,534)  | 1:85:A:TYR:HE1   | 1:151:A:VAL:H    | 4        | 0.15          |
| (2,534)  | 1:85:A:TYR:HE2   | 1:151:A:VAL:H    | 4        | 0.15          |
| (1,2370) | 1:174:A:ILE:HG21 | 1:175:A:PHE:HA   | 2        | 0.15          |
| (1,2370) | 1:174:A:ILE:HG22 | 1:175:A:PHE:HA   | 2        | 0.15          |
| (1,2370) | 1:174:A:ILE:HG23 | 1:175:A:PHE:HA   | 2        | 0.15          |
| (1,2349) | 1:173:A:VAL:HB   | 1:174:A:ILE:H    | 3        | 0.15          |
| (1,2299) | 1:169:A:ASP:H    | 1:170:A:SER:H    | 8        | 0.15          |
| (1,2270) | 1:166:A:MET:HA   | 1:167:A:LEU:H    | 4        | 0.15          |
| (1,2270) | 1:166:A:MET:HA   | 1:167:A:LEU:H    | 7        | 0.15          |
| (1,2270) | 1:166:A:MET:HA   | 1:167:A:LEU:H    | 8        | 0.15          |
| (1,2258) | 1:163:A:LYS:HG2  | 1:163:A:LYS:H    | 10       | 0.15          |
| (1,2139) | 1:155:A:ASN:H    | 1:156:A:PHE:HZ   | 6        | 0.15          |
| (1,2013) | 1:142:A:ILE:HG21 | 1:143:A:ILE:H    | 7        | 0.15          |
| (1,2013) | 1:142:A:ILE:HG22 | 1:143:A:ILE:H    | 7        | 0.15          |
| (1,2013) | 1:142:A:ILE:HG23 | 1:143:A:ILE:H    | 7        | 0.15          |
| (1,1894) | 1:134:A:TRP:HB3  | 1:142:A:ILE:HA   | 4        | 0.15          |
| (1,1894) | 1:134:A:TRP:HB3  | 1:142:A:ILE:HA   | 5        | 0.15          |
| (1,1790) | 1:126:A:THR:HA   | 1:126:A:THR:HG21 | 5        | 0.15          |
| (1,1790) | 1:126:A:THR:HA   | 1:126:A:THR:HG22 | 5        | 0.15          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1790) | 1:126:A:THR:HA   | 1:126:A:THR:HG23 | 5        | 0.15          |
| (1,1787) | 1:123:A:PRO:HD2  | 1:124:A:ASP:H    | 4        | 0.15          |
| (1,1778) | 1:121:A:LEU:HG   | 1:121:A:LEU:H    | 1        | 0.15          |
| (1,1747) | 1:118:A:ILE:HD11 | 1:118:A:ILE:H    | 5        | 0.15          |
| (1,1747) | 1:118:A:ILE:HD12 | 1:118:A:ILE:H    | 5        | 0.15          |
| (1,1747) | 1:118:A:ILE:HD13 | 1:118:A:ILE:H    | 5        | 0.15          |
| (1,1677) | 1:114:A:ASP:HA   | 1:118:A:ILE:H    | 6        | 0.15          |
| (1,1677) | 1:114:A:ASP:HA   | 1:118:A:ILE:H    | 7        | 0.15          |
| (1,1639) | 1:111:A:ILE:HG21 | 1:111:A:ILE:H    | 8        | 0.15          |
| (1,1639) | 1:111:A:ILE:HG22 | 1:111:A:ILE:H    | 8        | 0.15          |
| (1,1639) | 1:111:A:ILE:HG23 | 1:111:A:ILE:H    | 8        | 0.15          |
| (1,1572) | 1:104:A:LEU:HD11 | 1:104:A:LEU:H    | 7        | 0.15          |
| (1,1572) | 1:104:A:LEU:HD12 | 1:104:A:LEU:H    | 7        | 0.15          |
| (1,1572) | 1:104:A:LEU:HD13 | 1:104:A:LEU:H    | 7        | 0.15          |
| (1,1534) | 1:102:A:ILE:HB   | 1:103:A:SER:H    | 4        | 0.15          |
| (1,1510) | 1:98:A:THR:HG21  | 1:100:A:ALA:H    | 3        | 0.15          |
| (1,1510) | 1:98:A:THR:HG22  | 1:100:A:ALA:H    | 3        | 0.15          |
| (1,1510) | 1:98:A:THR:HG23  | 1:100:A:ALA:H    | 3        | 0.15          |
| (1,1505) | 1:98:A:THR:HA    | 1:100:A:ALA:H    | 8        | 0.15          |
| (1,1460) | 1:92:A:LEU:HG    | 1:93:A:GLY:H     | 4        | 0.15          |
| (1,1425) | 1:88:A:ASN:HD21  | 1:88:A:ASN:HD22  | 1        | 0.15          |
| (1,1425) | 1:88:A:ASN:HD21  | 1:88:A:ASN:HD22  | 2        | 0.15          |
| (1,1425) | 1:88:A:ASN:HD21  | 1:88:A:ASN:HD22  | 3        | 0.15          |
| (1,1425) | 1:88:A:ASN:HD21  | 1:88:A:ASN:HD22  | 4        | 0.15          |
| (1,1425) | 1:88:A:ASN:HD21  | 1:88:A:ASN:HD22  | 5        | 0.15          |
| (1,1425) | 1:88:A:ASN:HD21  | 1:88:A:ASN:HD22  | 6        | 0.15          |
| (1,1425) | 1:88:A:ASN:HD21  | 1:88:A:ASN:HD22  | 8        | 0.15          |
| (1,1425) | 1:88:A:ASN:HD21  | 1:88:A:ASN:HD22  | 9        | 0.15          |
| (1,1425) | 1:88:A:ASN:HD21  | 1:88:A:ASN:HD22  | 10       | 0.15          |
| (1,1402) | 1:87:A:THR:HG21  | 1:89:A:SER:H     | 2        | 0.15          |
| (1,1402) | 1:87:A:THR:HG22  | 1:89:A:SER:H     | 2        | 0.15          |
| (1,1402) | 1:87:A:THR:HG23  | 1:89:A:SER:H     | 2        | 0.15          |
| (1,1363) | 1:86:A:GLU:HG3   | 1:86:A:GLU:H     | 1        | 0.15          |
| (1,1363) | 1:86:A:GLU:HG3   | 1:86:A:GLU:H     | 8        | 0.15          |
| (1,1343) | 1:85:A:TYR:HE1   | 1:152:A:ALA:HA   | 6        | 0.15          |
| (1,1343) | 1:85:A:TYR:HE2   | 1:152:A:ALA:HA   | 6        | 0.15          |
| (1,1338) | 1:85:A:TYR:HD1   | 1:86:A:GLU:H     | 7        | 0.15          |
| (1,1338) | 1:85:A:TYR:HD2   | 1:86:A:GLU:H     | 7        | 0.15          |
| (1,1314) | 1:83:A:SER:H     | 1:99:A:LYS:HE2   | 4        | 0.15          |
| (1,1233) | 1:81:A:ILE:HG21  | 1:100:A:ALA:HB1  | 1        | 0.15          |
| (1,1233) | 1:81:A:ILE:HG21  | 1:100:A:ALA:HB2  | 1        | 0.15          |
| (1,1233) | 1:81:A:ILE:HG21  | 1:100:A:ALA:HB3  | 1        | 0.15          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1233) | 1:81:A:ILE:HG22 | 1:100:A:ALA:HB1 | 1        | 0.15          |
| (1,1233) | 1:81:A:ILE:HG22 | 1:100:A:ALA:HB2 | 1        | 0.15          |
| (1,1233) | 1:81:A:ILE:HG22 | 1:100:A:ALA:HB3 | 1        | 0.15          |
| (1,1233) | 1:81:A:ILE:HG23 | 1:100:A:ALA:HB1 | 1        | 0.15          |
| (1,1233) | 1:81:A:ILE:HG23 | 1:100:A:ALA:HB2 | 1        | 0.15          |
| (1,1233) | 1:81:A:ILE:HG23 | 1:100:A:ALA:HB3 | 1        | 0.15          |
| (1,1207) | 1:81:A:ILE:HA   | 1:82:A:THR:H    | 2        | 0.15          |
| (1,1128) | 1:78:A:GLN:H    | 1:158:A:ALA:HA  | 3        | 0.15          |
| (1,1128) | 1:78:A:GLN:H    | 1:158:A:ALA:HA  | 7        | 0.15          |
| (1,1127) | 1:78:A:GLN:H    | 1:104:A:LEU:H   | 9        | 0.15          |
| (1,1100) | 1:77:A:LEU:HG   | 1:78:A:GLN:H    | 4        | 0.15          |
| (1,1097) | 1:77:A:LEU:HD11 | 1:160:A:TYR:HB3 | 4        | 0.15          |
| (1,1097) | 1:77:A:LEU:HD12 | 1:160:A:TYR:HB3 | 4        | 0.15          |
| (1,1097) | 1:77:A:LEU:HD13 | 1:160:A:TYR:HB3 | 4        | 0.15          |
| (1,1097) | 1:77:A:LEU:HD21 | 1:160:A:TYR:HB3 | 4        | 0.15          |
| (1,1097) | 1:77:A:LEU:HD22 | 1:160:A:TYR:HB3 | 4        | 0.15          |
| (1,1097) | 1:77:A:LEU:HD23 | 1:160:A:TYR:HB3 | 4        | 0.15          |
| (1,1006) | 1:74:A:PHE:HA   | 1:163:A:LYS:H   | 1        | 0.15          |
| (1,1006) | 1:74:A:PHE:HA   | 1:163:A:LYS:H   | 4        | 0.15          |
| (1,1006) | 1:74:A:PHE:HA   | 1:163:A:LYS:H   | 10       | 0.15          |
| (1,989)  | 1:73:A:TYR:HD1  | 1:74:A:PHE:HE1  | 3        | 0.15          |
| (1,989)  | 1:73:A:TYR:HD1  | 1:74:A:PHE:HE2  | 3        | 0.15          |
| (1,989)  | 1:73:A:TYR:HD2  | 1:74:A:PHE:HE1  | 3        | 0.15          |
| (1,989)  | 1:73:A:TYR:HD2  | 1:74:A:PHE:HE2  | 3        | 0.15          |
| (1,922)  | 1:70:A:LEU:HD11 | 1:70:A:LEU:H    | 1        | 0.15          |
| (1,922)  | 1:70:A:LEU:HD12 | 1:70:A:LEU:H    | 1        | 0.15          |
| (1,922)  | 1:70:A:LEU:HD13 | 1:70:A:LEU:H    | 1        | 0.15          |
| (1,912)  | 1:69:A:GLN:HG3  | 1:69:A:GLN:HE21 | 10       | 0.15          |
| (1,909)  | 1:69:A:GLN:HB2  | 1:70:A:LEU:H    | 8        | 0.15          |
| (1,899)  | 1:69:A:GLN:HA   | 1:69:A:GLN:HE22 | 9        | 0.15          |
| (1,894)  | 1:68:A:GLU:H    | 1:69:A:GLN:H    | 3        | 0.15          |
| (1,894)  | 1:68:A:GLU:H    | 1:69:A:GLN:H    | 5        | 0.15          |
| (1,856)  | 1:66:A:ASN:HD22 | 1:173:A:VAL:HA  | 9        | 0.15          |
| (1,854)  | 1:66:A:ASN:HD22 | 1:172:A:PRO:HD3 | 10       | 0.15          |
| (1,831)  | 1:66:A:ASN:HA   | 1:174:A:ILE:HB  | 3        | 0.15          |
| (1,831)  | 1:66:A:ASN:HA   | 1:174:A:ILE:HB  | 8        | 0.15          |
| (1,710)  | 1:62:A:VAL:HA   | 1:62:A:VAL:HG21 | 9        | 0.15          |
| (1,710)  | 1:62:A:VAL:HA   | 1:62:A:VAL:HG22 | 9        | 0.15          |
| (1,710)  | 1:62:A:VAL:HA   | 1:62:A:VAL:HG23 | 9        | 0.15          |
| (1,651)  | 1:58:A:VAL:HG11 | 1:59:A:LYS:H    | 7        | 0.15          |
| (1,651)  | 1:58:A:VAL:HG12 | 1:59:A:LYS:H    | 7        | 0.15          |
| (1,651)  | 1:58:A:VAL:HG13 | 1:59:A:LYS:H    | 7        | 0.15          |

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| Key     | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,651) | 1:58:A:VAL:HG21 | 1:59:A:LYS:H     | 7        | 0.15          |
| (1,651) | 1:58:A:VAL:HG22 | 1:59:A:LYS:H     | 7        | 0.15          |
| (1,651) | 1:58:A:VAL:HG23 | 1:59:A:LYS:H     | 7        | 0.15          |
| (1,633) | 1:56:A:ASN:HD22 | 1:57:A:ASP:H     | 6        | 0.15          |
| (1,632) | 1:56:A:ASN:HD21 | 1:56:A:ASN:HD22  | 3        | 0.15          |
| (1,632) | 1:56:A:ASN:HD21 | 1:56:A:ASN:HD22  | 5        | 0.15          |
| (1,632) | 1:56:A:ASN:HD21 | 1:56:A:ASN:HD22  | 8        | 0.15          |
| (1,632) | 1:56:A:ASN:HD21 | 1:56:A:ASN:HD22  | 9        | 0.15          |
| (1,623) | 1:55:A:VAL:H    | 1:115:A:LYS:HA   | 2        | 0.15          |
| (1,623) | 1:55:A:VAL:H    | 1:115:A:LYS:HA   | 8        | 0.15          |
| (1,579) | 1:51:A:ILE:HG21 | 1:53:A:ASP:HB2   | 3        | 0.15          |
| (1,579) | 1:51:A:ILE:HG21 | 1:53:A:ASP:HB3   | 3        | 0.15          |
| (1,579) | 1:51:A:ILE:HG22 | 1:53:A:ASP:HB2   | 3        | 0.15          |
| (1,579) | 1:51:A:ILE:HG22 | 1:53:A:ASP:HB3   | 3        | 0.15          |
| (1,579) | 1:51:A:ILE:HG23 | 1:53:A:ASP:HB2   | 3        | 0.15          |
| (1,579) | 1:51:A:ILE:HG23 | 1:53:A:ASP:HB3   | 3        | 0.15          |
| (1,573) | 1:51:A:ILE:HD11 | 1:55:A:VAL:H     | 10       | 0.15          |
| (1,573) | 1:51:A:ILE:HD12 | 1:55:A:VAL:H     | 10       | 0.15          |
| (1,573) | 1:51:A:ILE:HD13 | 1:55:A:VAL:H     | 10       | 0.15          |
| (1,561) | 1:50:A:TRP:HE3  | 1:151:A:VAL:HG21 | 6        | 0.15          |
| (1,561) | 1:50:A:TRP:HE3  | 1:151:A:VAL:HG22 | 6        | 0.15          |
| (1,561) | 1:50:A:TRP:HE3  | 1:151:A:VAL:HG23 | 6        | 0.15          |
| (1,553) | 1:50:A:TRP:HB2  | 1:52:A:LYS:H     | 7        | 0.15          |
| (1,513) | 1:49:A:VAL:HA   | 1:49:A:VAL:HG11  | 10       | 0.15          |
| (1,513) | 1:49:A:VAL:HA   | 1:49:A:VAL:HG12  | 10       | 0.15          |
| (1,513) | 1:49:A:VAL:HA   | 1:49:A:VAL:HG13  | 10       | 0.15          |
| (1,470) | 1:48:A:ILE:HA   | 1:48:A:ILE:HG21  | 6        | 0.15          |
| (1,470) | 1:48:A:ILE:HA   | 1:48:A:ILE:HG22  | 6        | 0.15          |
| (1,470) | 1:48:A:ILE:HA   | 1:48:A:ILE:HG23  | 6        | 0.15          |
| (1,292) | 1:37:A:GLY:HA2  | 1:37:A:GLY:H     | 8        | 0.15          |
| (1,268) | 1:34:A:PRO:HD3  | 1:35:A:ALA:H     | 10       | 0.15          |
| (1,241) | 1:32:A:ILE:HG21 | 1:160:A:TYR:HD1  | 1        | 0.15          |
| (1,241) | 1:32:A:ILE:HG21 | 1:160:A:TYR:HD2  | 1        | 0.15          |
| (1,241) | 1:32:A:ILE:HG22 | 1:160:A:TYR:HD1  | 1        | 0.15          |
| (1,241) | 1:32:A:ILE:HG22 | 1:160:A:TYR:HD2  | 1        | 0.15          |
| (1,241) | 1:32:A:ILE:HG23 | 1:160:A:TYR:HD1  | 1        | 0.15          |
| (1,241) | 1:32:A:ILE:HG23 | 1:160:A:TYR:HD2  | 1        | 0.15          |
| (1,230) | 1:32:A:ILE:HG12 | 1:32:A:ILE:H     | 8        | 0.15          |
| (1,227) | 1:32:A:ILE:HG13 | 1:33:A:THR:H     | 1        | 0.15          |
| (1,227) | 1:32:A:ILE:HG13 | 1:33:A:THR:H     | 9        | 0.15          |
| (1,208) | 1:32:A:ILE:HA   | 1:32:A:ILE:HG12  | 10       | 0.15          |
| (1,100) | 1:26:A:GLU:HB2  | 1:50:A:TRP:HE1   | 10       | 0.15          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,54)   | 1:24:A:ASP:HB2   | 1:50:A:TRP:HB2   | 6        | 0.15          |
| (1,51)   | 1:24:A:ASP:HB2   | 1:25:A:VAL:H     | 3        | 0.15          |
| (3,12)   | 1:181:A:GLN:HA   | 1:181:A:GLN:HB3  | 5        | 0.14          |
| (2,628)  | 1:122:A:TYR:HB3  | 1:123:A:PRO:HD2  | 7        | 0.14          |
| (2,628)  | 1:122:A:TYR:HB3  | 1:123:A:PRO:HD2  | 10       | 0.14          |
| (2,607)  | 1:115:A:LYS:H    | 1:116:A:GLU:HG2  | 4        | 0.14          |
| (2,607)  | 1:115:A:LYS:H    | 1:116:A:GLU:HG3  | 4        | 0.14          |
| (2,518)  | 1:84:A:GLY:HA2   | 1:95:A:PHE:HE1   | 2        | 0.14          |
| (2,518)  | 1:84:A:GLY:HA2   | 1:95:A:PHE:HE2   | 2        | 0.14          |
| (2,518)  | 1:84:A:GLY:HA3   | 1:95:A:PHE:HE1   | 2        | 0.14          |
| (2,518)  | 1:84:A:GLY:HA3   | 1:95:A:PHE:HE2   | 2        | 0.14          |
| (2,517)  | 1:84:A:GLY:HA2   | 1:85:A:TYR:HD1   | 1        | 0.14          |
| (2,517)  | 1:84:A:GLY:HA2   | 1:85:A:TYR:HD2   | 1        | 0.14          |
| (2,517)  | 1:84:A:GLY:HA3   | 1:85:A:TYR:HD1   | 1        | 0.14          |
| (2,517)  | 1:84:A:GLY:HA3   | 1:85:A:TYR:HD2   | 1        | 0.14          |
| (2,510)  | 1:83:A:SER:HB3   | 1:154:A:LEU:HA   | 2        | 0.14          |
| (2,298)  | 1:54:A:GLN:HB3   | 1:54:A:GLN:HE21  | 8        | 0.14          |
| (2,206)  | 1:39:A:GLN:HB2   | 1:39:A:GLN:HE21  | 1        | 0.14          |
| (2,206)  | 1:39:A:GLN:HB2   | 1:39:A:GLN:HE21  | 6        | 0.14          |
| (2,206)  | 1:39:A:GLN:HB2   | 1:39:A:GLN:HE21  | 7        | 0.14          |
| (2,205)  | 1:39:A:GLN:HB3   | 1:39:A:GLN:HE21  | 3        | 0.14          |
| (2,205)  | 1:39:A:GLN:HB3   | 1:39:A:GLN:HE21  | 4        | 0.14          |
| (2,205)  | 1:39:A:GLN:HB3   | 1:39:A:GLN:HE21  | 5        | 0.14          |
| (2,205)  | 1:39:A:GLN:HB3   | 1:39:A:GLN:HE21  | 8        | 0.14          |
| (2,205)  | 1:39:A:GLN:HB3   | 1:39:A:GLN:HE21  | 9        | 0.14          |
| (2,178)  | 1:36:A:ALA:H     | 1:37:A:GLY:H     | 2        | 0.14          |
| (2,12)   | 1:17:A:GLN:HB2   | 1:17:A:GLN:HE21  | 5        | 0.14          |
| (2,12)   | 1:17:A:GLN:HB2   | 1:17:A:GLN:HE21  | 7        | 0.14          |
| (2,11)   | 1:17:A:GLN:HB3   | 1:17:A:GLN:HE21  | 8        | 0.14          |
| (1,2371) | 1:174:A:ILE:HG21 | 1:175:A:PHE:H    | 4        | 0.14          |
| (1,2371) | 1:174:A:ILE:HG22 | 1:175:A:PHE:H    | 4        | 0.14          |
| (1,2371) | 1:174:A:ILE:HG23 | 1:175:A:PHE:H    | 4        | 0.14          |
| (1,2370) | 1:174:A:ILE:HG21 | 1:175:A:PHE:HA   | 1        | 0.14          |
| (1,2370) | 1:174:A:ILE:HG22 | 1:175:A:PHE:HA   | 1        | 0.14          |
| (1,2370) | 1:174:A:ILE:HG23 | 1:175:A:PHE:HA   | 1        | 0.14          |
| (1,2354) | 1:173:A:VAL:HG11 | 1:175:A:PHE:HE1  | 8        | 0.14          |
| (1,2354) | 1:173:A:VAL:HG11 | 1:175:A:PHE:HE2  | 8        | 0.14          |
| (1,2354) | 1:173:A:VAL:HG12 | 1:175:A:PHE:HE1  | 8        | 0.14          |
| (1,2354) | 1:173:A:VAL:HG12 | 1:175:A:PHE:HE2  | 8        | 0.14          |
| (1,2354) | 1:173:A:VAL:HG13 | 1:175:A:PHE:HE1  | 8        | 0.14          |
| (1,2354) | 1:173:A:VAL:HG13 | 1:175:A:PHE:HE2  | 8        | 0.14          |
| (1,2342) | 1:173:A:VAL:HA   | 1:173:A:VAL:HG11 | 6        | 0.14          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2342) | 1:173:A:VAL:HA   | 1:173:A:VAL:HG12 | 6        | 0.14          |
| (1,2342) | 1:173:A:VAL:HA   | 1:173:A:VAL:HG13 | 6        | 0.14          |
| (1,2299) | 1:169:A:ASP:H    | 1:170:A:SER:H    | 10       | 0.14          |
| (1,2283) | 1:168:A:PHE:HB2  | 1:168:A:PHE:H    | 2        | 0.14          |
| (1,2260) | 1:163:A:LYS:H    | 1:168:A:PHE:HZ   | 2        | 0.14          |
| (1,2258) | 1:163:A:LYS:HG2  | 1:163:A:LYS:H    | 5        | 0.14          |
| (1,2258) | 1:163:A:LYS:HG2  | 1:163:A:LYS:H    | 8        | 0.14          |
| (1,2190) | 1:158:A:ALA:HB1  | 1:160:A:TYR:HD1  | 2        | 0.14          |
| (1,2190) | 1:158:A:ALA:HB1  | 1:160:A:TYR:HD2  | 2        | 0.14          |
| (1,2190) | 1:158:A:ALA:HB2  | 1:160:A:TYR:HD1  | 2        | 0.14          |
| (1,2190) | 1:158:A:ALA:HB2  | 1:160:A:TYR:HD2  | 2        | 0.14          |
| (1,2190) | 1:158:A:ALA:HB3  | 1:160:A:TYR:HD1  | 2        | 0.14          |
| (1,2190) | 1:158:A:ALA:HB3  | 1:160:A:TYR:HD2  | 2        | 0.14          |
| (1,2139) | 1:155:A:ASN:H    | 1:156:A:PHE:HZ   | 5        | 0.14          |
| (1,2089) | 1:152:A:ALA:HB1  | 1:152:A:ALA:H    | 6        | 0.14          |
| (1,2089) | 1:152:A:ALA:HB2  | 1:152:A:ALA:H    | 6        | 0.14          |
| (1,2089) | 1:152:A:ALA:HB3  | 1:152:A:ALA:H    | 6        | 0.14          |
| (1,2069) | 1:148:A:THR:HG21 | 1:148:A:THR:H    | 5        | 0.14          |
| (1,2069) | 1:148:A:THR:HG22 | 1:148:A:THR:H    | 5        | 0.14          |
| (1,2069) | 1:148:A:THR:HG23 | 1:148:A:THR:H    | 5        | 0.14          |
| (1,2013) | 1:142:A:ILE:HG21 | 1:143:A:ILE:H    | 6        | 0.14          |
| (1,2013) | 1:142:A:ILE:HG22 | 1:143:A:ILE:H    | 6        | 0.14          |
| (1,2013) | 1:142:A:ILE:HG23 | 1:143:A:ILE:H    | 6        | 0.14          |
| (1,1894) | 1:134:A:TRP:HB3  | 1:142:A:ILE:HA   | 7        | 0.14          |
| (1,1892) | 1:134:A:TRP:HB3  | 1:135:A:VAL:H    | 1        | 0.14          |
| (1,1847) | 1:132:A:SER:H    | 1:134:A:TRP:HH2  | 8        | 0.14          |
| (1,1834) | 1:132:A:SER:HA   | 1:145:A:TYR:HB3  | 5        | 0.14          |
| (1,1793) | 1:128:A:TYR:HA   | 1:128:A:TYR:HB3  | 6        | 0.14          |
| (1,1790) | 1:126:A:THR:HA   | 1:126:A:THR:HG21 | 3        | 0.14          |
| (1,1790) | 1:126:A:THR:HA   | 1:126:A:THR:HG22 | 3        | 0.14          |
| (1,1790) | 1:126:A:THR:HA   | 1:126:A:THR:HG23 | 3        | 0.14          |
| (1,1790) | 1:126:A:THR:HA   | 1:126:A:THR:HG21 | 7        | 0.14          |
| (1,1790) | 1:126:A:THR:HA   | 1:126:A:THR:HG22 | 7        | 0.14          |
| (1,1790) | 1:126:A:THR:HA   | 1:126:A:THR:HG23 | 7        | 0.14          |
| (1,1775) | 1:121:A:LEU:HB2  | 1:121:A:LEU:H    | 8        | 0.14          |
| (1,1774) | 1:121:A:LEU:HB3  | 1:121:A:LEU:H    | 5        | 0.14          |
| (1,1640) | 1:111:A:ILE:HG21 | 1:112:A:VAL:H    | 5        | 0.14          |
| (1,1640) | 1:111:A:ILE:HG22 | 1:112:A:VAL:H    | 5        | 0.14          |
| (1,1640) | 1:111:A:ILE:HG23 | 1:112:A:VAL:H    | 5        | 0.14          |
| (1,1510) | 1:98:A:THR:HG21  | 1:100:A:ALA:H    | 6        | 0.14          |
| (1,1510) | 1:98:A:THR:HG22  | 1:100:A:ALA:H    | 6        | 0.14          |
| (1,1510) | 1:98:A:THR:HG23  | 1:100:A:ALA:H    | 6        | 0.14          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1443) | 1:89:A:SER:H    | 1:134:A:TRP:HH2 | 5        | 0.14          |
| (1,1419) | 1:88:A:ASN:HB3  | 1:88:A:ASN:HD21 | 5        | 0.14          |
| (1,1399) | 1:87:A:THR:HG21 | 1:87:A:THR:H    | 4        | 0.14          |
| (1,1399) | 1:87:A:THR:HG22 | 1:87:A:THR:H    | 4        | 0.14          |
| (1,1399) | 1:87:A:THR:HG23 | 1:87:A:THR:H    | 4        | 0.14          |
| (1,1380) | 1:87:A:THR:HA   | 1:134:A:TRP:HH2 | 2        | 0.14          |
| (1,1343) | 1:85:A:TYR:HE1  | 1:152:A:ALA:HA  | 10       | 0.14          |
| (1,1343) | 1:85:A:TYR:HE2  | 1:152:A:ALA:HA  | 10       | 0.14          |
| (1,1335) | 1:85:A:TYR:HB2  | 1:86:A:GLU:H    | 2        | 0.14          |
| (1,1335) | 1:85:A:TYR:HB2  | 1:86:A:GLU:H    | 4        | 0.14          |
| (1,1273) | 1:82:A:THR:HG21 | 1:96:A:SER:HA   | 7        | 0.14          |
| (1,1273) | 1:82:A:THR:HG22 | 1:96:A:SER:HA   | 7        | 0.14          |
| (1,1273) | 1:82:A:THR:HG23 | 1:96:A:SER:HA   | 7        | 0.14          |
| (1,1273) | 1:82:A:THR:HG21 | 1:96:A:SER:HA   | 8        | 0.14          |
| (1,1273) | 1:82:A:THR:HG22 | 1:96:A:SER:HA   | 8        | 0.14          |
| (1,1273) | 1:82:A:THR:HG23 | 1:96:A:SER:HA   | 8        | 0.14          |
| (1,1272) | 1:82:A:THR:HG21 | 1:96:A:SER:HA   | 7        | 0.14          |
| (1,1272) | 1:82:A:THR:HG22 | 1:96:A:SER:HA   | 7        | 0.14          |
| (1,1272) | 1:82:A:THR:HG23 | 1:96:A:SER:HA   | 7        | 0.14          |
| (1,1272) | 1:82:A:THR:HG21 | 1:96:A:SER:HA   | 8        | 0.14          |
| (1,1272) | 1:82:A:THR:HG22 | 1:96:A:SER:HA   | 8        | 0.14          |
| (1,1272) | 1:82:A:THR:HG23 | 1:96:A:SER:HA   | 8        | 0.14          |
| (1,1250) | 1:81:A:ILE:H    | 1:156:A:PHE:HA  | 3        | 0.14          |
| (1,1250) | 1:81:A:ILE:H    | 1:156:A:PHE:HA  | 6        | 0.14          |
| (1,1250) | 1:81:A:ILE:H    | 1:156:A:PHE:HA  | 9        | 0.14          |
| (1,1207) | 1:81:A:ILE:HA   | 1:82:A:THR:H    | 3        | 0.14          |
| (1,1207) | 1:81:A:ILE:HA   | 1:82:A:THR:H    | 7        | 0.14          |
| (1,1207) | 1:81:A:ILE:HA   | 1:82:A:THR:H    | 9        | 0.14          |
| (1,975)  | 1:73:A:TYR:HA   | 1:73:A:TYR:HB3  | 1        | 0.14          |
| (1,975)  | 1:73:A:TYR:HA   | 1:73:A:TYR:HB3  | 7        | 0.14          |
| (1,926)  | 1:70:A:LEU:HD21 | 1:70:A:LEU:H    | 4        | 0.14          |
| (1,926)  | 1:70:A:LEU:HD22 | 1:70:A:LEU:H    | 4        | 0.14          |
| (1,926)  | 1:70:A:LEU:HD23 | 1:70:A:LEU:H    | 4        | 0.14          |
| (1,909)  | 1:69:A:GLN:HB2  | 1:70:A:LEU:H    | 2        | 0.14          |
| (1,886)  | 1:68:A:GLU:HA   | 1:71:A:LYS:HD2  | 10       | 0.14          |
| (1,886)  | 1:68:A:GLU:HA   | 1:71:A:LYS:HD3  | 10       | 0.14          |
| (1,880)  | 1:68:A:GLU:HA   | 1:68:A:GLU:HG3  | 6        | 0.14          |
| (1,863)  | 1:66:A:ASN:H    | 1:175:A:PHE:HA  | 1        | 0.14          |
| (1,779)  | 1:64:A:LEU:HD11 | 1:64:A:LEU:HD21 | 6        | 0.14          |
| (1,779)  | 1:64:A:LEU:HD11 | 1:64:A:LEU:HD22 | 6        | 0.14          |
| (1,779)  | 1:64:A:LEU:HD11 | 1:64:A:LEU:HD23 | 6        | 0.14          |
| (1,779)  | 1:64:A:LEU:HD12 | 1:64:A:LEU:HD21 | 6        | 0.14          |

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| Key     | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,779) | 1:64:A:LEU:HD12 | 1:64:A:LEU:HD22  | 6        | 0.14          |
| (1,779) | 1:64:A:LEU:HD12 | 1:64:A:LEU:HD23  | 6        | 0.14          |
| (1,779) | 1:64:A:LEU:HD13 | 1:64:A:LEU:HD21  | 6        | 0.14          |
| (1,779) | 1:64:A:LEU:HD13 | 1:64:A:LEU:HD22  | 6        | 0.14          |
| (1,779) | 1:64:A:LEU:HD13 | 1:64:A:LEU:HD23  | 6        | 0.14          |
| (1,683) | 1:60:A:LEU:HG   | 1:60:A:LEU:H     | 6        | 0.14          |
| (1,683) | 1:60:A:LEU:HG   | 1:60:A:LEU:H     | 9        | 0.14          |
| (1,597) | 1:53:A:ASP:HB2  | 1:54:A:GLN:H     | 4        | 0.14          |
| (1,597) | 1:53:A:ASP:HB3  | 1:54:A:GLN:H     | 4        | 0.14          |
| (1,579) | 1:51:A:ILE:HG21 | 1:53:A:ASP:HB2   | 2        | 0.14          |
| (1,579) | 1:51:A:ILE:HG21 | 1:53:A:ASP:HB3   | 2        | 0.14          |
| (1,579) | 1:51:A:ILE:HG22 | 1:53:A:ASP:HB2   | 2        | 0.14          |
| (1,579) | 1:51:A:ILE:HG22 | 1:53:A:ASP:HB3   | 2        | 0.14          |
| (1,579) | 1:51:A:ILE:HG23 | 1:53:A:ASP:HB2   | 2        | 0.14          |
| (1,579) | 1:51:A:ILE:HG23 | 1:53:A:ASP:HB3   | 2        | 0.14          |
| (1,554) | 1:50:A:TRP:HD1  | 1:50:A:TRP:H     | 7        | 0.14          |
| (1,529) | 1:49:A:VAL:H    | 1:151:A:VAL:HA   | 3        | 0.14          |
| (1,513) | 1:49:A:VAL:HA   | 1:49:A:VAL:HG11  | 6        | 0.14          |
| (1,513) | 1:49:A:VAL:HA   | 1:49:A:VAL:HG12  | 6        | 0.14          |
| (1,513) | 1:49:A:VAL:HA   | 1:49:A:VAL:HG13  | 6        | 0.14          |
| (1,461) | 1:47:A:ALA:H    | 1:153:A:ILE:HG21 | 5        | 0.14          |
| (1,461) | 1:47:A:ALA:H    | 1:153:A:ILE:HG22 | 5        | 0.14          |
| (1,461) | 1:47:A:ALA:H    | 1:153:A:ILE:HG23 | 5        | 0.14          |
| (1,447) | 1:46:A:TYR:HE1  | 1:141:A:LYS:HG3  | 3        | 0.14          |
| (1,447) | 1:46:A:TYR:HE2  | 1:141:A:LYS:HG3  | 3        | 0.14          |
| (1,436) | 1:46:A:TYR:HB2  | 1:153:A:ILE:HG21 | 9        | 0.14          |
| (1,436) | 1:46:A:TYR:HB2  | 1:153:A:ILE:HG22 | 9        | 0.14          |
| (1,436) | 1:46:A:TYR:HB2  | 1:153:A:ILE:HG23 | 9        | 0.14          |
| (1,426) | 1:46:A:TYR:HA   | 1:156:A:PHE:HA   | 5        | 0.14          |
| (1,337) | 1:41:A:SER:HB2  | 1:42:A:ASP:HA    | 5        | 0.14          |
| (1,337) | 1:41:A:SER:HB2  | 1:42:A:ASP:HA    | 9        | 0.14          |
| (1,268) | 1:34:A:PRO:HD3  | 1:35:A:ALA:H     | 6        | 0.14          |
| (1,256) | 1:33:A:THR:HA   | 1:168:A:PHE:HZ   | 6        | 0.14          |
| (1,230) | 1:32:A:ILE:HG12 | 1:32:A:ILE:H     | 4        | 0.14          |
| (1,230) | 1:32:A:ILE:HG12 | 1:32:A:ILE:H     | 9        | 0.14          |
| (1,227) | 1:32:A:ILE:HG13 | 1:33:A:THR:H     | 8        | 0.14          |
| (1,139) | 1:28:A:HIS:HD2  | 1:46:A:TYR:HE1   | 8        | 0.14          |
| (1,139) | 1:28:A:HIS:HD2  | 1:46:A:TYR:HE2   | 8        | 0.14          |
| (1,92)  | 1:25:A:VAL:H    | 1:50:A:TRP:HE1   | 10       | 0.14          |
| (1,51)  | 1:24:A:ASP:HB2  | 1:25:A:VAL:H     | 4        | 0.14          |
| (1,12)  | 1:21:A:GLU:HA   | 1:21:A:GLU:HG2   | 1        | 0.14          |
| (1,12)  | 1:21:A:GLU:HA   | 1:21:A:GLU:HG3   | 1        | 0.14          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (3,4)    | 1:57:A:ASP:HA    | 1:114:A:ASP:HA   | 5        | 0.13          |
| (2,761)  | 1:168:A:PHE:H    | 1:169:A:ASP:H    | 2        | 0.13          |
| (2,760)  | 1:168:A:PHE:HE1  | 1:171:A:LEU:HG   | 6        | 0.13          |
| (2,760)  | 1:168:A:PHE:HE2  | 1:171:A:LEU:HG   | 6        | 0.13          |
| (2,731)  | 1:155:A:ASN:H    | 1:156:A:PHE:HD1  | 4        | 0.13          |
| (2,731)  | 1:155:A:ASN:H    | 1:156:A:PHE:HD2  | 4        | 0.13          |
| (2,625)  | 1:121:A:LEU:H    | 1:122:A:TYR:HD1  | 8        | 0.13          |
| (2,625)  | 1:121:A:LEU:H    | 1:122:A:TYR:HD2  | 8        | 0.13          |
| (2,574)  | 1:92:A:LEU:H     | 1:94:A:ASN:H     | 7        | 0.13          |
| (2,383)  | 1:70:A:LEU:HA    | 1:74:A:PHE:HD1   | 2        | 0.13          |
| (2,383)  | 1:70:A:LEU:HA    | 1:74:A:PHE:HD2   | 2        | 0.13          |
| (2,298)  | 1:54:A:GLN:HB3   | 1:54:A:GLN:HE21  | 10       | 0.13          |
| (1,2313) | 1:171:A:LEU:HA   | 1:171:A:LEU:HD11 | 7        | 0.13          |
| (1,2313) | 1:171:A:LEU:HA   | 1:171:A:LEU:HD12 | 7        | 0.13          |
| (1,2313) | 1:171:A:LEU:HA   | 1:171:A:LEU:HD13 | 7        | 0.13          |
| (1,2271) | 1:166:A:MET:HB3  | 1:167:A:LEU:H    | 6        | 0.13          |
| (1,2270) | 1:166:A:MET:HA   | 1:167:A:LEU:H    | 1        | 0.13          |
| (1,2270) | 1:166:A:MET:HA   | 1:167:A:LEU:H    | 6        | 0.13          |
| (1,2260) | 1:163:A:LYS:H    | 1:168:A:PHE:HZ   | 8        | 0.13          |
| (1,2258) | 1:163:A:LYS:HG2  | 1:163:A:LYS:H    | 3        | 0.13          |
| (1,2207) | 1:159:A:PHE:HB2  | 1:159:A:PHE:H    | 2        | 0.13          |
| (1,2191) | 1:158:A:ALA:HB1  | 1:160:A:TYR:HE1  | 4        | 0.13          |
| (1,2191) | 1:158:A:ALA:HB1  | 1:160:A:TYR:HE2  | 4        | 0.13          |
| (1,2191) | 1:158:A:ALA:HB2  | 1:160:A:TYR:HE1  | 4        | 0.13          |
| (1,2191) | 1:158:A:ALA:HB2  | 1:160:A:TYR:HE2  | 4        | 0.13          |
| (1,2191) | 1:158:A:ALA:HB3  | 1:160:A:TYR:HE1  | 4        | 0.13          |
| (1,2191) | 1:158:A:ALA:HB3  | 1:160:A:TYR:HE2  | 4        | 0.13          |
| (1,2139) | 1:155:A:ASN:H    | 1:156:A:PHE:HZ   | 3        | 0.13          |
| (1,2139) | 1:155:A:ASN:H    | 1:156:A:PHE:HZ   | 4        | 0.13          |
| (1,2028) | 1:143:A:ILE:HD11 | 1:143:A:ILE:H    | 9        | 0.13          |
| (1,2028) | 1:143:A:ILE:HD12 | 1:143:A:ILE:H    | 9        | 0.13          |
| (1,2028) | 1:143:A:ILE:HD13 | 1:143:A:ILE:H    | 9        | 0.13          |
| (1,2015) | 1:142:A:ILE:HG21 | 1:144:A:VAL:H    | 1        | 0.13          |
| (1,2015) | 1:142:A:ILE:HG22 | 1:144:A:VAL:H    | 1        | 0.13          |
| (1,2015) | 1:142:A:ILE:HG23 | 1:144:A:VAL:H    | 1        | 0.13          |
| (1,2015) | 1:142:A:ILE:HG21 | 1:144:A:VAL:H    | 10       | 0.13          |
| (1,2015) | 1:142:A:ILE:HG22 | 1:144:A:VAL:H    | 10       | 0.13          |
| (1,2015) | 1:142:A:ILE:HG23 | 1:144:A:VAL:H    | 10       | 0.13          |
| (1,2013) | 1:142:A:ILE:HG21 | 1:143:A:ILE:H    | 1        | 0.13          |
| (1,2013) | 1:142:A:ILE:HG22 | 1:143:A:ILE:H    | 1        | 0.13          |
| (1,2013) | 1:142:A:ILE:HG23 | 1:143:A:ILE:H    | 1        | 0.13          |
| (1,1953) | 1:136:A:PRO:HG3  | 1:155:A:ASN:HD21 | 2        | 0.13          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1953) | 1:136:A:PRO:HG3  | 1:155:A:ASN:HD22 | 2        | 0.13          |
| (1,1880) | 1:134:A:TRP:HA   | 1:142:A:ILE:HG21 | 5        | 0.13          |
| (1,1880) | 1:134:A:TRP:HA   | 1:142:A:ILE:HG22 | 5        | 0.13          |
| (1,1880) | 1:134:A:TRP:HA   | 1:142:A:ILE:HG23 | 5        | 0.13          |
| (1,1859) | 1:133:A:ILE:HD11 | 1:144:A:VAL:HB   | 4        | 0.13          |
| (1,1859) | 1:133:A:ILE:HD12 | 1:144:A:VAL:HB   | 4        | 0.13          |
| (1,1859) | 1:133:A:ILE:HD13 | 1:144:A:VAL:HB   | 4        | 0.13          |
| (1,1826) | 1:132:A:SER:HA   | 1:133:A:ILE:HB   | 2        | 0.13          |
| (1,1826) | 1:132:A:SER:HA   | 1:133:A:ILE:HB   | 9        | 0.13          |
| (1,1818) | 1:131:A:THR:HG21 | 1:131:A:THR:H    | 6        | 0.13          |
| (1,1818) | 1:131:A:THR:HG22 | 1:131:A:THR:H    | 6        | 0.13          |
| (1,1818) | 1:131:A:THR:HG23 | 1:131:A:THR:H    | 6        | 0.13          |
| (1,1818) | 1:131:A:THR:HG21 | 1:131:A:THR:H    | 8        | 0.13          |
| (1,1818) | 1:131:A:THR:HG22 | 1:131:A:THR:H    | 8        | 0.13          |
| (1,1818) | 1:131:A:THR:HG23 | 1:131:A:THR:H    | 8        | 0.13          |
| (1,1799) | 1:128:A:TYR:HD1  | 1:128:A:TYR:H    | 5        | 0.13          |
| (1,1799) | 1:128:A:TYR:HD2  | 1:128:A:TYR:H    | 5        | 0.13          |
| (1,1723) | 1:116:A:GLU:HG2  | 1:116:A:GLU:H    | 8        | 0.13          |
| (1,1723) | 1:116:A:GLU:HG3  | 1:116:A:GLU:H    | 8        | 0.13          |
| (1,1702) | 1:115:A:LYS:HB2  | 1:116:A:GLU:H    | 5        | 0.13          |
| (1,1690) | 1:115:A:LYS:HA   | 1:115:A:LYS:HG2  | 7        | 0.13          |
| (1,1690) | 1:115:A:LYS:HA   | 1:115:A:LYS:HG3  | 7        | 0.13          |
| (1,1640) | 1:111:A:ILE:HG21 | 1:112:A:VAL:H    | 10       | 0.13          |
| (1,1640) | 1:111:A:ILE:HG22 | 1:112:A:VAL:H    | 10       | 0.13          |
| (1,1640) | 1:111:A:ILE:HG23 | 1:112:A:VAL:H    | 10       | 0.13          |
| (1,1532) | 1:102:A:ILE:HB   | 1:102:A:ILE:H    | 3        | 0.13          |
| (1,1505) | 1:98:A:THR:HA    | 1:100:A:ALA:H    | 1        | 0.13          |
| (1,1474) | 1:95:A:PHE:HB2   | 1:95:A:PHE:H     | 7        | 0.13          |
| (1,1474) | 1:95:A:PHE:HB3   | 1:95:A:PHE:H     | 7        | 0.13          |
| (1,1446) | 1:90:A:THR:HA    | 1:93:A:GLY:H     | 2        | 0.13          |
| (1,1439) | 1:88:A:ASN:H     | 1:134:A:TRP:HZ3  | 5        | 0.13          |
| (1,1380) | 1:87:A:THR:HA    | 1:134:A:TRP:HH2  | 5        | 0.13          |
| (1,1379) | 1:87:A:THR:HA    | 1:134:A:TRP:HE3  | 5        | 0.13          |
| (1,1379) | 1:87:A:THR:HA    | 1:134:A:TRP:HE3  | 8        | 0.13          |
| (1,1371) | 1:86:A:GLU:H     | 1:134:A:TRP:HE1  | 3        | 0.13          |
| (1,1371) | 1:86:A:GLU:H     | 1:134:A:TRP:HE1  | 4        | 0.13          |
| (1,1371) | 1:86:A:GLU:H     | 1:134:A:TRP:HE1  | 10       | 0.13          |
| (1,1369) | 1:86:A:GLU:H     | 1:133:A:ILE:HG21 | 1        | 0.13          |
| (1,1369) | 1:86:A:GLU:H     | 1:133:A:ILE:HG22 | 1        | 0.13          |
| (1,1369) | 1:86:A:GLU:H     | 1:133:A:ILE:HG23 | 1        | 0.13          |
| (1,1363) | 1:86:A:GLU:HG3   | 1:86:A:GLU:H     | 3        | 0.13          |
| (1,1363) | 1:86:A:GLU:HG3   | 1:86:A:GLU:H     | 6        | 0.13          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1343) | 1:85:A:TYR:HE1  | 1:152:A:ALA:HA  | 3        | 0.13          |
| (1,1343) | 1:85:A:TYR:HE2  | 1:152:A:ALA:HA  | 3        | 0.13          |
| (1,1333) | 1:85:A:TYR:HA   | 1:86:A:GLU:H    | 4        | 0.13          |
| (1,1250) | 1:81:A:ILE:H    | 1:156:A:PHE:HA  | 4        | 0.13          |
| (1,1241) | 1:81:A:ILE:HG21 | 1:156:A:PHE:HD1 | 2        | 0.13          |
| (1,1241) | 1:81:A:ILE:HG21 | 1:156:A:PHE:HD2 | 2        | 0.13          |
| (1,1241) | 1:81:A:ILE:HG22 | 1:156:A:PHE:HD1 | 2        | 0.13          |
| (1,1241) | 1:81:A:ILE:HG22 | 1:156:A:PHE:HD2 | 2        | 0.13          |
| (1,1241) | 1:81:A:ILE:HG23 | 1:156:A:PHE:HD1 | 2        | 0.13          |
| (1,1241) | 1:81:A:ILE:HG23 | 1:156:A:PHE:HD2 | 2        | 0.13          |
| (1,1241) | 1:81:A:ILE:HG21 | 1:156:A:PHE:HD1 | 4        | 0.13          |
| (1,1241) | 1:81:A:ILE:HG21 | 1:156:A:PHE:HD2 | 4        | 0.13          |
| (1,1241) | 1:81:A:ILE:HG22 | 1:156:A:PHE:HD1 | 4        | 0.13          |
| (1,1241) | 1:81:A:ILE:HG22 | 1:156:A:PHE:HD2 | 4        | 0.13          |
| (1,1241) | 1:81:A:ILE:HG23 | 1:156:A:PHE:HD1 | 4        | 0.13          |
| (1,1241) | 1:81:A:ILE:HG23 | 1:156:A:PHE:HD2 | 4        | 0.13          |
| (1,1216) | 1:81:A:ILE:HD11 | 1:100:A:ALA:H   | 8        | 0.13          |
| (1,1216) | 1:81:A:ILE:HD12 | 1:100:A:ALA:H   | 8        | 0.13          |
| (1,1216) | 1:81:A:ILE:HD13 | 1:100:A:ALA:H   | 8        | 0.13          |
| (1,1216) | 1:81:A:ILE:HD11 | 1:100:A:ALA:H   | 10       | 0.13          |
| (1,1216) | 1:81:A:ILE:HD12 | 1:100:A:ALA:H   | 10       | 0.13          |
| (1,1216) | 1:81:A:ILE:HD13 | 1:100:A:ALA:H   | 10       | 0.13          |
| (1,1215) | 1:81:A:ILE:HD11 | 1:100:A:ALA:HB1 | 5        | 0.13          |
| (1,1215) | 1:81:A:ILE:HD11 | 1:100:A:ALA:HB2 | 5        | 0.13          |
| (1,1215) | 1:81:A:ILE:HD11 | 1:100:A:ALA:HB3 | 5        | 0.13          |
| (1,1215) | 1:81:A:ILE:HD12 | 1:100:A:ALA:HB1 | 5        | 0.13          |
| (1,1215) | 1:81:A:ILE:HD12 | 1:100:A:ALA:HB2 | 5        | 0.13          |
| (1,1215) | 1:81:A:ILE:HD12 | 1:100:A:ALA:HB3 | 5        | 0.13          |
| (1,1215) | 1:81:A:ILE:HD13 | 1:100:A:ALA:HB1 | 5        | 0.13          |
| (1,1215) | 1:81:A:ILE:HD13 | 1:100:A:ALA:HB2 | 5        | 0.13          |
| (1,1215) | 1:81:A:ILE:HD13 | 1:100:A:ALA:HB3 | 5        | 0.13          |
| (1,1207) | 1:81:A:ILE:HA   | 1:82:A:THR:H    | 4        | 0.13          |
| (1,1207) | 1:81:A:ILE:HA   | 1:82:A:THR:H    | 5        | 0.13          |
| (1,1207) | 1:81:A:ILE:HA   | 1:82:A:THR:H    | 6        | 0.13          |
| (1,1207) | 1:81:A:ILE:HA   | 1:82:A:THR:H    | 8        | 0.13          |
| (1,1207) | 1:81:A:ILE:HA   | 1:82:A:THR:H    | 10       | 0.13          |
| (1,1169) | 1:79:A:ILE:HG21 | 1:79:A:ILE:HD11 | 8        | 0.13          |
| (1,1169) | 1:79:A:ILE:HG21 | 1:79:A:ILE:HD12 | 8        | 0.13          |
| (1,1169) | 1:79:A:ILE:HG21 | 1:79:A:ILE:HD13 | 8        | 0.13          |
| (1,1169) | 1:79:A:ILE:HG22 | 1:79:A:ILE:HD11 | 8        | 0.13          |
| (1,1169) | 1:79:A:ILE:HG22 | 1:79:A:ILE:HD12 | 8        | 0.13          |
| (1,1169) | 1:79:A:ILE:HG22 | 1:79:A:ILE:HD13 | 8        | 0.13          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1169) | 1:79:A:ILE:HG23 | 1:79:A:ILE:HD11  | 8        | 0.13          |
| (1,1169) | 1:79:A:ILE:HG23 | 1:79:A:ILE:HD12  | 8        | 0.13          |
| (1,1169) | 1:79:A:ILE:HG23 | 1:79:A:ILE:HD13  | 8        | 0.13          |
| (1,1127) | 1:78:A:GLN:H    | 1:104:A:LEU:H    | 2        | 0.13          |
| (1,1127) | 1:78:A:GLN:H    | 1:104:A:LEU:H    | 4        | 0.13          |
| (1,1127) | 1:78:A:GLN:H    | 1:104:A:LEU:H    | 10       | 0.13          |
| (1,1006) | 1:74:A:PHE:HA   | 1:163:A:LYS:H    | 2        | 0.13          |
| (1,975)  | 1:73:A:TYR:HA   | 1:73:A:TYR:HB3   | 2        | 0.13          |
| (1,922)  | 1:70:A:LEU:HD11 | 1:70:A:LEU:H     | 2        | 0.13          |
| (1,922)  | 1:70:A:LEU:HD12 | 1:70:A:LEU:H     | 2        | 0.13          |
| (1,922)  | 1:70:A:LEU:HD13 | 1:70:A:LEU:H     | 2        | 0.13          |
| (1,894)  | 1:68:A:GLU:H    | 1:69:A:GLN:H     | 1        | 0.13          |
| (1,857)  | 1:66:A:ASN:HD22 | 1:174:A:ILE:H    | 5        | 0.13          |
| (1,857)  | 1:66:A:ASN:HD22 | 1:174:A:ILE:H    | 6        | 0.13          |
| (1,834)  | 1:66:A:ASN:HB3  | 1:66:A:ASN:H     | 3        | 0.13          |
| (1,834)  | 1:66:A:ASN:HB3  | 1:66:A:ASN:H     | 4        | 0.13          |
| (1,834)  | 1:66:A:ASN:HB3  | 1:66:A:ASN:H     | 10       | 0.13          |
| (1,831)  | 1:66:A:ASN:HA   | 1:174:A:ILE:HB   | 4        | 0.13          |
| (1,831)  | 1:66:A:ASN:HA   | 1:174:A:ILE:HB   | 5        | 0.13          |
| (1,795)  | 1:64:A:LEU:HG   | 1:67:A:ALA:HA    | 10       | 0.13          |
| (1,761)  | 1:63:A:THR:H    | 1:175:A:PHE:HA   | 1        | 0.13          |
| (1,643)  | 1:57:A:ASP:HB2  | 1:115:A:LYS:H    | 9        | 0.13          |
| (1,623)  | 1:55:A:VAL:H    | 1:115:A:LYS:HA   | 1        | 0.13          |
| (1,554)  | 1:50:A:TRP:HD1  | 1:50:A:TRP:H     | 1        | 0.13          |
| (1,553)  | 1:50:A:TRP:HB2  | 1:52:A:LYS:H     | 4        | 0.13          |
| (1,553)  | 1:50:A:TRP:HB2  | 1:52:A:LYS:H     | 6        | 0.13          |
| (1,548)  | 1:50:A:TRP:HB3  | 1:50:A:TRP:H     | 4        | 0.13          |
| (1,548)  | 1:50:A:TRP:HB3  | 1:50:A:TRP:H     | 7        | 0.13          |
| (1,513)  | 1:49:A:VAL:HA   | 1:49:A:VAL:HG11  | 5        | 0.13          |
| (1,513)  | 1:49:A:VAL:HA   | 1:49:A:VAL:HG12  | 5        | 0.13          |
| (1,513)  | 1:49:A:VAL:HA   | 1:49:A:VAL:HG13  | 5        | 0.13          |
| (1,503)  | 1:48:A:ILE:HG21 | 1:143:A:ILE:HG21 | 10       | 0.13          |
| (1,503)  | 1:48:A:ILE:HG21 | 1:143:A:ILE:HG22 | 10       | 0.13          |
| (1,503)  | 1:48:A:ILE:HG21 | 1:143:A:ILE:HG23 | 10       | 0.13          |
| (1,503)  | 1:48:A:ILE:HG22 | 1:143:A:ILE:HG21 | 10       | 0.13          |
| (1,503)  | 1:48:A:ILE:HG22 | 1:143:A:ILE:HG22 | 10       | 0.13          |
| (1,503)  | 1:48:A:ILE:HG22 | 1:143:A:ILE:HG23 | 10       | 0.13          |
| (1,503)  | 1:48:A:ILE:HG23 | 1:143:A:ILE:HG21 | 10       | 0.13          |
| (1,503)  | 1:48:A:ILE:HG23 | 1:143:A:ILE:HG22 | 10       | 0.13          |
| (1,503)  | 1:48:A:ILE:HG23 | 1:143:A:ILE:HG23 | 10       | 0.13          |
| (1,480)  | 1:48:A:ILE:HB   | 1:50:A:TRP:HE1   | 5        | 0.13          |
| (1,436)  | 1:46:A:TYR:HB2  | 1:153:A:ILE:HG21 | 2        | 0.13          |

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| Key     | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,436) | 1:46:A:TYR:HB2  | 1:153:A:ILE:HG22 | 2        | 0.13          |
| (1,436) | 1:46:A:TYR:HB2  | 1:153:A:ILE:HG23 | 2        | 0.13          |
| (1,432) | 1:46:A:TYR:HB3  | 1:154:A:LEU:H    | 1        | 0.13          |
| (1,426) | 1:46:A:TYR:HA   | 1:156:A:PHE:HA   | 6        | 0.13          |
| (1,426) | 1:46:A:TYR:HA   | 1:156:A:PHE:HA   | 7        | 0.13          |
| (1,424) | 1:46:A:TYR:HA   | 1:155:A:ASN:HB2  | 3        | 0.13          |
| (1,259) | 1:33:A:THR:HB   | 1:35:A:ALA:H     | 5        | 0.13          |
| (1,259) | 1:33:A:THR:HB   | 1:35:A:ALA:H     | 6        | 0.13          |
| (1,240) | 1:32:A:ILE:HG21 | 1:74:A:PHE:HE1   | 5        | 0.13          |
| (1,240) | 1:32:A:ILE:HG21 | 1:74:A:PHE:HE2   | 5        | 0.13          |
| (1,240) | 1:32:A:ILE:HG22 | 1:74:A:PHE:HE1   | 5        | 0.13          |
| (1,240) | 1:32:A:ILE:HG22 | 1:74:A:PHE:HE2   | 5        | 0.13          |
| (1,240) | 1:32:A:ILE:HG23 | 1:74:A:PHE:HE1   | 5        | 0.13          |
| (1,240) | 1:32:A:ILE:HG23 | 1:74:A:PHE:HE2   | 5        | 0.13          |
| (1,235) | 1:32:A:ILE:HG21 | 1:33:A:THR:H     | 2        | 0.13          |
| (1,235) | 1:32:A:ILE:HG22 | 1:33:A:THR:H     | 2        | 0.13          |
| (1,235) | 1:32:A:ILE:HG23 | 1:33:A:THR:H     | 2        | 0.13          |
| (1,230) | 1:32:A:ILE:HG12 | 1:32:A:ILE:H     | 2        | 0.13          |
| (1,230) | 1:32:A:ILE:HG12 | 1:32:A:ILE:H     | 3        | 0.13          |
| (1,230) | 1:32:A:ILE:HG12 | 1:32:A:ILE:H     | 7        | 0.13          |
| (1,230) | 1:32:A:ILE:HG12 | 1:32:A:ILE:H     | 10       | 0.13          |
| (1,227) | 1:32:A:ILE:HG13 | 1:33:A:THR:H     | 2        | 0.13          |
| (1,227) | 1:32:A:ILE:HG13 | 1:33:A:THR:H     | 5        | 0.13          |
| (1,220) | 1:32:A:ILE:HD11 | 1:158:A:ALA:HB1  | 9        | 0.13          |
| (1,220) | 1:32:A:ILE:HD11 | 1:158:A:ALA:HB2  | 9        | 0.13          |
| (1,220) | 1:32:A:ILE:HD11 | 1:158:A:ALA:HB3  | 9        | 0.13          |
| (1,220) | 1:32:A:ILE:HD12 | 1:158:A:ALA:HB1  | 9        | 0.13          |
| (1,220) | 1:32:A:ILE:HD12 | 1:158:A:ALA:HB2  | 9        | 0.13          |
| (1,220) | 1:32:A:ILE:HD12 | 1:158:A:ALA:HB3  | 9        | 0.13          |
| (1,220) | 1:32:A:ILE:HD13 | 1:158:A:ALA:HB1  | 9        | 0.13          |
| (1,220) | 1:32:A:ILE:HD13 | 1:158:A:ALA:HB2  | 9        | 0.13          |
| (1,220) | 1:32:A:ILE:HD13 | 1:158:A:ALA:HB3  | 9        | 0.13          |
| (1,51)  | 1:24:A:ASP:HB2  | 1:25:A:VAL:H     | 7        | 0.13          |
| (1,32)  | 1:23:A:ILE:HG12 | 1:23:A:ILE:H     | 10       | 0.13          |
| (1,25)  | 1:23:A:ILE:HA   | 1:23:A:ILE:HG21  | 4        | 0.13          |
| (1,25)  | 1:23:A:ILE:HA   | 1:23:A:ILE:HG22  | 4        | 0.13          |
| (1,25)  | 1:23:A:ILE:HA   | 1:23:A:ILE:HG23  | 4        | 0.13          |
| (1,12)  | 1:21:A:GLU:HA   | 1:21:A:GLU:HG2   | 6        | 0.13          |
| (1,12)  | 1:21:A:GLU:HA   | 1:21:A:GLU:HG3   | 6        | 0.13          |
| (1,12)  | 1:21:A:GLU:HA   | 1:21:A:GLU:HG2   | 9        | 0.13          |
| (1,12)  | 1:21:A:GLU:HA   | 1:21:A:GLU:HG3   | 9        | 0.13          |
| (4,21)  | 1:59:A:LYS:O    | 1:180:A:LEU:H    | 5        | 0.12          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (3,2)    | 1:33:A:THR:HA    | 1:34:A:PRO:HD3   | 8        | 0.12          |
| (2,761)  | 1:168:A:PHE:H    | 1:169:A:ASP:H    | 5        | 0.12          |
| (2,761)  | 1:168:A:PHE:H    | 1:169:A:ASP:H    | 8        | 0.12          |
| (2,732)  | 1:155:A:ASN:H    | 1:156:A:PHE:HE1  | 8        | 0.12          |
| (2,732)  | 1:155:A:ASN:H    | 1:156:A:PHE:HE2  | 8        | 0.12          |
| (2,718)  | 1:142:A:ILE:HD11 | 1:145:A:TYR:HE1  | 10       | 0.12          |
| (2,718)  | 1:142:A:ILE:HD11 | 1:145:A:TYR:HE2  | 10       | 0.12          |
| (2,718)  | 1:142:A:ILE:HD12 | 1:145:A:TYR:HE1  | 10       | 0.12          |
| (2,718)  | 1:142:A:ILE:HD12 | 1:145:A:TYR:HE2  | 10       | 0.12          |
| (2,718)  | 1:142:A:ILE:HD13 | 1:145:A:TYR:HE1  | 10       | 0.12          |
| (2,718)  | 1:142:A:ILE:HD13 | 1:145:A:TYR:HE2  | 10       | 0.12          |
| (2,592)  | 1:114:A:ASP:HB3  | 1:116:A:GLU:HG2  | 5        | 0.12          |
| (2,592)  | 1:114:A:ASP:HB3  | 1:116:A:GLU:HG3  | 5        | 0.12          |
| (2,592)  | 1:114:A:ASP:HB3  | 1:116:A:GLU:HG2  | 8        | 0.12          |
| (2,592)  | 1:114:A:ASP:HB3  | 1:116:A:GLU:HG3  | 8        | 0.12          |
| (2,443)  | 1:76:A:TYR:HE1   | 1:78:A:GLN:HE22  | 4        | 0.12          |
| (2,443)  | 1:76:A:TYR:HE2   | 1:78:A:GLN:HE22  | 4        | 0.12          |
| (2,425)  | 1:74:A:PHE:HZ    | 1:160:A:TYR:HE1  | 3        | 0.12          |
| (2,425)  | 1:74:A:PHE:HZ    | 1:160:A:TYR:HE2  | 3        | 0.12          |
| (2,178)  | 1:36:A:ALA:H     | 1:37:A:GLY:H     | 1        | 0.12          |
| (2,94)   | 1:23:A:ILE:HD11  | 1:53:A:ASP:H     | 1        | 0.12          |
| (2,94)   | 1:23:A:ILE:HD12  | 1:53:A:ASP:H     | 1        | 0.12          |
| (2,94)   | 1:23:A:ILE:HD13  | 1:53:A:ASP:H     | 1        | 0.12          |
| (2,27)   | 1:19:A:VAL:H     | 1:20:A:SER:H     | 4        | 0.12          |
| (2,26)   | 1:19:A:VAL:H     | 1:20:A:SER:HB2   | 5        | 0.12          |
| (2,26)   | 1:19:A:VAL:H     | 1:20:A:SER:HB3   | 5        | 0.12          |
| (2,26)   | 1:19:A:VAL:H     | 1:20:A:SER:HB2   | 7        | 0.12          |
| (2,26)   | 1:19:A:VAL:H     | 1:20:A:SER:HB3   | 7        | 0.12          |
| (1,2270) | 1:166:A:MET:HA   | 1:167:A:LEU:H    | 10       | 0.12          |
| (1,2207) | 1:159:A:PHE:HB2  | 1:159:A:PHE:H    | 6        | 0.12          |
| (1,2183) | 1:158:A:ALA:HA   | 1:159:A:PHE:HB3  | 4        | 0.12          |
| (1,2106) | 1:153:A:ILE:HG21 | 1:155:A:ASN:HD21 | 9        | 0.12          |
| (1,2106) | 1:153:A:ILE:HG21 | 1:155:A:ASN:HD22 | 9        | 0.12          |
| (1,2106) | 1:153:A:ILE:HG22 | 1:155:A:ASN:HD21 | 9        | 0.12          |
| (1,2106) | 1:153:A:ILE:HG22 | 1:155:A:ASN:HD22 | 9        | 0.12          |
| (1,2106) | 1:153:A:ILE:HG23 | 1:155:A:ASN:HD21 | 9        | 0.12          |
| (1,2106) | 1:153:A:ILE:HG23 | 1:155:A:ASN:HD22 | 9        | 0.12          |
| (1,2079) | 1:151:A:VAL:HG11 | 1:151:A:VAL:H    | 7        | 0.12          |
| (1,2079) | 1:151:A:VAL:HG12 | 1:151:A:VAL:H    | 7        | 0.12          |
| (1,2079) | 1:151:A:VAL:HG13 | 1:151:A:VAL:H    | 7        | 0.12          |
| (1,2054) | 1:145:A:TYR:HD1  | 1:146:A:ASN:H    | 10       | 0.12          |
| (1,2054) | 1:145:A:TYR:HD2  | 1:146:A:ASN:H    | 10       | 0.12          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1923) | 1:134:A:TRP:HE1  | 1:139:A:PRO:HD2  | 4        | 0.12          |
| (1,1923) | 1:134:A:TRP:HE1  | 1:139:A:PRO:HD2  | 5        | 0.12          |
| (1,1894) | 1:134:A:TRP:HB3  | 1:142:A:ILE:HA   | 10       | 0.12          |
| (1,1826) | 1:132:A:SER:HA   | 1:133:A:ILE:HB   | 3        | 0.12          |
| (1,1826) | 1:132:A:SER:HA   | 1:133:A:ILE:HB   | 5        | 0.12          |
| (1,1826) | 1:132:A:SER:HA   | 1:133:A:ILE:HB   | 6        | 0.12          |
| (1,1817) | 1:131:A:THR:HB   | 1:132:A:SER:H    | 3        | 0.12          |
| (1,1817) | 1:131:A:THR:HB   | 1:132:A:SER:H    | 10       | 0.12          |
| (1,1794) | 1:128:A:TYR:HA   | 1:128:A:TYR:HB2  | 3        | 0.12          |
| (1,1787) | 1:123:A:PRO:HD2  | 1:124:A:ASP:H    | 2        | 0.12          |
| (1,1778) | 1:121:A:LEU:HG   | 1:121:A:LEU:H    | 4        | 0.12          |
| (1,1778) | 1:121:A:LEU:HG   | 1:121:A:LEU:H    | 6        | 0.12          |
| (1,1777) | 1:121:A:LEU:HD21 | 1:121:A:LEU:H    | 7        | 0.12          |
| (1,1777) | 1:121:A:LEU:HD22 | 1:121:A:LEU:H    | 7        | 0.12          |
| (1,1777) | 1:121:A:LEU:HD23 | 1:121:A:LEU:H    | 7        | 0.12          |
| (1,1723) | 1:116:A:GLU:HG2  | 1:116:A:GLU:H    | 4        | 0.12          |
| (1,1723) | 1:116:A:GLU:HG3  | 1:116:A:GLU:H    | 4        | 0.12          |
| (1,1723) | 1:116:A:GLU:HG2  | 1:116:A:GLU:H    | 9        | 0.12          |
| (1,1723) | 1:116:A:GLU:HG3  | 1:116:A:GLU:H    | 9        | 0.12          |
| (1,1681) | 1:114:A:ASP:HB2  | 1:116:A:GLU:H    | 6        | 0.12          |
| (1,1677) | 1:114:A:ASP:HA   | 1:118:A:ILE:H    | 4        | 0.12          |
| (1,1653) | 1:113:A:LEU:HA   | 1:113:A:LEU:HD21 | 5        | 0.12          |
| (1,1653) | 1:113:A:LEU:HA   | 1:113:A:LEU:HD22 | 5        | 0.12          |
| (1,1653) | 1:113:A:LEU:HA   | 1:113:A:LEU:HD23 | 5        | 0.12          |
| (1,1629) | 1:110:A:VAL:HG11 | 1:111:A:ILE:H    | 1        | 0.12          |
| (1,1629) | 1:110:A:VAL:HG12 | 1:111:A:ILE:H    | 1        | 0.12          |
| (1,1629) | 1:110:A:VAL:HG13 | 1:111:A:ILE:H    | 1        | 0.12          |
| (1,1574) | 1:104:A:LEU:HG   | 1:104:A:LEU:H    | 7        | 0.12          |
| (1,1532) | 1:102:A:ILE:HB   | 1:102:A:ILE:H    | 8        | 0.12          |
| (1,1532) | 1:102:A:ILE:HB   | 1:102:A:ILE:H    | 10       | 0.12          |
| (1,1505) | 1:98:A:THR:HA    | 1:100:A:ALA:H    | 10       | 0.12          |
| (1,1432) | 1:88:A:ASN:H     | 1:89:A:SER:H     | 9        | 0.12          |
| (1,1422) | 1:88:A:ASN:HB2   | 1:88:A:ASN:HD21  | 6        | 0.12          |
| (1,1422) | 1:88:A:ASN:HB2   | 1:88:A:ASN:HD21  | 10       | 0.12          |
| (1,1379) | 1:87:A:THR:HA    | 1:134:A:TRP:HE3  | 9        | 0.12          |
| (1,1371) | 1:86:A:GLU:H     | 1:134:A:TRP:HE1  | 8        | 0.12          |
| (1,1333) | 1:85:A:TYR:HA    | 1:86:A:GLU:H     | 8        | 0.12          |
| (1,1317) | 1:83:A:SER:H     | 1:99:A:LYS:H     | 2        | 0.12          |
| (1,1282) | 1:82:A:THR:H     | 1:155:A:ASN:HB3  | 8        | 0.12          |
| (1,1282) | 1:82:A:THR:H     | 1:155:A:ASN:HB3  | 10       | 0.12          |
| (1,1271) | 1:82:A:THR:HG21  | 1:83:A:SER:H     | 9        | 0.12          |
| (1,1271) | 1:82:A:THR:HG22  | 1:83:A:SER:H     | 9        | 0.12          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1271) | 1:82:A:THR:HG23 | 1:83:A:SER:H     | 9        | 0.12          |
| (1,1250) | 1:81:A:ILE:H    | 1:156:A:PHE:HA   | 8        | 0.12          |
| (1,1250) | 1:81:A:ILE:H    | 1:156:A:PHE:HA   | 10       | 0.12          |
| (1,1241) | 1:81:A:ILE:HG21 | 1:156:A:PHE:HD1  | 8        | 0.12          |
| (1,1241) | 1:81:A:ILE:HG21 | 1:156:A:PHE:HD2  | 8        | 0.12          |
| (1,1241) | 1:81:A:ILE:HG22 | 1:156:A:PHE:HD1  | 8        | 0.12          |
| (1,1241) | 1:81:A:ILE:HG22 | 1:156:A:PHE:HD2  | 8        | 0.12          |
| (1,1241) | 1:81:A:ILE:HG23 | 1:156:A:PHE:HD1  | 8        | 0.12          |
| (1,1241) | 1:81:A:ILE:HG23 | 1:156:A:PHE:HD2  | 8        | 0.12          |
| (1,1207) | 1:81:A:ILE:HA   | 1:82:A:THR:H     | 1        | 0.12          |
| (1,1086) | 1:77:A:LEU:HB2  | 1:78:A:GLN:H     | 5        | 0.12          |
| (1,1086) | 1:77:A:LEU:HB2  | 1:78:A:GLN:H     | 6        | 0.12          |
| (1,1055) | 1:76:A:TYR:HB3  | 1:77:A:LEU:H     | 10       | 0.12          |
| (1,1004) | 1:74:A:PHE:HA   | 1:162:A:ALA:HA   | 4        | 0.12          |
| (1,975)  | 1:73:A:TYR:HA   | 1:73:A:TYR:HB3   | 3        | 0.12          |
| (1,975)  | 1:73:A:TYR:HA   | 1:73:A:TYR:HB3   | 4        | 0.12          |
| (1,975)  | 1:73:A:TYR:HA   | 1:73:A:TYR:HB3   | 5        | 0.12          |
| (1,975)  | 1:73:A:TYR:HA   | 1:73:A:TYR:HB3   | 9        | 0.12          |
| (1,914)  | 1:69:A:GLN:HG3  | 1:69:A:GLN:H     | 10       | 0.12          |
| (1,881)  | 1:68:A:GLU:HA   | 1:68:A:GLU:HG2   | 1        | 0.12          |
| (1,863)  | 1:66:A:ASN:H    | 1:175:A:PHE:HA   | 9        | 0.12          |
| (1,795)  | 1:64:A:LEU:HG   | 1:67:A:ALA:HA    | 2        | 0.12          |
| (1,795)  | 1:64:A:LEU:HG   | 1:67:A:ALA:HA    | 6        | 0.12          |
| (1,761)  | 1:63:A:THR:H    | 1:175:A:PHE:HA   | 2        | 0.12          |
| (1,735)  | 1:62:A:VAL:H    | 1:108:A:SER:HA   | 4        | 0.12          |
| (1,683)  | 1:60:A:LEU:HG   | 1:60:A:LEU:H     | 2        | 0.12          |
| (1,683)  | 1:60:A:LEU:HG   | 1:60:A:LEU:H     | 7        | 0.12          |
| (1,643)  | 1:57:A:ASP:HB2  | 1:115:A:LYS:H    | 3        | 0.12          |
| (1,643)  | 1:57:A:ASP:HB2  | 1:115:A:LYS:H    | 7        | 0.12          |
| (1,643)  | 1:57:A:ASP:HB2  | 1:115:A:LYS:H    | 10       | 0.12          |
| (1,640)  | 1:57:A:ASP:HB3  | 1:115:A:LYS:H    | 6        | 0.12          |
| (1,568)  | 1:51:A:ILE:HA   | 1:51:A:ILE:HG21  | 4        | 0.12          |
| (1,568)  | 1:51:A:ILE:HA   | 1:51:A:ILE:HG22  | 4        | 0.12          |
| (1,568)  | 1:51:A:ILE:HA   | 1:51:A:ILE:HG23  | 4        | 0.12          |
| (1,568)  | 1:51:A:ILE:HA   | 1:51:A:ILE:HG21  | 6        | 0.12          |
| (1,568)  | 1:51:A:ILE:HA   | 1:51:A:ILE:HG22  | 6        | 0.12          |
| (1,568)  | 1:51:A:ILE:HA   | 1:51:A:ILE:HG23  | 6        | 0.12          |
| (1,568)  | 1:51:A:ILE:HA   | 1:51:A:ILE:HG21  | 7        | 0.12          |
| (1,568)  | 1:51:A:ILE:HA   | 1:51:A:ILE:HG22  | 7        | 0.12          |
| (1,568)  | 1:51:A:ILE:HA   | 1:51:A:ILE:HG23  | 7        | 0.12          |
| (1,567)  | 1:50:A:TRP:HZ3  | 1:151:A:VAL:HG21 | 10       | 0.12          |
| (1,567)  | 1:50:A:TRP:HZ3  | 1:151:A:VAL:HG22 | 10       | 0.12          |

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| Key     | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,567) | 1:50:A:TRP:HZ3  | 1:151:A:VAL:HG23 | 10       | 0.12          |
| (1,548) | 1:50:A:TRP:HB3  | 1:50:A:TRP:H     | 1        | 0.12          |
| (1,548) | 1:50:A:TRP:HB3  | 1:50:A:TRP:H     | 2        | 0.12          |
| (1,548) | 1:50:A:TRP:HB3  | 1:50:A:TRP:H     | 3        | 0.12          |
| (1,548) | 1:50:A:TRP:HB3  | 1:50:A:TRP:H     | 8        | 0.12          |
| (1,513) | 1:49:A:VAL:HA   | 1:49:A:VAL:HG11  | 2        | 0.12          |
| (1,513) | 1:49:A:VAL:HA   | 1:49:A:VAL:HG12  | 2        | 0.12          |
| (1,513) | 1:49:A:VAL:HA   | 1:49:A:VAL:HG13  | 2        | 0.12          |
| (1,513) | 1:49:A:VAL:HA   | 1:49:A:VAL:HG11  | 9        | 0.12          |
| (1,513) | 1:49:A:VAL:HA   | 1:49:A:VAL:HG12  | 9        | 0.12          |
| (1,513) | 1:49:A:VAL:HA   | 1:49:A:VAL:HG13  | 9        | 0.12          |
| (1,426) | 1:46:A:TYR:HA   | 1:156:A:PHE:HA   | 3        | 0.12          |
| (1,424) | 1:46:A:TYR:HA   | 1:155:A:ASN:HB2  | 6        | 0.12          |
| (1,292) | 1:37:A:GLY:HA2  | 1:37:A:GLY:H     | 5        | 0.12          |
| (1,291) | 1:37:A:GLY:HA2  | 1:37:A:GLY:HA3   | 1        | 0.12          |
| (1,291) | 1:37:A:GLY:HA2  | 1:37:A:GLY:HA3   | 2        | 0.12          |
| (1,291) | 1:37:A:GLY:HA2  | 1:37:A:GLY:HA3   | 3        | 0.12          |
| (1,291) | 1:37:A:GLY:HA2  | 1:37:A:GLY:HA3   | 4        | 0.12          |
| (1,291) | 1:37:A:GLY:HA2  | 1:37:A:GLY:HA3   | 5        | 0.12          |
| (1,291) | 1:37:A:GLY:HA2  | 1:37:A:GLY:HA3   | 6        | 0.12          |
| (1,291) | 1:37:A:GLY:HA2  | 1:37:A:GLY:HA3   | 7        | 0.12          |
| (1,291) | 1:37:A:GLY:HA2  | 1:37:A:GLY:HA3   | 8        | 0.12          |
| (1,291) | 1:37:A:GLY:HA2  | 1:37:A:GLY:HA3   | 9        | 0.12          |
| (1,291) | 1:37:A:GLY:HA2  | 1:37:A:GLY:HA3   | 10       | 0.12          |
| (1,272) | 1:34:A:PRO:HD2  | 1:35:A:ALA:H     | 1        | 0.12          |
| (1,272) | 1:34:A:PRO:HD2  | 1:35:A:ALA:H     | 9        | 0.12          |
| (1,254) | 1:33:A:THR:HA   | 1:33:A:THR:HG21  | 2        | 0.12          |
| (1,254) | 1:33:A:THR:HA   | 1:33:A:THR:HG22  | 2        | 0.12          |
| (1,254) | 1:33:A:THR:HA   | 1:33:A:THR:HG23  | 2        | 0.12          |
| (1,254) | 1:33:A:THR:HA   | 1:33:A:THR:HG21  | 4        | 0.12          |
| (1,254) | 1:33:A:THR:HA   | 1:33:A:THR:HG22  | 4        | 0.12          |
| (1,254) | 1:33:A:THR:HA   | 1:33:A:THR:HG23  | 4        | 0.12          |
| (1,230) | 1:32:A:ILE:HG12 | 1:32:A:ILE:H     | 6        | 0.12          |
| (1,202) | 1:31:A:SER:HB2  | 1:173:A:VAL:H    | 1        | 0.12          |
| (1,82)  | 1:25:A:VAL:HG21 | 1:25:A:VAL:HG11  | 7        | 0.12          |
| (1,82)  | 1:25:A:VAL:HG21 | 1:25:A:VAL:HG12  | 7        | 0.12          |
| (1,82)  | 1:25:A:VAL:HG21 | 1:25:A:VAL:HG13  | 7        | 0.12          |
| (1,82)  | 1:25:A:VAL:HG22 | 1:25:A:VAL:HG11  | 7        | 0.12          |
| (1,82)  | 1:25:A:VAL:HG22 | 1:25:A:VAL:HG12  | 7        | 0.12          |
| (1,82)  | 1:25:A:VAL:HG22 | 1:25:A:VAL:HG13  | 7        | 0.12          |
| (1,82)  | 1:25:A:VAL:HG23 | 1:25:A:VAL:HG11  | 7        | 0.12          |
| (1,82)  | 1:25:A:VAL:HG23 | 1:25:A:VAL:HG12  | 7        | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,82)   | 1:25:A:VAL:HG23 | 1:25:A:VAL:HG13 | 7        | 0.12          |
| (1,77)   | 1:25:A:VAL:HG11 | 1:25:A:VAL:H    | 2        | 0.12          |
| (1,77)   | 1:25:A:VAL:HG12 | 1:25:A:VAL:H    | 2        | 0.12          |
| (1,77)   | 1:25:A:VAL:HG13 | 1:25:A:VAL:H    | 2        | 0.12          |
| (1,77)   | 1:25:A:VAL:HG11 | 1:25:A:VAL:H    | 8        | 0.12          |
| (1,77)   | 1:25:A:VAL:HG12 | 1:25:A:VAL:H    | 8        | 0.12          |
| (1,77)   | 1:25:A:VAL:HG13 | 1:25:A:VAL:H    | 8        | 0.12          |
| (1,51)   | 1:24:A:ASP:HB2  | 1:25:A:VAL:H    | 5        | 0.12          |
| (1,51)   | 1:24:A:ASP:HB2  | 1:25:A:VAL:H    | 9        | 0.12          |
| (1,48)   | 1:24:A:ASP:HB3  | 1:50:A:TRP:HD1  | 5        | 0.12          |
| (2,632)  | 1:122:A:TYR:HD1 | 1:125:A:LYS:H   | 3        | 0.11          |
| (2,632)  | 1:122:A:TYR:HD2 | 1:125:A:LYS:H   | 3        | 0.11          |
| (2,518)  | 1:84:A:GLY:HA2  | 1:95:A:PHE:HE1  | 5        | 0.11          |
| (2,518)  | 1:84:A:GLY:HA2  | 1:95:A:PHE:HE2  | 5        | 0.11          |
| (2,518)  | 1:84:A:GLY:HA3  | 1:95:A:PHE:HE1  | 5        | 0.11          |
| (2,518)  | 1:84:A:GLY:HA3  | 1:95:A:PHE:HE2  | 5        | 0.11          |
| (2,397)  | 1:73:A:TYR:HD1  | 1:74:A:PHE:HA   | 4        | 0.11          |
| (2,397)  | 1:73:A:TYR:HD2  | 1:74:A:PHE:HA   | 4        | 0.11          |
| (2,389)  | 1:70:A:LEU:HD21 | 1:172:A:PRO:HD2 | 1        | 0.11          |
| (2,389)  | 1:70:A:LEU:HD22 | 1:172:A:PRO:HD2 | 1        | 0.11          |
| (2,389)  | 1:70:A:LEU:HD23 | 1:172:A:PRO:HD2 | 1        | 0.11          |
| (2,178)  | 1:36:A:ALA:H    | 1:37:A:GLY:H    | 3        | 0.11          |
| (2,123)  | 1:28:A:HIS:HD2  | 1:46:A:TYR:HE1  | 1        | 0.11          |
| (2,123)  | 1:28:A:HIS:HD2  | 1:46:A:TYR:HE2  | 1        | 0.11          |
| (2,123)  | 1:28:A:HIS:HD2  | 1:46:A:TYR:HE1  | 7        | 0.11          |
| (2,123)  | 1:28:A:HIS:HD2  | 1:46:A:TYR:HE2  | 7        | 0.11          |
| (1,2459) | 1:182:A:VAL:HB  | 1:183:A:GLY:H   | 3        | 0.11          |
| (1,2459) | 1:182:A:VAL:HB  | 1:183:A:GLY:H   | 4        | 0.11          |
| (1,2459) | 1:182:A:VAL:HB  | 1:183:A:GLY:H   | 5        | 0.11          |
| (1,2425) | 1:177:A:PHE:HD1 | 1:177:A:PHE:H   | 8        | 0.11          |
| (1,2425) | 1:177:A:PHE:HD2 | 1:177:A:PHE:H   | 8        | 0.11          |
| (1,2316) | 1:171:A:LEU:HA  | 1:172:A:PRO:HD3 | 9        | 0.11          |
| (1,2295) | 1:169:A:ASP:HB3 | 1:170:A:SER:H   | 1        | 0.11          |
| (1,2276) | 1:167:A:LEU:H   | 1:168:A:PHE:H   | 10       | 0.11          |
| (1,2275) | 1:167:A:LEU:HA  | 1:168:A:PHE:H   | 3        | 0.11          |
| (1,2275) | 1:167:A:LEU:HA  | 1:168:A:PHE:H   | 5        | 0.11          |
| (1,2271) | 1:166:A:MET:HB3 | 1:167:A:LEU:H   | 8        | 0.11          |
| (1,2260) | 1:163:A:LYS:H   | 1:168:A:PHE:HZ  | 10       | 0.11          |
| (1,2258) | 1:163:A:LYS:HG2 | 1:163:A:LYS:H   | 7        | 0.11          |
| (1,2257) | 1:163:A:LYS:HG3 | 1:163:A:LYS:H   | 9        | 0.11          |
| (1,2207) | 1:159:A:PHE:HB2 | 1:159:A:PHE:H   | 1        | 0.11          |
| (1,2207) | 1:159:A:PHE:HB2 | 1:159:A:PHE:H   | 9        | 0.11          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2183) | 1:158:A:ALA:HA   | 1:159:A:PHE:HB3 | 2        | 0.11          |
| (1,2183) | 1:158:A:ALA:HA   | 1:159:A:PHE:HB3 | 3        | 0.11          |
| (1,2183) | 1:158:A:ALA:HA   | 1:159:A:PHE:HB3 | 7        | 0.11          |
| (1,2183) | 1:158:A:ALA:HA   | 1:159:A:PHE:HB3 | 8        | 0.11          |
| (1,2183) | 1:158:A:ALA:HA   | 1:159:A:PHE:HB3 | 10       | 0.11          |
| (1,2139) | 1:155:A:ASN:H    | 1:156:A:PHE:HZ  | 8        | 0.11          |
| (1,2139) | 1:155:A:ASN:H    | 1:156:A:PHE:HZ  | 10       | 0.11          |
| (1,2089) | 1:152:A:ALA:HB1  | 1:152:A:ALA:H   | 4        | 0.11          |
| (1,2089) | 1:152:A:ALA:HB2  | 1:152:A:ALA:H   | 4        | 0.11          |
| (1,2089) | 1:152:A:ALA:HB3  | 1:152:A:ALA:H   | 4        | 0.11          |
| (1,2086) | 1:152:A:ALA:HA   | 1:152:A:ALA:HB1 | 6        | 0.11          |
| (1,2086) | 1:152:A:ALA:HA   | 1:152:A:ALA:HB2 | 6        | 0.11          |
| (1,2086) | 1:152:A:ALA:HA   | 1:152:A:ALA:HB3 | 6        | 0.11          |
| (1,2086) | 1:152:A:ALA:HA   | 1:152:A:ALA:HB1 | 7        | 0.11          |
| (1,2086) | 1:152:A:ALA:HA   | 1:152:A:ALA:HB2 | 7        | 0.11          |
| (1,2086) | 1:152:A:ALA:HA   | 1:152:A:ALA:HB3 | 7        | 0.11          |
| (1,2086) | 1:152:A:ALA:HA   | 1:152:A:ALA:HB1 | 10       | 0.11          |
| (1,2086) | 1:152:A:ALA:HA   | 1:152:A:ALA:HB2 | 10       | 0.11          |
| (1,2086) | 1:152:A:ALA:HA   | 1:152:A:ALA:HB3 | 10       | 0.11          |
| (1,2079) | 1:151:A:VAL:HG11 | 1:151:A:VAL:H   | 8        | 0.11          |
| (1,2079) | 1:151:A:VAL:HG12 | 1:151:A:VAL:H   | 8        | 0.11          |
| (1,2079) | 1:151:A:VAL:HG13 | 1:151:A:VAL:H   | 8        | 0.11          |
| (1,2028) | 1:143:A:ILE:HD11 | 1:143:A:ILE:H   | 3        | 0.11          |
| (1,2028) | 1:143:A:ILE:HD12 | 1:143:A:ILE:H   | 3        | 0.11          |
| (1,2028) | 1:143:A:ILE:HD13 | 1:143:A:ILE:H   | 3        | 0.11          |
| (1,1974) | 1:138:A:GLU:H    | 1:139:A:PRO:HD2 | 1        | 0.11          |
| (1,1974) | 1:138:A:GLU:H    | 1:139:A:PRO:HD2 | 5        | 0.11          |
| (1,1974) | 1:138:A:GLU:H    | 1:139:A:PRO:HD2 | 7        | 0.11          |
| (1,1974) | 1:138:A:GLU:H    | 1:139:A:PRO:HD2 | 9        | 0.11          |
| (1,1923) | 1:134:A:TRP:HE1  | 1:139:A:PRO:HD2 | 2        | 0.11          |
| (1,1923) | 1:134:A:TRP:HE1  | 1:139:A:PRO:HD2 | 3        | 0.11          |
| (1,1923) | 1:134:A:TRP:HE1  | 1:139:A:PRO:HD2 | 10       | 0.11          |
| (1,1917) | 1:134:A:TRP:HE1  | 1:136:A:PRO:HA  | 1        | 0.11          |
| (1,1894) | 1:134:A:TRP:HB3  | 1:142:A:ILE:HA  | 3        | 0.11          |
| (1,1894) | 1:134:A:TRP:HB3  | 1:142:A:ILE:HA  | 6        | 0.11          |
| (1,1826) | 1:132:A:SER:HA   | 1:133:A:ILE:HB  | 1        | 0.11          |
| (1,1826) | 1:132:A:SER:HA   | 1:133:A:ILE:HB  | 7        | 0.11          |
| (1,1826) | 1:132:A:SER:HA   | 1:133:A:ILE:HB  | 8        | 0.11          |
| (1,1826) | 1:132:A:SER:HA   | 1:133:A:ILE:HB  | 10       | 0.11          |
| (1,1778) | 1:121:A:LEU:HG   | 1:121:A:LEU:H   | 3        | 0.11          |
| (1,1778) | 1:121:A:LEU:HG   | 1:121:A:LEU:H   | 10       | 0.11          |
| (1,1761) | 1:119:A:ALA:H    | 1:151:A:VAL:H   | 10       | 0.11          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1734) | 1:117:A:ASP:H    | 1:118:A:ILE:HB   | 10       | 0.11          |
| (1,1723) | 1:116:A:GLU:HG2  | 1:116:A:GLU:H    | 1        | 0.11          |
| (1,1723) | 1:116:A:GLU:HG3  | 1:116:A:GLU:H    | 1        | 0.11          |
| (1,1699) | 1:115:A:LYS:HB3  | 1:115:A:LYS:H    | 4        | 0.11          |
| (1,1690) | 1:115:A:LYS:HA   | 1:115:A:LYS:HG2  | 9        | 0.11          |
| (1,1690) | 1:115:A:LYS:HA   | 1:115:A:LYS:HG3  | 9        | 0.11          |
| (1,1677) | 1:114:A:ASP:HA   | 1:118:A:ILE:H    | 1        | 0.11          |
| (1,1677) | 1:114:A:ASP:HA   | 1:118:A:ILE:H    | 5        | 0.11          |
| (1,1677) | 1:114:A:ASP:HA   | 1:118:A:ILE:H    | 8        | 0.11          |
| (1,1629) | 1:110:A:VAL:HG11 | 1:111:A:ILE:H    | 9        | 0.11          |
| (1,1629) | 1:110:A:VAL:HG12 | 1:111:A:ILE:H    | 9        | 0.11          |
| (1,1629) | 1:110:A:VAL:HG13 | 1:111:A:ILE:H    | 9        | 0.11          |
| (1,1629) | 1:110:A:VAL:HG11 | 1:111:A:ILE:H    | 10       | 0.11          |
| (1,1629) | 1:110:A:VAL:HG12 | 1:111:A:ILE:H    | 10       | 0.11          |
| (1,1629) | 1:110:A:VAL:HG13 | 1:111:A:ILE:H    | 10       | 0.11          |
| (1,1618) | 1:108:A:SER:H    | 1:109:A:ALA:H    | 1        | 0.11          |
| (1,1618) | 1:108:A:SER:H    | 1:109:A:ALA:H    | 7        | 0.11          |
| (1,1618) | 1:108:A:SER:H    | 1:109:A:ALA:H    | 8        | 0.11          |
| (1,1532) | 1:102:A:ILE:HB   | 1:102:A:ILE:H    | 2        | 0.11          |
| (1,1531) | 1:102:A:ILE:HB   | 1:102:A:ILE:HG21 | 4        | 0.11          |
| (1,1531) | 1:102:A:ILE:HB   | 1:102:A:ILE:HG22 | 4        | 0.11          |
| (1,1531) | 1:102:A:ILE:HB   | 1:102:A:ILE:HG23 | 4        | 0.11          |
| (1,1399) | 1:87:A:THR:HG21  | 1:87:A:THR:H     | 2        | 0.11          |
| (1,1399) | 1:87:A:THR:HG22  | 1:87:A:THR:H     | 2        | 0.11          |
| (1,1399) | 1:87:A:THR:HG23  | 1:87:A:THR:H     | 2        | 0.11          |
| (1,1399) | 1:87:A:THR:HG21  | 1:87:A:THR:H     | 7        | 0.11          |
| (1,1399) | 1:87:A:THR:HG22  | 1:87:A:THR:H     | 7        | 0.11          |
| (1,1399) | 1:87:A:THR:HG23  | 1:87:A:THR:H     | 7        | 0.11          |
| (1,1380) | 1:87:A:THR:HA    | 1:134:A:TRP:HH2  | 8        | 0.11          |
| (1,1379) | 1:87:A:THR:HA    | 1:134:A:TRP:HE3  | 1        | 0.11          |
| (1,1379) | 1:87:A:THR:HA    | 1:134:A:TRP:HE3  | 4        | 0.11          |
| (1,1371) | 1:86:A:GLU:H     | 1:134:A:TRP:HE1  | 1        | 0.11          |
| (1,1369) | 1:86:A:GLU:H     | 1:133:A:ILE:HG21 | 3        | 0.11          |
| (1,1369) | 1:86:A:GLU:H     | 1:133:A:ILE:HG22 | 3        | 0.11          |
| (1,1369) | 1:86:A:GLU:H     | 1:133:A:ILE:HG23 | 3        | 0.11          |
| (1,1363) | 1:86:A:GLU:HG3   | 1:86:A:GLU:H     | 4        | 0.11          |
| (1,1343) | 1:85:A:TYR:HE1   | 1:152:A:ALA:HA   | 9        | 0.11          |
| (1,1343) | 1:85:A:TYR:HE2   | 1:152:A:ALA:HA   | 9        | 0.11          |
| (1,1315) | 1:83:A:SER:H     | 1:99:A:LYS:HG3   | 9        | 0.11          |
| (1,1271) | 1:82:A:THR:HG21  | 1:83:A:SER:H     | 2        | 0.11          |
| (1,1271) | 1:82:A:THR:HG22  | 1:83:A:SER:H     | 2        | 0.11          |
| (1,1271) | 1:82:A:THR:HG23  | 1:83:A:SER:H     | 2        | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1250) | 1:81:A:ILE:H    | 1:156:A:PHE:HA  | 1        | 0.11          |
| (1,1250) | 1:81:A:ILE:H    | 1:156:A:PHE:HA  | 7        | 0.11          |
| (1,1232) | 1:81:A:ILE:HG21 | 1:99:A:LYS:H    | 7        | 0.11          |
| (1,1232) | 1:81:A:ILE:HG22 | 1:99:A:LYS:H    | 7        | 0.11          |
| (1,1232) | 1:81:A:ILE:HG23 | 1:99:A:LYS:H    | 7        | 0.11          |
| (1,1169) | 1:79:A:ILE:HG21 | 1:79:A:ILE:HD11 | 1        | 0.11          |
| (1,1169) | 1:79:A:ILE:HG21 | 1:79:A:ILE:HD12 | 1        | 0.11          |
| (1,1169) | 1:79:A:ILE:HG21 | 1:79:A:ILE:HD13 | 1        | 0.11          |
| (1,1169) | 1:79:A:ILE:HG22 | 1:79:A:ILE:HD11 | 1        | 0.11          |
| (1,1169) | 1:79:A:ILE:HG22 | 1:79:A:ILE:HD12 | 1        | 0.11          |
| (1,1169) | 1:79:A:ILE:HG22 | 1:79:A:ILE:HD13 | 1        | 0.11          |
| (1,1169) | 1:79:A:ILE:HG23 | 1:79:A:ILE:HD11 | 1        | 0.11          |
| (1,1169) | 1:79:A:ILE:HG23 | 1:79:A:ILE:HD12 | 1        | 0.11          |
| (1,1169) | 1:79:A:ILE:HG23 | 1:79:A:ILE:HD13 | 1        | 0.11          |
| (1,1128) | 1:78:A:GLN:H    | 1:158:A:ALA:HA  | 6        | 0.11          |
| (1,1127) | 1:78:A:GLN:H    | 1:104:A:LEU:H   | 1        | 0.11          |
| (1,1100) | 1:77:A:LEU:HG   | 1:78:A:GLN:H    | 8        | 0.11          |
| (1,1078) | 1:77:A:LEU:HA   | 1:77:A:LEU:HB2  | 4        | 0.11          |
| (1,1075) | 1:76:A:TYR:H    | 1:162:A:ALA:HA  | 2        | 0.11          |
| (1,1075) | 1:76:A:TYR:H    | 1:162:A:ALA:HA  | 4        | 0.11          |
| (1,1075) | 1:76:A:TYR:H    | 1:162:A:ALA:HA  | 6        | 0.11          |
| (1,1075) | 1:76:A:TYR:H    | 1:162:A:ALA:HA  | 7        | 0.11          |
| (1,1037) | 1:74:A:PHE:HZ   | 1:162:A:ALA:HA  | 5        | 0.11          |
| (1,1006) | 1:74:A:PHE:HA   | 1:163:A:LYS:H   | 9        | 0.11          |
| (1,975)  | 1:73:A:TYR:HA   | 1:73:A:TYR:HB3  | 6        | 0.11          |
| (1,921)  | 1:70:A:LEU:HA   | 1:73:A:TYR:HD1  | 8        | 0.11          |
| (1,921)  | 1:70:A:LEU:HA   | 1:73:A:TYR:HD2  | 8        | 0.11          |
| (1,894)  | 1:68:A:GLU:H    | 1:69:A:GLN:H    | 7        | 0.11          |
| (1,886)  | 1:68:A:GLU:HA   | 1:71:A:LYS:HD2  | 7        | 0.11          |
| (1,886)  | 1:68:A:GLU:HA   | 1:71:A:LYS:HD3  | 7        | 0.11          |
| (1,857)  | 1:66:A:ASN:HD22 | 1:174:A:ILE:H   | 4        | 0.11          |
| (1,854)  | 1:66:A:ASN:HD22 | 1:172:A:PRO:HD3 | 4        | 0.11          |
| (1,854)  | 1:66:A:ASN:HD22 | 1:172:A:PRO:HD3 | 8        | 0.11          |
| (1,845)  | 1:66:A:ASN:HD21 | 1:173:A:VAL:HA  | 7        | 0.11          |
| (1,834)  | 1:66:A:ASN:HB3  | 1:66:A:ASN:H    | 5        | 0.11          |
| (1,830)  | 1:66:A:ASN:HA   | 1:69:A:GLN:H    | 10       | 0.11          |
| (1,828)  | 1:66:A:ASN:HA   | 1:69:A:GLN:HG3  | 9        | 0.11          |
| (1,795)  | 1:64:A:LEU:HG   | 1:67:A:ALA:HA   | 7        | 0.11          |
| (1,761)  | 1:63:A:THR:H    | 1:175:A:PHE:HA  | 7        | 0.11          |
| (1,761)  | 1:63:A:THR:H    | 1:175:A:PHE:HA  | 8        | 0.11          |
| (1,761)  | 1:63:A:THR:H    | 1:175:A:PHE:HA  | 10       | 0.11          |
| (1,755)  | 1:63:A:THR:HG21 | 1:108:A:SER:HA  | 7        | 0.11          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,755) | 1:63:A:THR:HG22 | 1:108:A:SER:HA  | 7        | 0.11          |
| (1,755) | 1:63:A:THR:HG23 | 1:108:A:SER:HA  | 7        | 0.11          |
| (1,755) | 1:63:A:THR:HG21 | 1:108:A:SER:HA  | 8        | 0.11          |
| (1,755) | 1:63:A:THR:HG22 | 1:108:A:SER:HA  | 8        | 0.11          |
| (1,755) | 1:63:A:THR:HG23 | 1:108:A:SER:HA  | 8        | 0.11          |
| (1,731) | 1:62:A:VAL:HG21 | 1:177:A:PHE:HD1 | 3        | 0.11          |
| (1,731) | 1:62:A:VAL:HG21 | 1:177:A:PHE:HD2 | 3        | 0.11          |
| (1,731) | 1:62:A:VAL:HG22 | 1:177:A:PHE:HD1 | 3        | 0.11          |
| (1,731) | 1:62:A:VAL:HG22 | 1:177:A:PHE:HD2 | 3        | 0.11          |
| (1,731) | 1:62:A:VAL:HG23 | 1:177:A:PHE:HD1 | 3        | 0.11          |
| (1,731) | 1:62:A:VAL:HG23 | 1:177:A:PHE:HD2 | 3        | 0.11          |
| (1,683) | 1:60:A:LEU:HG   | 1:60:A:LEU:H    | 10       | 0.11          |
| (1,639) | 1:57:A:ASP:HB3  | 1:58:A:VAL:H    | 7        | 0.11          |
| (1,597) | 1:53:A:ASP:HB2  | 1:54:A:GLN:H    | 7        | 0.11          |
| (1,597) | 1:53:A:ASP:HB3  | 1:54:A:GLN:H    | 7        | 0.11          |
| (1,554) | 1:50:A:TRP:HD1  | 1:50:A:TRP:H    | 3        | 0.11          |
| (1,548) | 1:50:A:TRP:HB3  | 1:50:A:TRP:H    | 9        | 0.11          |
| (1,541) | 1:50:A:TRP:HA   | 1:51:A:ILE:HB   | 3        | 0.11          |
| (1,529) | 1:49:A:VAL:H    | 1:151:A:VAL:HA  | 7        | 0.11          |
| (1,513) | 1:49:A:VAL:HA   | 1:49:A:VAL:HG11 | 3        | 0.11          |
| (1,513) | 1:49:A:VAL:HA   | 1:49:A:VAL:HG12 | 3        | 0.11          |
| (1,513) | 1:49:A:VAL:HA   | 1:49:A:VAL:HG13 | 3        | 0.11          |
| (1,513) | 1:49:A:VAL:HA   | 1:49:A:VAL:HG11 | 4        | 0.11          |
| (1,513) | 1:49:A:VAL:HA   | 1:49:A:VAL:HG12 | 4        | 0.11          |
| (1,513) | 1:49:A:VAL:HA   | 1:49:A:VAL:HG13 | 4        | 0.11          |
| (1,513) | 1:49:A:VAL:HA   | 1:49:A:VAL:HG11 | 8        | 0.11          |
| (1,513) | 1:49:A:VAL:HA   | 1:49:A:VAL:HG12 | 8        | 0.11          |
| (1,513) | 1:49:A:VAL:HA   | 1:49:A:VAL:HG13 | 8        | 0.11          |
| (1,493) | 1:48:A:ILE:HG21 | 1:50:A:TRP:HA   | 6        | 0.11          |
| (1,493) | 1:48:A:ILE:HG22 | 1:50:A:TRP:HA   | 6        | 0.11          |
| (1,493) | 1:48:A:ILE:HG23 | 1:50:A:TRP:HA   | 6        | 0.11          |
| (1,447) | 1:46:A:TYR:HE1  | 1:141:A:LYS:HG3 | 9        | 0.11          |
| (1,447) | 1:46:A:TYR:HE2  | 1:141:A:LYS:HG3 | 9        | 0.11          |
| (1,432) | 1:46:A:TYR:HB3  | 1:154:A:LEU:H   | 2        | 0.11          |
| (1,424) | 1:46:A:TYR:HA   | 1:155:A:ASN:HB2 | 5        | 0.11          |
| (1,356) | 1:42:A:ASP:HB2  | 1:160:A:TYR:HE1 | 8        | 0.11          |
| (1,356) | 1:42:A:ASP:HB2  | 1:160:A:TYR:HE2 | 8        | 0.11          |
| (1,356) | 1:42:A:ASP:HB3  | 1:160:A:TYR:HE1 | 8        | 0.11          |
| (1,356) | 1:42:A:ASP:HB3  | 1:160:A:TYR:HE2 | 8        | 0.11          |
| (1,292) | 1:37:A:GLY:HA2  | 1:37:A:GLY:H    | 6        | 0.11          |
| (1,290) | 1:37:A:GLY:HA3  | 1:38:A:ALA:H    | 7        | 0.11          |
| (1,268) | 1:34:A:PRO:HD3  | 1:35:A:ALA:H    | 3        | 0.11          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,240) | 1:32:A:ILE:HG21 | 1:74:A:PHE:HE1  | 3        | 0.11          |
| (1,240) | 1:32:A:ILE:HG21 | 1:74:A:PHE:HE2  | 3        | 0.11          |
| (1,240) | 1:32:A:ILE:HG22 | 1:74:A:PHE:HE1  | 3        | 0.11          |
| (1,240) | 1:32:A:ILE:HG22 | 1:74:A:PHE:HE2  | 3        | 0.11          |
| (1,240) | 1:32:A:ILE:HG23 | 1:74:A:PHE:HE1  | 3        | 0.11          |
| (1,240) | 1:32:A:ILE:HG23 | 1:74:A:PHE:HE2  | 3        | 0.11          |
| (1,227) | 1:32:A:ILE:HG13 | 1:33:A:THR:H    | 6        | 0.11          |
| (1,190) | 1:31:A:SER:HA   | 1:32:A:ILE:HD11 | 6        | 0.11          |
| (1,190) | 1:31:A:SER:HA   | 1:32:A:ILE:HD12 | 6        | 0.11          |
| (1,190) | 1:31:A:SER:HA   | 1:32:A:ILE:HD13 | 6        | 0.11          |
| (1,188) | 1:30:A:GLY:H    | 1:46:A:TYR:H    | 2        | 0.11          |
| (1,188) | 1:30:A:GLY:H    | 1:46:A:TYR:H    | 5        | 0.11          |
| (1,166) | 1:29:A:LEU:HD11 | 1:175:A:PHE:H   | 5        | 0.11          |
| (1,166) | 1:29:A:LEU:HD12 | 1:175:A:PHE:H   | 5        | 0.11          |
| (1,166) | 1:29:A:LEU:HD13 | 1:175:A:PHE:H   | 5        | 0.11          |
| (1,141) | 1:28:A:HIS:HD2  | 1:48:A:ILE:HA   | 7        | 0.11          |
| (1,82)  | 1:25:A:VAL:HG21 | 1:25:A:VAL:HG11 | 3        | 0.11          |
| (1,82)  | 1:25:A:VAL:HG21 | 1:25:A:VAL:HG12 | 3        | 0.11          |
| (1,82)  | 1:25:A:VAL:HG21 | 1:25:A:VAL:HG13 | 3        | 0.11          |
| (1,82)  | 1:25:A:VAL:HG22 | 1:25:A:VAL:HG11 | 3        | 0.11          |
| (1,82)  | 1:25:A:VAL:HG22 | 1:25:A:VAL:HG12 | 3        | 0.11          |
| (1,82)  | 1:25:A:VAL:HG22 | 1:25:A:VAL:HG13 | 3        | 0.11          |
| (1,82)  | 1:25:A:VAL:HG23 | 1:25:A:VAL:HG11 | 3        | 0.11          |
| (1,82)  | 1:25:A:VAL:HG23 | 1:25:A:VAL:HG12 | 3        | 0.11          |
| (1,82)  | 1:25:A:VAL:HG23 | 1:25:A:VAL:HG13 | 3        | 0.11          |
| (1,82)  | 1:25:A:VAL:HG21 | 1:25:A:VAL:HG11 | 5        | 0.11          |
| (1,82)  | 1:25:A:VAL:HG21 | 1:25:A:VAL:HG12 | 5        | 0.11          |
| (1,82)  | 1:25:A:VAL:HG21 | 1:25:A:VAL:HG13 | 5        | 0.11          |
| (1,82)  | 1:25:A:VAL:HG22 | 1:25:A:VAL:HG11 | 5        | 0.11          |
| (1,82)  | 1:25:A:VAL:HG22 | 1:25:A:VAL:HG12 | 5        | 0.11          |
| (1,82)  | 1:25:A:VAL:HG22 | 1:25:A:VAL:HG13 | 5        | 0.11          |
| (1,82)  | 1:25:A:VAL:HG23 | 1:25:A:VAL:HG11 | 5        | 0.11          |
| (1,82)  | 1:25:A:VAL:HG23 | 1:25:A:VAL:HG12 | 5        | 0.11          |
| (1,82)  | 1:25:A:VAL:HG23 | 1:25:A:VAL:HG13 | 5        | 0.11          |
| (1,82)  | 1:25:A:VAL:HG21 | 1:25:A:VAL:HG11 | 6        | 0.11          |
| (1,82)  | 1:25:A:VAL:HG21 | 1:25:A:VAL:HG12 | 6        | 0.11          |
| (1,82)  | 1:25:A:VAL:HG21 | 1:25:A:VAL:HG13 | 6        | 0.11          |
| (1,82)  | 1:25:A:VAL:HG22 | 1:25:A:VAL:HG11 | 6        | 0.11          |
| (1,82)  | 1:25:A:VAL:HG22 | 1:25:A:VAL:HG12 | 6        | 0.11          |
| (1,82)  | 1:25:A:VAL:HG22 | 1:25:A:VAL:HG13 | 6        | 0.11          |
| (1,82)  | 1:25:A:VAL:HG23 | 1:25:A:VAL:HG11 | 6        | 0.11          |
| (1,82)  | 1:25:A:VAL:HG23 | 1:25:A:VAL:HG12 | 6        | 0.11          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,82)  | 1:25:A:VAL:HG23 | 1:25:A:VAL:HG13 | 6        | 0.11          |
| (1,82)  | 1:25:A:VAL:HG21 | 1:25:A:VAL:HG11 | 8        | 0.11          |
| (1,82)  | 1:25:A:VAL:HG21 | 1:25:A:VAL:HG12 | 8        | 0.11          |
| (1,82)  | 1:25:A:VAL:HG21 | 1:25:A:VAL:HG13 | 8        | 0.11          |
| (1,82)  | 1:25:A:VAL:HG22 | 1:25:A:VAL:HG11 | 8        | 0.11          |
| (1,82)  | 1:25:A:VAL:HG22 | 1:25:A:VAL:HG12 | 8        | 0.11          |
| (1,82)  | 1:25:A:VAL:HG22 | 1:25:A:VAL:HG13 | 8        | 0.11          |
| (1,82)  | 1:25:A:VAL:HG23 | 1:25:A:VAL:HG11 | 8        | 0.11          |
| (1,82)  | 1:25:A:VAL:HG23 | 1:25:A:VAL:HG12 | 8        | 0.11          |
| (1,82)  | 1:25:A:VAL:HG23 | 1:25:A:VAL:HG13 | 8        | 0.11          |
| (1,82)  | 1:25:A:VAL:HG21 | 1:25:A:VAL:HG11 | 9        | 0.11          |
| (1,82)  | 1:25:A:VAL:HG21 | 1:25:A:VAL:HG12 | 9        | 0.11          |
| (1,82)  | 1:25:A:VAL:HG21 | 1:25:A:VAL:HG13 | 9        | 0.11          |
| (1,82)  | 1:25:A:VAL:HG22 | 1:25:A:VAL:HG11 | 9        | 0.11          |
| (1,82)  | 1:25:A:VAL:HG22 | 1:25:A:VAL:HG12 | 9        | 0.11          |
| (1,82)  | 1:25:A:VAL:HG22 | 1:25:A:VAL:HG13 | 9        | 0.11          |
| (1,82)  | 1:25:A:VAL:HG23 | 1:25:A:VAL:HG11 | 9        | 0.11          |
| (1,82)  | 1:25:A:VAL:HG23 | 1:25:A:VAL:HG12 | 9        | 0.11          |
| (1,82)  | 1:25:A:VAL:HG23 | 1:25:A:VAL:HG13 | 9        | 0.11          |
| (1,82)  | 1:25:A:VAL:HG21 | 1:25:A:VAL:HG11 | 10       | 0.11          |
| (1,82)  | 1:25:A:VAL:HG21 | 1:25:A:VAL:HG12 | 10       | 0.11          |
| (1,82)  | 1:25:A:VAL:HG21 | 1:25:A:VAL:HG13 | 10       | 0.11          |
| (1,82)  | 1:25:A:VAL:HG22 | 1:25:A:VAL:HG11 | 10       | 0.11          |
| (1,82)  | 1:25:A:VAL:HG22 | 1:25:A:VAL:HG12 | 10       | 0.11          |
| (1,82)  | 1:25:A:VAL:HG22 | 1:25:A:VAL:HG13 | 10       | 0.11          |
| (1,82)  | 1:25:A:VAL:HG23 | 1:25:A:VAL:HG11 | 10       | 0.11          |
| (1,82)  | 1:25:A:VAL:HG23 | 1:25:A:VAL:HG12 | 10       | 0.11          |
| (1,82)  | 1:25:A:VAL:HG23 | 1:25:A:VAL:HG13 | 10       | 0.11          |
| (1,77)  | 1:25:A:VAL:HG11 | 1:25:A:VAL:H    | 5        | 0.11          |
| (1,77)  | 1:25:A:VAL:HG12 | 1:25:A:VAL:H    | 5        | 0.11          |
| (1,77)  | 1:25:A:VAL:HG13 | 1:25:A:VAL:H    | 5        | 0.11          |
| (1,51)  | 1:24:A:ASP:HB2  | 1:25:A:VAL:H    | 8        | 0.11          |
| (1,48)  | 1:24:A:ASP:HB3  | 1:50:A:TRP:HD1  | 7        | 0.11          |
| (1,25)  | 1:23:A:ILE:HA   | 1:23:A:ILE:HG21 | 7        | 0.11          |
| (1,25)  | 1:23:A:ILE:HA   | 1:23:A:ILE:HG22 | 7        | 0.11          |
| (1,25)  | 1:23:A:ILE:HA   | 1:23:A:ILE:HG23 | 7        | 0.11          |
| (1,9)   | 1:19:A:VAL:HB   | 1:19:A:VAL:H    | 5        | 0.11          |
| (2,732) | 1:155:A:ASN:H   | 1:156:A:PHE:HE1 | 7        | 0.1           |
| (2,732) | 1:155:A:ASN:H   | 1:156:A:PHE:HE2 | 7        | 0.1           |
| (2,512) | 1:83:A:SER:HB2  | 1:154:A:LEU:HA  | 6        | 0.1           |
| (2,206) | 1:39:A:GLN:HB2  | 1:39:A:GLN:HE21 | 10       | 0.1           |
| (2,27)  | 1:19:A:VAL:H    | 1:20:A:SER:H    | 5        | 0.1           |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2459) | 1:182:A:VAL:HB  | 1:183:A:GLY:H    | 2        | 0.1           |
| (1,2459) | 1:182:A:VAL:HB  | 1:183:A:GLY:H    | 7        | 0.1           |
| (1,2459) | 1:182:A:VAL:HB  | 1:183:A:GLY:H    | 10       | 0.1           |
| (1,2450) | 1:180:A:LEU:H   | 1:181:A:GLN:H    | 5        | 0.1           |
| (1,2303) | 1:170:A:SER:HA  | 1:171:A:LEU:HD11 | 7        | 0.1           |
| (1,2303) | 1:170:A:SER:HA  | 1:171:A:LEU:HD12 | 7        | 0.1           |
| (1,2303) | 1:170:A:SER:HA  | 1:171:A:LEU:HD13 | 7        | 0.1           |
| (1,2299) | 1:169:A:ASP:H   | 1:170:A:SER:H    | 3        | 0.1           |
| (1,2299) | 1:169:A:ASP:H   | 1:170:A:SER:H    | 5        | 0.1           |
| (1,2295) | 1:169:A:ASP:HB3 | 1:170:A:SER:H    | 6        | 0.1           |
| (1,2275) | 1:167:A:LEU:HA  | 1:168:A:PHE:H    | 2        | 0.1           |
| (1,2275) | 1:167:A:LEU:HA  | 1:168:A:PHE:H    | 4        | 0.1           |
| (1,2275) | 1:167:A:LEU:HA  | 1:168:A:PHE:H    | 10       | 0.1           |
| (1,2260) | 1:163:A:LYS:H   | 1:168:A:PHE:HZ   | 5        | 0.1           |
| (1,2246) | 1:162:A:ALA:HB1 | 1:168:A:PHE:HZ   | 8        | 0.1           |
| (1,2246) | 1:162:A:ALA:HB2 | 1:168:A:PHE:HZ   | 8        | 0.1           |
| (1,2246) | 1:162:A:ALA:HB3 | 1:168:A:PHE:HZ   | 8        | 0.1           |
| (1,2183) | 1:158:A:ALA:HA  | 1:159:A:PHE:HB3  | 1        | 0.1           |
| (1,2183) | 1:158:A:ALA:HA  | 1:159:A:PHE:HB3  | 5        | 0.1           |
| (1,2124) | 1:155:A:ASN:HA  | 1:155:A:ASN:HD21 | 5        | 0.1           |
| (1,2124) | 1:155:A:ASN:HA  | 1:155:A:ASN:HD22 | 5        | 0.1           |
| (1,2089) | 1:152:A:ALA:HB1 | 1:152:A:ALA:H    | 1        | 0.1           |
| (1,2089) | 1:152:A:ALA:HB2 | 1:152:A:ALA:H    | 1        | 0.1           |
| (1,2089) | 1:152:A:ALA:HB3 | 1:152:A:ALA:H    | 1        | 0.1           |
| (1,2089) | 1:152:A:ALA:HB1 | 1:152:A:ALA:H    | 2        | 0.1           |
| (1,2089) | 1:152:A:ALA:HB2 | 1:152:A:ALA:H    | 2        | 0.1           |
| (1,2089) | 1:152:A:ALA:HB3 | 1:152:A:ALA:H    | 2        | 0.1           |
| (1,2089) | 1:152:A:ALA:HB1 | 1:152:A:ALA:H    | 9        | 0.1           |
| (1,2089) | 1:152:A:ALA:HB2 | 1:152:A:ALA:H    | 9        | 0.1           |
| (1,2089) | 1:152:A:ALA:HB3 | 1:152:A:ALA:H    | 9        | 0.1           |
| (1,2089) | 1:152:A:ALA:HB1 | 1:152:A:ALA:H    | 10       | 0.1           |
| (1,2089) | 1:152:A:ALA:HB2 | 1:152:A:ALA:H    | 10       | 0.1           |
| (1,2089) | 1:152:A:ALA:HB3 | 1:152:A:ALA:H    | 10       | 0.1           |
| (1,1974) | 1:138:A:GLU:H   | 1:139:A:PRO:HD2  | 6        | 0.1           |
| (1,1923) | 1:134:A:TRP:HE1 | 1:139:A:PRO:HD2  | 6        | 0.1           |
| (1,1894) | 1:134:A:TRP:HB3 | 1:142:A:ILE:HA   | 9        | 0.1           |
| (1,1826) | 1:132:A:SER:HA  | 1:133:A:ILE:HB   | 4        | 0.1           |
| (1,1787) | 1:123:A:PRO:HD2 | 1:124:A:ASP:H    | 5        | 0.1           |
| (1,1787) | 1:123:A:PRO:HD2 | 1:124:A:ASP:H    | 7        | 0.1           |
| (1,1787) | 1:123:A:PRO:HD2 | 1:124:A:ASP:H    | 9        | 0.1           |
| (1,1787) | 1:123:A:PRO:HD2 | 1:124:A:ASP:H    | 10       | 0.1           |
| (1,1761) | 1:119:A:ALA:H   | 1:151:A:VAL:H    | 6        | 0.1           |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1684) | 1:114:A:ASP:H    | 1:116:A:GLU:H   | 5        | 0.1           |
| (1,1677) | 1:114:A:ASP:HA   | 1:118:A:ILE:H   | 2        | 0.1           |
| (1,1677) | 1:114:A:ASP:HA   | 1:118:A:ILE:H   | 3        | 0.1           |
| (1,1640) | 1:111:A:ILE:HG21 | 1:112:A:VAL:H   | 3        | 0.1           |
| (1,1640) | 1:111:A:ILE:HG22 | 1:112:A:VAL:H   | 3        | 0.1           |
| (1,1640) | 1:111:A:ILE:HG23 | 1:112:A:VAL:H   | 3        | 0.1           |
| (1,1618) | 1:108:A:SER:H    | 1:109:A:ALA:H   | 3        | 0.1           |
| (1,1618) | 1:108:A:SER:H    | 1:109:A:ALA:H   | 5        | 0.1           |
| (1,1618) | 1:108:A:SER:H    | 1:109:A:ALA:H   | 6        | 0.1           |
| (1,1618) | 1:108:A:SER:H    | 1:109:A:ALA:H   | 10       | 0.1           |
| (1,1532) | 1:102:A:ILE:HB   | 1:102:A:ILE:H   | 7        | 0.1           |
| (1,1532) | 1:102:A:ILE:HB   | 1:102:A:ILE:H   | 9        | 0.1           |
| (1,1439) | 1:88:A:ASN:H     | 1:134:A:TRP:HZ3 | 7        | 0.1           |
| (1,1436) | 1:88:A:ASN:H     | 1:133:A:ILE:HA  | 3        | 0.1           |
| (1,1422) | 1:88:A:ASN:HB2   | 1:88:A:ASN:HD21 | 1        | 0.1           |
| (1,1408) | 1:87:A:THR:H     | 1:134:A:TRP:HH2 | 7        | 0.1           |
| (1,1380) | 1:87:A:THR:HA    | 1:134:A:TRP:HH2 | 7        | 0.1           |
| (1,1365) | 1:86:A:GLU:HG2   | 1:86:A:GLU:H    | 4        | 0.1           |
| (1,1250) | 1:81:A:ILE:H     | 1:156:A:PHE:HA  | 5        | 0.1           |
| (1,1127) | 1:78:A:GLN:H     | 1:104:A:LEU:H   | 5        | 0.1           |
| (1,1127) | 1:78:A:GLN:H     | 1:104:A:LEU:H   | 8        | 0.1           |
| (1,1020) | 1:74:A:PHE:HD1   | 1:162:A:ALA:HA  | 5        | 0.1           |
| (1,1020) | 1:74:A:PHE:HD2   | 1:162:A:ALA:HA  | 5        | 0.1           |
| (1,1006) | 1:74:A:PHE:HA    | 1:163:A:LYS:H   | 6        | 0.1           |
| (1,914)  | 1:69:A:GLN:HG3   | 1:69:A:GLN:H    | 2        | 0.1           |
| (1,828)  | 1:66:A:ASN:HA    | 1:69:A:GLN:HG3  | 10       | 0.1           |
| (1,795)  | 1:64:A:LEU:HG    | 1:67:A:ALA:HA   | 1        | 0.1           |
| (1,795)  | 1:64:A:LEU:HG    | 1:67:A:ALA:HA   | 4        | 0.1           |
| (1,710)  | 1:62:A:VAL:HA    | 1:62:A:VAL:HG21 | 5        | 0.1           |
| (1,710)  | 1:62:A:VAL:HA    | 1:62:A:VAL:HG22 | 5        | 0.1           |
| (1,710)  | 1:62:A:VAL:HA    | 1:62:A:VAL:HG23 | 5        | 0.1           |
| (1,678)  | 1:60:A:LEU:HA    | 1:111:A:ILE:H   | 6        | 0.1           |
| (1,678)  | 1:60:A:LEU:HA    | 1:111:A:ILE:H   | 7        | 0.1           |
| (1,678)  | 1:60:A:LEU:HA    | 1:111:A:ILE:H   | 8        | 0.1           |
| (1,643)  | 1:57:A:ASP:HB2   | 1:115:A:LYS:H   | 8        | 0.1           |
| (1,639)  | 1:57:A:ASP:HB3   | 1:58:A:VAL:H    | 5        | 0.1           |
| (1,541)  | 1:50:A:TRP:HA    | 1:51:A:ILE:HB   | 1        | 0.1           |
| (1,513)  | 1:49:A:VAL:HA    | 1:49:A:VAL:HG11 | 1        | 0.1           |
| (1,513)  | 1:49:A:VAL:HA    | 1:49:A:VAL:HG12 | 1        | 0.1           |
| (1,513)  | 1:49:A:VAL:HA    | 1:49:A:VAL:HG13 | 1        | 0.1           |
| (1,455)  | 1:47:A:ALA:HB1   | 1:48:A:ILE:H    | 3        | 0.1           |
| (1,455)  | 1:47:A:ALA:HB2   | 1:48:A:ILE:H    | 3        | 0.1           |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,455) | 1:47:A:ALA:HB3  | 1:48:A:ILE:H    | 3        | 0.1           |
| (1,454) | 1:47:A:ALA:HB1  | 1:47:A:ALA:H    | 7        | 0.1           |
| (1,454) | 1:47:A:ALA:HB2  | 1:47:A:ALA:H    | 7        | 0.1           |
| (1,454) | 1:47:A:ALA:HB3  | 1:47:A:ALA:H    | 7        | 0.1           |
| (1,432) | 1:46:A:TYR:HB3  | 1:154:A:LEU:H   | 5        | 0.1           |
| (1,427) | 1:46:A:TYR:HA   | 1:156:A:PHE:HE1 | 10       | 0.1           |
| (1,427) | 1:46:A:TYR:HA   | 1:156:A:PHE:HE2 | 10       | 0.1           |
| (1,426) | 1:46:A:TYR:HA   | 1:156:A:PHE:HA  | 10       | 0.1           |
| (1,356) | 1:42:A:ASP:HB2  | 1:160:A:TYR:HE1 | 9        | 0.1           |
| (1,356) | 1:42:A:ASP:HB2  | 1:160:A:TYR:HE2 | 9        | 0.1           |
| (1,356) | 1:42:A:ASP:HB3  | 1:160:A:TYR:HE1 | 9        | 0.1           |
| (1,356) | 1:42:A:ASP:HB3  | 1:160:A:TYR:HE2 | 9        | 0.1           |
| (1,290) | 1:37:A:GLY:HA3  | 1:38:A:ALA:H    | 4        | 0.1           |
| (1,272) | 1:34:A:PRO:HD2  | 1:35:A:ALA:H    | 3        | 0.1           |
| (1,256) | 1:33:A:THR:HA   | 1:168:A:PHE:HZ  | 5        | 0.1           |
| (1,209) | 1:32:A:ILE:HA   | 1:32:A:ILE:HG21 | 10       | 0.1           |
| (1,209) | 1:32:A:ILE:HA   | 1:32:A:ILE:HG22 | 10       | 0.1           |
| (1,209) | 1:32:A:ILE:HA   | 1:32:A:ILE:HG23 | 10       | 0.1           |
| (1,170) | 1:29:A:LEU:HD21 | 1:175:A:PHE:HD1 | 7        | 0.1           |
| (1,170) | 1:29:A:LEU:HD21 | 1:175:A:PHE:HD2 | 7        | 0.1           |
| (1,170) | 1:29:A:LEU:HD22 | 1:175:A:PHE:HD1 | 7        | 0.1           |
| (1,170) | 1:29:A:LEU:HD22 | 1:175:A:PHE:HD2 | 7        | 0.1           |
| (1,170) | 1:29:A:LEU:HD23 | 1:175:A:PHE:HD1 | 7        | 0.1           |
| (1,170) | 1:29:A:LEU:HD23 | 1:175:A:PHE:HD2 | 7        | 0.1           |
| (1,141) | 1:28:A:HIS:HD2  | 1:48:A:ILE:HA   | 2        | 0.1           |
| (1,92)  | 1:25:A:VAL:H    | 1:50:A:TRP:HE1  | 6        | 0.1           |
| (1,82)  | 1:25:A:VAL:HG21 | 1:25:A:VAL:HG11 | 4        | 0.1           |
| (1,82)  | 1:25:A:VAL:HG21 | 1:25:A:VAL:HG12 | 4        | 0.1           |
| (1,82)  | 1:25:A:VAL:HG21 | 1:25:A:VAL:HG13 | 4        | 0.1           |
| (1,82)  | 1:25:A:VAL:HG22 | 1:25:A:VAL:HG11 | 4        | 0.1           |
| (1,82)  | 1:25:A:VAL:HG22 | 1:25:A:VAL:HG12 | 4        | 0.1           |
| (1,82)  | 1:25:A:VAL:HG22 | 1:25:A:VAL:HG13 | 4        | 0.1           |
| (1,82)  | 1:25:A:VAL:HG23 | 1:25:A:VAL:HG11 | 4        | 0.1           |
| (1,82)  | 1:25:A:VAL:HG23 | 1:25:A:VAL:HG12 | 4        | 0.1           |
| (1,82)  | 1:25:A:VAL:HG23 | 1:25:A:VAL:HG13 | 4        | 0.1           |
| (1,54)  | 1:24:A:ASP:HB2  | 1:50:A:TRP:HB2  | 2        | 0.1           |

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

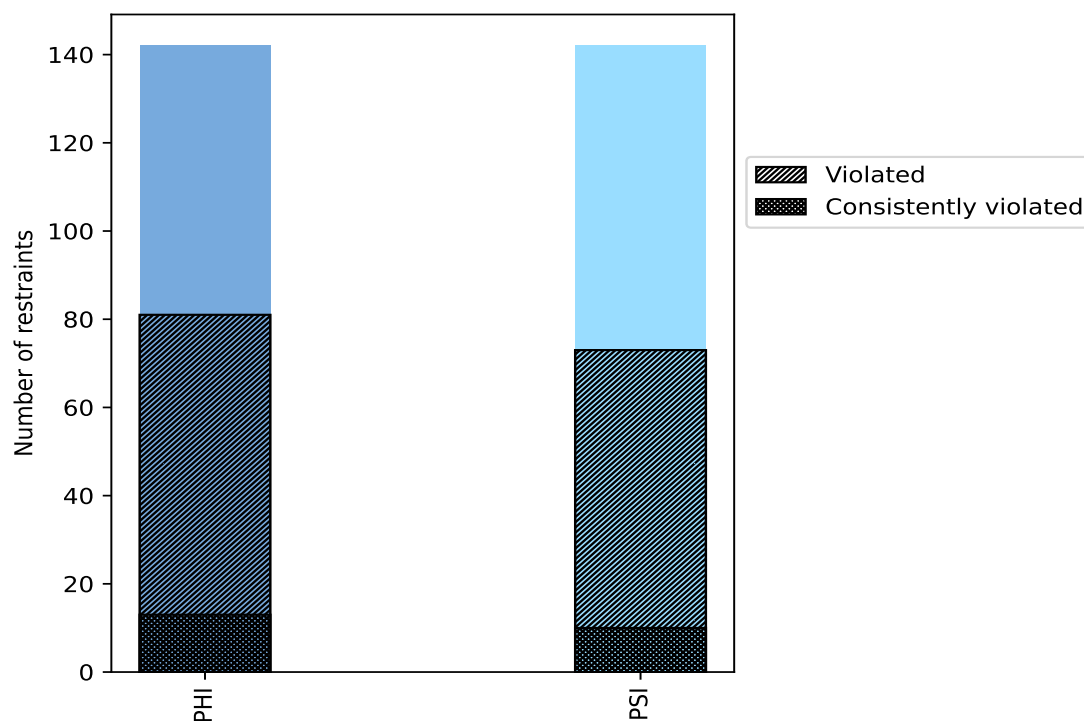
### 10.1 Summary of dihedral-angle violations [i](#)

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        | 142   | 50.0           | 81                    | 57.0           | 28.5           | 13                                 | 9.2            | 4.6            |
| PSI        | 142   | 50.0           | 73                    | 51.4           | 25.7           | 10                                 | 7.0            | 3.5            |
| Total      | 284   | 100.0          | 154                   | 54.2           | 54.2           | 23                                 | 8.1            | 8.1            |

<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](#)



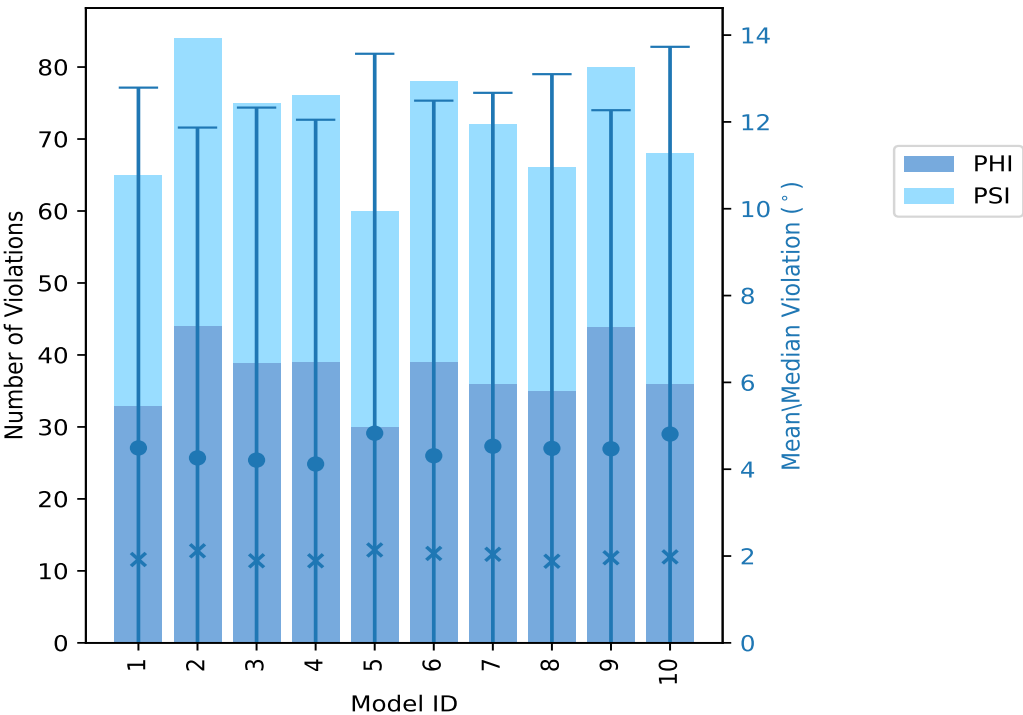
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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        | 33                   | 32  | 65    | 4.49     | 40.03   | 8.3    | 1.92       |
| 2        | 44                   | 40  | 84    | 4.26     | 39.91   | 7.61   | 2.12       |
| 3        | 39                   | 36  | 75    | 4.21     | 40.34   | 8.12   | 1.89       |
| 4        | 39                   | 37  | 76    | 4.12     | 40.62   | 7.93   | 1.89       |
| 5        | 30                   | 30  | 60    | 4.83     | 40.21   | 8.74   | 2.14       |
| 6        | 39                   | 39  | 78    | 4.31     | 43.13   | 8.18   | 2.06       |
| 7        | 36                   | 36  | 72    | 4.53     | 39.99   | 8.14   | 2.04       |
| 8        | 35                   | 31  | 66    | 4.48     | 41.94   | 8.62   | 1.88       |
| 9        | 44                   | 36  | 80    | 4.47     | 40.52   | 7.8    | 1.96       |
| 10       | 36                   | 32  | 68    | 4.81     | 43.26   | 8.92   | 1.98       |

10.2.1 Bar graph : Dihedral 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

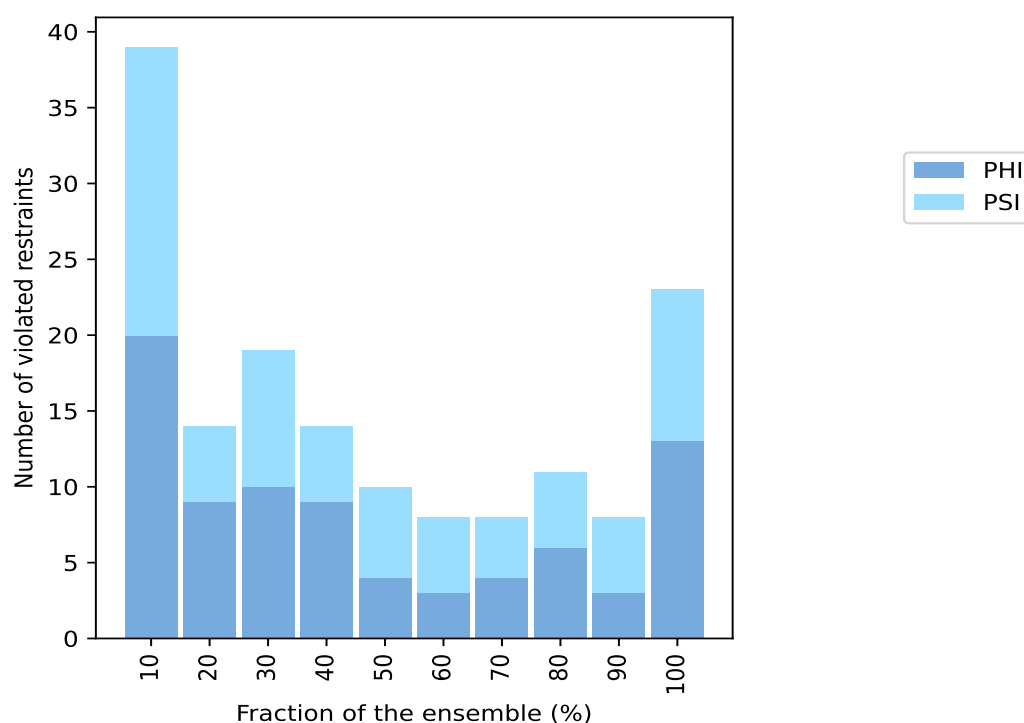
### 10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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>       | %     |
| 20                            | 19  | 39    | 1                        | 10.0  |
| 9                             | 5   | 14    | 2                        | 20.0  |
| 10                            | 9   | 19    | 3                        | 30.0  |
| 9                             | 5   | 14    | 4                        | 40.0  |
| 4                             | 6   | 10    | 5                        | 50.0  |
| 3                             | 5   | 8     | 6                        | 60.0  |
| 4                             | 4   | 8     | 7                        | 70.0  |
| 6                             | 5   | 11    | 8                        | 80.0  |
| 3                             | 5   | 8     | 9                        | 90.0  |
| 13                            | 10  | 23    | 10                       | 100.0 |

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

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

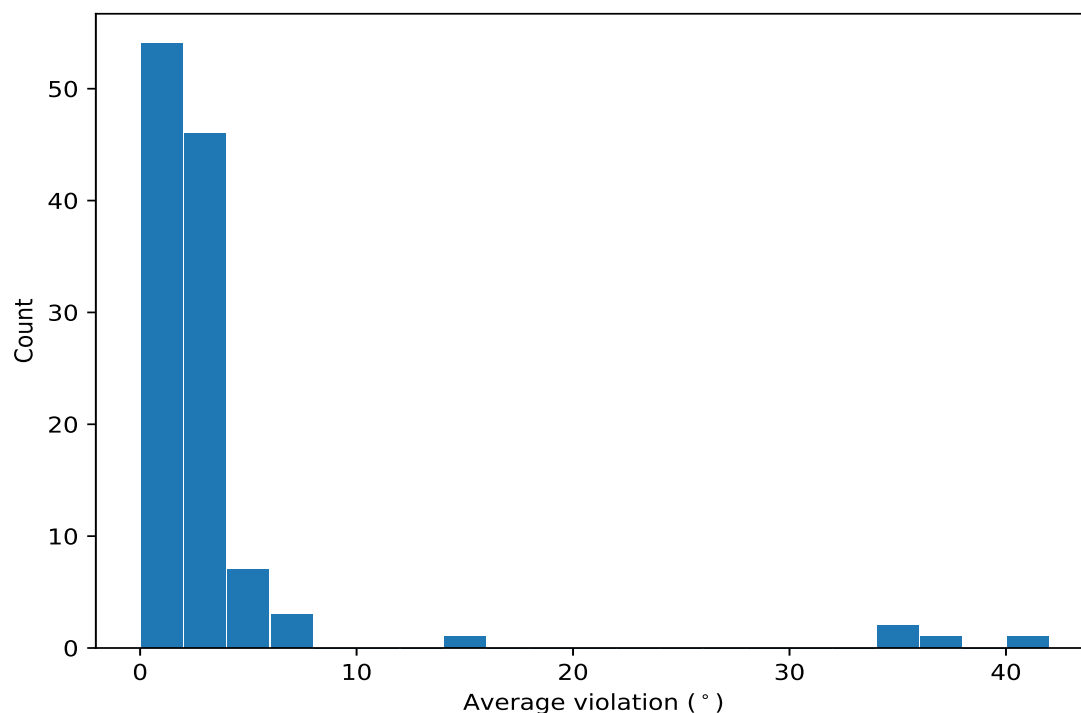




## 10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

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

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



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

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

| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Models <sup>1</sup> | Mean  | SD <sup>2</sup> | Median |
|---------|---------------|----------------|----------------|---------------|---------------------|-------|-----------------|--------|
| (1,222) | 1:150:A:PRO:N | 1:150:A:PRO:CA | 1:150:A:PRO:C  | 1:151:A:VAL:N | 10                  | 40.3  | 0.62            | 40.12  |
| (1,226) | 1:152:A:ALA:N | 1:152:A:ALA:CA | 1:152:A:ALA:C  | 1:153:A:ILE:N | 10                  | 37.47 | 2.93            | 36.34  |
| (1,14)  | 1:28:A:HIS:N  | 1:28:A:HIS:CA  | 1:28:A:HIS:C   | 1:29:A:LEU:N  | 10                  | 35.8  | 0.19            | 35.86  |
| (1,157) | 1:112:A:VAL:C | 1:113:A:LEU:N  | 1:113:A:LEU:CA | 1:113:A:LEU:C | 10                  | 35.28 | 0.86            | 35.57  |
| (1,9)   | 1:25:A:VAL:C  | 1:26:A:GLU:N   | 1:26:A:GLU:CA  | 1:26:A:GLU:C  | 10                  | 15.78 | 2.3             | 14.58  |
| (1,196) | 1:134:A:TRP:N | 1:134:A:TRP:CA | 1:134:A:TRP:C  | 1:135:A:VAL:N | 10                  | 6.09  | 0.71            | 6.04   |
| (1,204) | 1:138:A:GLU:N | 1:138:A:GLU:CA | 1:138:A:GLU:C  | 1:139:A:PRO:N | 10                  | 5.55  | 0.38            | 5.64   |
| (1,24)  | 1:33:A:THR:N  | 1:33:A:THR:CA  | 1:33:A:THR:C   | 1:34:A:PRO:N  | 10                  | 5.27  | 0.91            | 5.23   |
| (1,223) | 1:150:A:PRO:C | 1:151:A:VAL:N  | 1:151:A:VAL:CA | 1:151:A:VAL:C | 10                  | 4.63  | 0.52            | 4.68   |
| (1,7)   | 1:24:A:ASP:C  | 1:25:A:VAL:N   | 1:25:A:VAL:CA  | 1:25:A:VAL:C  | 10                  | 4.04  | 0.42            | 4.19   |
| (1,12)  | 1:27:A:SER:N  | 1:27:A:SER:CA  | 1:27:A:SER:C   | 1:28:A:HIS:N  | 10                  | 3.7   | 0.52            | 3.71   |
| (1,13)  | 1:27:A:SER:C  | 1:28:A:HIS:N   | 1:28:A:HIS:CA  | 1:28:A:HIS:C  | 10                  | 3.08  | 0.46            | 3.14   |
| (1,176) | 1:122:A:TYR:N | 1:122:A:TYR:CA | 1:122:A:TYR:C  | 1:123:A:PRO:N | 10                  | 2.68  | 0.72            | 2.56   |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Models <sup>1</sup> | Mean | SD <sup>2</sup> | Median |
|---------|---------------|----------------|----------------|---------------|---------------------|------|-----------------|--------|
| (1,53)  | 1:56:A:ASN:C  | 1:57:A:ASP:N   | 1:57:A:ASP:CA  | 1:57:A:ASP:C  | 10                  | 2.5  | 0.76            | 2.68   |
| (1,26)  | 1:34:A:PRO:N  | 1:34:A:PRO:CA  | 1:34:A:PRO:C   | 1:35:A:ALA:N  | 10                  | 2.31 | 0.51            | 2.17   |
| (1,69)  | 1:64:A:LEU:C  | 1:65:A:ALA:N   | 1:65:A:ALA:CA  | 1:65:A:ALA:C  | 10                  | 2.29 | 0.86            | 2.16   |
| (1,11)  | 1:26:A:GLU:C  | 1:27:A:SER:N   | 1:27:A:SER:CA  | 1:27:A:SER:C  | 10                  | 2.23 | 0.43            | 2.3    |
| (1,127) | 1:96:A:SER:C  | 1:97:A:GLU:N   | 1:97:A:GLU:CA  | 1:97:A:GLU:C  | 10                  | 2.21 | 0.34            | 2.23   |
| (1,197) | 1:134:A:TRP:C | 1:135:A:VAL:N  | 1:135:A:VAL:CA | 1:135:A:VAL:C | 10                  | 2.21 | 0.48            | 2.08   |
| (1,240) | 1:159:A:PHE:N | 1:159:A:PHE:CA | 1:159:A:PHE:C  | 1:160:A:TYR:N | 10                  | 2.01 | 0.73            | 1.76   |
| (1,237) | 1:157:A:LYS:C | 1:158:A:ALA:N  | 1:158:A:ALA:CA | 1:158:A:ALA:C | 10                  | 2.0  | 0.22            | 2.0    |
| (1,203) | 1:137:A:GLY:C | 1:138:A:GLU:N  | 1:138:A:GLU:CA | 1:138:A:GLU:C | 10                  | 1.67 | 0.25            | 1.7    |
| (1,103) | 1:81:A:ILE:C  | 1:82:A:THR:N   | 1:82:A:THR:CA  | 1:82:A:THR:C  | 10                  | 1.6  | 0.34            | 1.56   |
| (1,93)  | 1:76:A:TYR:C  | 1:77:A:LEU:N   | 1:77:A:LEU:CA  | 1:77:A:LEU:C  | 9                   | 3.02 | 1.41            | 2.93   |
| (1,83)  | 1:71:A:LYS:C  | 1:72:A:PRO:N   | 1:72:A:PRO:CA  | 1:72:A:PRO:C  | 9                   | 2.58 | 0.89            | 2.4    |
| (1,75)  | 1:67:A:ALA:C  | 1:68:A:GLU:N   | 1:68:A:GLU:CA  | 1:68:A:GLU:C  | 9                   | 2.19 | 0.48            | 2.21   |
| (1,206) | 1:141:A:LYS:N | 1:141:A:LYS:CA | 1:141:A:LYS:C  | 1:142:A:ILE:N | 9                   | 2.12 | 0.66            | 1.84   |
| (1,52)  | 1:56:A:ASN:N  | 1:56:A:ASN:CA  | 1:56:A:ASN:C   | 1:57:A:ASP:N  | 9                   | 2.06 | 1.05            | 1.72   |
| (1,144) | 1:105:A:ASP:N | 1:105:A:ASP:CA | 1:105:A:ASP:C  | 1:106:A:ASN:N | 9                   | 1.96 | 0.17            | 1.98   |
| (1,68)  | 1:64:A:LEU:N  | 1:64:A:LEU:CA  | 1:64:A:LEU:C   | 1:65:A:ALA:N  | 9                   | 1.71 | 0.6             | 1.49   |
| (1,244) | 1:161:A:GLU:N | 1:161:A:GLU:CA | 1:161:A:GLU:C  | 1:162:A:ALA:N | 9                   | 1.65 | 0.37            | 1.76   |
| (1,82)  | 1:71:A:LYS:N  | 1:71:A:LYS:CA  | 1:71:A:LYS:C   | 1:72:A:PRO:N  | 8                   | 2.44 | 1.13            | 2.08   |
| (1,105) | 1:82:A:THR:C  | 1:83:A:SER:N   | 1:83:A:SER:CA  | 1:83:A:SER:C  | 8                   | 2.32 | 1.0             | 2.43   |
| (1,249) | 1:163:A:LYS:C | 1:164:A:GLU:N  | 1:164:A:GLU:CA | 1:164:A:GLU:C | 8                   | 2.19 | 0.67            | 1.94   |
| (1,160) | 1:114:A:ASP:N | 1:114:A:ASP:CA | 1:114:A:ASP:C  | 1:115:A:LYS:N | 8                   | 2.12 | 1.01            | 1.94   |
| (1,207) | 1:141:A:LYS:C | 1:142:A:ILE:N  | 1:142:A:ILE:CA | 1:142:A:ILE:C | 8                   | 1.92 | 0.57            | 1.8    |
| (1,248) | 1:163:A:LYS:N | 1:163:A:LYS:CA | 1:163:A:LYS:C  | 1:164:A:GLU:N | 8                   | 1.72 | 0.44            | 1.53   |
| (1,255) | 1:166:A:MET:C | 1:167:A:LEU:N  | 1:167:A:LEU:CA | 1:167:A:LEU:C | 8                   | 1.7  | 0.28            | 1.7    |
| (1,8)   | 1:25:A:VAL:N  | 1:25:A:VAL:CA  | 1:25:A:VAL:C   | 1:26:A:GLU:N  | 8                   | 1.61 | 0.39            | 1.52   |
| (1,114) | 1:87:A:THR:N  | 1:87:A:THR:CA  | 1:87:A:THR:C   | 1:88:A:ASN:N  | 8                   | 1.48 | 0.41            | 1.46   |
| (1,145) | 1:105:A:ASP:C | 1:106:A:ASN:N  | 1:106:A:ASN:CA | 1:106:A:ASN:C | 8                   | 1.37 | 0.15            | 1.44   |
| (1,141) | 1:103:A:SER:C | 1:104:A:LEU:N  | 1:104:A:LEU:CA | 1:104:A:LEU:C | 8                   | 1.19 | 0.14            | 1.14   |
| (1,79)  | 1:69:A:GLN:C  | 1:70:A:LEU:N   | 1:70:A:LEU:CA  | 1:70:A:LEU:C  | 7                   | 2.27 | 1.27            | 2.0    |
| (1,81)  | 1:70:A:LEU:C  | 1:71:A:LYS:N   | 1:71:A:LYS:CA  | 1:71:A:LYS:C  | 7                   | 2.26 | 1.09            | 1.75   |
| (1,47)  | 1:51:A:ILE:C  | 1:52:A:LYS:N   | 1:52:A:LYS:CA  | 1:52:A:LYS:C  | 7                   | 2.11 | 0.23            | 2.04   |
| (1,22)  | 1:32:A:ILE:N  | 1:32:A:ILE:CA  | 1:32:A:ILE:C   | 1:33:A:THR:N  | 7                   | 2.11 | 0.83            | 2.72   |
| (1,254) | 1:166:A:MET:N | 1:166:A:MET:CA | 1:166:A:MET:C  | 1:167:A:LEU:N | 7                   | 1.98 | 0.89            | 1.46   |
| (1,20)  | 1:31:A:SER:N  | 1:31:A:SER:CA  | 1:31:A:SER:C   | 1:32:A:ILE:N  | 7                   | 1.95 | 0.39            | 1.95   |
| (1,263) | 1:171:A:LEU:C | 1:172:A:PRO:N  | 1:172:A:PRO:CA | 1:172:A:PRO:C | 7                   | 1.85 | 0.22            | 1.8    |
| (1,172) | 1:120:A:VAL:N | 1:120:A:VAL:CA | 1:120:A:VAL:C  | 1:121:A:LEU:N | 7                   | 1.72 | 0.58            | 1.59   |
| (1,186) | 1:129:A:THR:N | 1:129:A:THR:CA | 1:129:A:THR:C  | 1:130:A:ASN:N | 6                   | 2.38 | 0.6             | 2.53   |
| (1,213) | 1:144:A:VAL:C | 1:145:A:TYR:N  | 1:145:A:TYR:CA | 1:145:A:TYR:C | 6                   | 2.09 | 0.53            | 2.36   |
| (1,225) | 1:151:A:VAL:C | 1:152:A:ALA:N  | 1:152:A:ALA:CA | 1:152:A:ALA:C | 6                   | 1.77 | 0.43            | 1.77   |
| (1,46)  | 1:51:A:ILE:N  | 1:51:A:ILE:CA  | 1:51:A:ILE:C   | 1:52:A:LYS:N  | 6                   | 1.61 | 0.4             | 1.48   |
| (1,183) | 1:126:A:THR:C | 1:127:A:GLY:N  | 1:127:A:GLY:CA | 1:127:A:GLY:C | 6                   | 1.34 | 0.22            | 1.4    |
| (1,36)  | 1:46:A:TYR:N  | 1:46:A:TYR:CA  | 1:46:A:TYR:C   | 1:47:A:ALA:N  | 6                   | 1.27 | 0.16            | 1.22   |
| (1,182) | 1:126:A:THR:N | 1:126:A:THR:CA | 1:126:A:THR:C  | 1:127:A:GLY:N | 6                   | 1.25 | 0.18            | 1.27   |
| (1,284) | 1:182:A:VAL:N | 1:182:A:VAL:CA | 1:182:A:VAL:C  | 1:183:A:GLY:N | 6                   | 1.12 | 0.09            | 1.12   |
| (1,96)  | 1:78:A:GLN:N  | 1:78:A:GLN:CA  | 1:78:A:GLN:C   | 1:79:A:ILE:N  | 5                   | 4.08 | 0.31            | 4.13   |
| (1,218) | 1:148:A:THR:N | 1:148:A:THR:CA | 1:148:A:THR:C  | 1:149:A:LYS:N | 5                   | 2.44 | 0.51            | 2.38   |
| (1,259) | 1:169:A:ASP:C | 1:170:A:SER:N  | 1:170:A:SER:CA | 1:170:A:SER:C | 5                   | 2.12 | 1.09            | 1.65   |
| (1,219) | 1:148:A:THR:C | 1:149:A:LYS:N  | 1:149:A:LYS:CA | 1:149:A:LYS:C | 5                   | 2.1  | 0.49            | 1.89   |
| (1,76)  | 1:68:A:GLU:N  | 1:68:A:GLU:CA  | 1:68:A:GLU:C   | 1:69:A:GLN:N  | 5                   | 2.08 | 0.74            | 1.91   |
| (1,104) | 1:82:A:THR:N  | 1:82:A:THR:CA  | 1:82:A:THR:C   | 1:83:A:SER:N  | 5                   | 1.67 | 0.44            | 1.47   |

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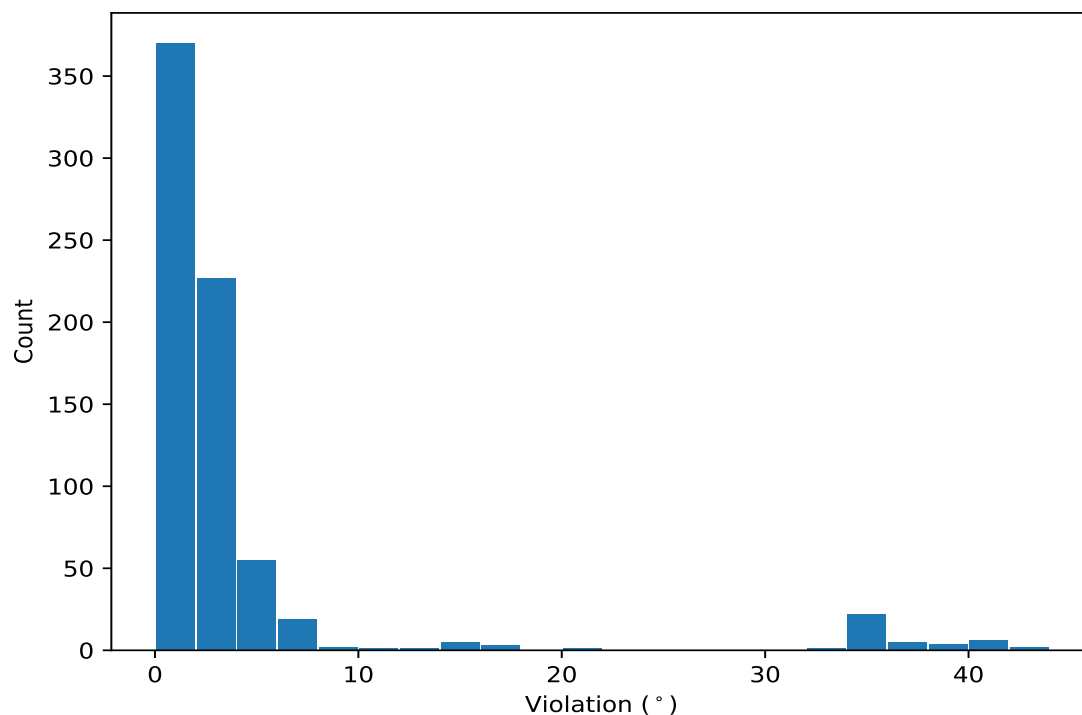
| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Models <sup>1</sup> | Mean | SD <sup>2</sup> | Median |
|---------|---------------|----------------|----------------|---------------|---------------------|------|-----------------|--------|
| (1,97)  | 1:78:A:GLN:C  | 1:79:A:ILE:N   | 1:79:A:ILE:CA  | 1:79:A:ILE:C  | 5                   | 1.63 | 0.19            | 1.72   |
| (1,42)  | 1:49:A:VAL:N  | 1:49:A:VAL:CA  | 1:49:A:VAL:C   | 1:50:A:TRP:N  | 5                   | 1.48 | 0.47            | 1.37   |
| (1,261) | 1:170:A:SER:C | 1:171:A:LEU:N  | 1:171:A:LEU:CA | 1:171:A:LEU:C | 5                   | 1.47 | 0.26            | 1.39   |
| (1,198) | 1:135:A:VAL:N | 1:135:A:VAL:CA | 1:135:A:VAL:C  | 1:136:A:PRO:N | 5                   | 1.29 | 0.13            | 1.34   |
| (1,78)  | 1:69:A:GLN:N  | 1:69:A:GLN:CA  | 1:69:A:GLN:C   | 1:70:A:LEU:N  | 4                   | 4.67 | 2.06            | 4.82   |
| (1,117) | 1:89:A:SER:C  | 1:90:A:THR:N   | 1:90:A:THR:CA  | 1:90:A:THR:C  | 4                   | 3.54 | 2.08            | 3.47   |
| (1,253) | 1:165:A:GLY:C | 1:166:A:MET:N  | 1:166:A:MET:CA | 1:166:A:MET:C | 4                   | 2.93 | 0.45            | 3.0    |
| (1,122) | 1:92:A:LEU:N  | 1:92:A:LEU:CA  | 1:92:A:LEU:C   | 1:93:A:GLY:N  | 4                   | 2.24 | 1.44            | 1.58   |
| (1,95)  | 1:77:A:LEU:C  | 1:78:A:GLN:N   | 1:78:A:GLN:CA  | 1:78:A:GLN:C  | 4                   | 2.16 | 0.35            | 2.25   |
| (1,187) | 1:129:A:THR:C | 1:130:A:ASN:N  | 1:130:A:ASN:CA | 1:130:A:ASN:C | 4                   | 2.09 | 0.24            | 1.98   |
| (1,106) | 1:83:A:SER:N  | 1:83:A:SER:CA  | 1:83:A:SER:C   | 1:84:A:GLY:N  | 4                   | 1.88 | 0.8             | 1.56   |
| (1,85)  | 1:72:A:PRO:C  | 1:73:A:TYR:N   | 1:73:A:TYR:CA  | 1:73:A:TYR:C  | 4                   | 1.87 | 0.65            | 1.66   |
| (1,188) | 1:130:A:ASN:N | 1:130:A:ASN:CA | 1:130:A:ASN:C  | 1:131:A:THR:N | 4                   | 1.7  | 0.26            | 1.66   |
| (1,133) | 1:99:A:LYS:C  | 1:100:A:ALA:N  | 1:100:A:ALA:CA | 1:100:A:ALA:C | 4                   | 1.5  | 0.32            | 1.38   |
| (1,165) | 1:116:A:GLU:C | 1:117:A:ASP:N  | 1:117:A:ASP:CA | 1:117:A:ASP:C | 4                   | 1.3  | 0.21            | 1.29   |
| (1,202) | 1:137:A:GLY:N | 1:137:A:GLY:CA | 1:137:A:GLY:C  | 1:138:A:GLU:N | 4                   | 1.29 | 0.08            | 1.28   |
| (1,267) | 1:173:A:VAL:C | 1:174:A:ILE:N  | 1:174:A:ILE:CA | 1:174:A:ILE:C | 4                   | 1.28 | 0.11            | 1.28   |
| (1,49)  | 1:54:A:GLN:C  | 1:55:A:VAL:N   | 1:55:A:VAL:CA  | 1:55:A:VAL:C  | 4                   | 1.24 | 0.1             | 1.24   |
| (1,121) | 1:91:A:ALA:C  | 1:92:A:LEU:N   | 1:92:A:LEU:CA  | 1:92:A:LEU:C  | 3                   | 7.19 | 4.35            | 9.99   |
| (1,120) | 1:91:A:ALA:N  | 1:91:A:ALA:CA  | 1:91:A:ALA:C   | 1:92:A:LEU:N  | 3                   | 6.09 | 2.63            | 7.49   |
| (1,116) | 1:89:A:SER:N  | 1:89:A:SER:CA  | 1:89:A:SER:C   | 1:90:A:THR:N  | 3                   | 5.68 | 3.03            | 7.67   |
| (1,124) | 1:95:A:PHE:N  | 1:95:A:PHE:CA  | 1:95:A:PHE:C   | 1:96:A:SER:N  | 3                   | 3.87 | 0.45            | 3.65   |
| (1,44)  | 1:50:A:TRP:N  | 1:50:A:TRP:CA  | 1:50:A:TRP:C   | 1:51:A:ILE:N  | 3                   | 3.81 | 0.25            | 3.77   |
| (1,45)  | 1:50:A:TRP:C  | 1:51:A:ILE:N   | 1:51:A:ILE:CA  | 1:51:A:ILE:C  | 3                   | 3.37 | 0.23            | 3.48   |
| (1,125) | 1:95:A:PHE:C  | 1:96:A:SER:N   | 1:96:A:SER:CA  | 1:96:A:SER:C  | 3                   | 3.25 | 0.39            | 3.13   |
| (1,92)  | 1:76:A:TYR:N  | 1:76:A:TYR:CA  | 1:76:A:TYR:C   | 1:77:A:LEU:N  | 3                   | 2.44 | 1.57            | 1.6    |
| (1,241) | 1:159:A:PHE:C | 1:160:A:TYR:N  | 1:160:A:TYR:CA | 1:160:A:TYR:C | 3                   | 2.31 | 0.19            | 2.18   |
| (1,86)  | 1:73:A:TYR:N  | 1:73:A:TYR:CA  | 1:73:A:TYR:C   | 1:74:A:PHE:N  | 3                   | 2.04 | 0.61            | 1.98   |
| (1,25)  | 1:33:A:THR:C  | 1:34:A:PRO:N   | 1:34:A:PRO:CA  | 1:34:A:PRO:C  | 3                   | 1.89 | 0.54            | 1.76   |
| (1,131) | 1:98:A:THR:C  | 1:99:A:LYS:N   | 1:99:A:LYS:CA  | 1:99:A:LYS:C  | 3                   | 1.73 | 0.38            | 1.88   |
| (1,189) | 1:130:A:ASN:C | 1:131:A:THR:N  | 1:131:A:THR:CA | 1:131:A:THR:C | 3                   | 1.55 | 0.28            | 1.45   |
| (1,184) | 1:127:A:GLY:N | 1:127:A:GLY:CA | 1:127:A:GLY:C  | 1:128:A:TYR:N | 3                   | 1.53 | 0.14            | 1.51   |
| (1,126) | 1:96:A:SER:N  | 1:96:A:SER:CA  | 1:96:A:SER:C   | 1:97:A:GLU:N  | 3                   | 1.51 | 0.04            | 1.5    |
| (1,212) | 1:144:A:VAL:N | 1:144:A:VAL:CA | 1:144:A:VAL:C  | 1:145:A:TYR:N | 3                   | 1.5  | 0.3             | 1.63   |
| (1,3)   | 1:22:A:PRO:C  | 1:23:A:ILE:N   | 1:23:A:ILE:CA  | 1:23:A:ILE:C  | 3                   | 1.48 | 0.35            | 1.35   |
| (1,169) | 1:118:A:ILE:C | 1:119:A:ALA:N  | 1:119:A:ALA:CA | 1:119:A:ALA:C | 3                   | 1.4  | 0.4             | 1.22   |
| (1,73)  | 1:66:A:ASN:C  | 1:67:A:ALA:N   | 1:67:A:ALA:CA  | 1:67:A:ALA:C  | 3                   | 1.22 | 0.15            | 1.17   |
| (1,113) | 1:86:A:GLU:C  | 1:87:A:THR:N   | 1:87:A:THR:CA  | 1:87:A:THR:C  | 2                   | 3.26 | 1.36            | 3.26   |
| (1,252) | 1:165:A:GLY:N | 1:165:A:GLY:CA | 1:165:A:GLY:C  | 1:166:A:MET:N | 2                   | 2.58 | 0.17            | 2.58   |
| (1,111) | 1:85:A:TYR:C  | 1:86:A:GLU:N   | 1:86:A:GLU:CA  | 1:86:A:GLU:C  | 2                   | 2.46 | 0.96            | 2.46   |
| (1,107) | 1:83:A:SER:C  | 1:84:A:GLY:N   | 1:84:A:GLY:CA  | 1:84:A:GLY:C  | 2                   | 2.22 | 0.84            | 2.22   |
| (1,87)  | 1:73:A:TYR:C  | 1:74:A:PHE:N   | 1:74:A:PHE:CA  | 1:74:A:PHE:C  | 2                   | 1.73 | 0.71            | 1.73   |
| (1,177) | 1:122:A:TYR:C | 1:123:A:PRO:N  | 1:123:A:PRO:CA | 1:123:A:PRO:C | 2                   | 1.5  | 0.4             | 1.5    |
| (1,118) | 1:90:A:THR:N  | 1:90:A:THR:CA  | 1:90:A:THR:C   | 1:91:A:ALA:N  | 2                   | 1.46 | 0.29            | 1.46   |
| (1,84)  | 1:72:A:PRO:N  | 1:72:A:PRO:CA  | 1:72:A:PRO:C   | 1:73:A:TYR:N  | 2                   | 1.45 | 0.24            | 1.45   |
| (1,148) | 1:108:A:SER:N | 1:108:A:SER:CA | 1:108:A:SER:C  | 1:109:A:ALA:N | 2                   | 1.32 | 0.21            | 1.32   |
| (1,173) | 1:120:A:VAL:C | 1:121:A:LEU:N  | 1:121:A:LEU:CA | 1:121:A:LEU:C | 2                   | 1.3  | 0.15            | 1.3    |
| (1,215) | 1:146:A:ASN:C | 1:147:A:GLU:N  | 1:147:A:GLU:CA | 1:147:A:GLU:C | 2                   | 1.3  | 0.08            | 1.3    |
| (1,146) | 1:106:A:ASN:N | 1:106:A:ASN:CA | 1:106:A:ASN:C  | 1:107:A:PRO:N | 2                   | 1.18 | 0.16            | 1.18   |
| (1,195) | 1:133:A:ILE:C | 1:134:A:TRP:N  | 1:134:A:TRP:CA | 1:134:A:TRP:C | 2                   | 1.11 | 0.06            | 1.11   |
| (1,119) | 1:90:A:THR:C  | 1:91:A:ALA:N   | 1:91:A:ALA:CA  | 1:91:A:ALA:C  | 2                   | 1.06 | 0.06            | 1.06   |

<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 (°) |
|---------|---------------|----------------|---------------|---------------|----------|---------------|
| (1,226) | 1:152:A:ALA:N | 1:152:A:ALA:CA | 1:152:A:ALA:C | 1:153:A:ILE:N | 10       | 43.26         |
| (1,226) | 1:152:A:ALA:N | 1:152:A:ALA:CA | 1:152:A:ALA:C | 1:153:A:ILE:N | 6        | 43.13         |
| (1,222) | 1:150:A:PRO:N | 1:150:A:PRO:CA | 1:150:A:PRO:C | 1:151:A:VAL:N | 8        | 41.94         |
| (1,222) | 1:150:A:PRO:N | 1:150:A:PRO:CA | 1:150:A:PRO:C | 1:151:A:VAL:N | 4        | 40.62         |
| (1,222) | 1:150:A:PRO:N | 1:150:A:PRO:CA | 1:150:A:PRO:C | 1:151:A:VAL:N | 9        | 40.52         |
| (1,222) | 1:150:A:PRO:N | 1:150:A:PRO:CA | 1:150:A:PRO:C | 1:151:A:VAL:N | 3        | 40.34         |
| (1,222) | 1:150:A:PRO:N | 1:150:A:PRO:CA | 1:150:A:PRO:C | 1:151:A:VAL:N | 5        | 40.21         |
| (1,222) | 1:150:A:PRO:N | 1:150:A:PRO:CA | 1:150:A:PRO:C | 1:151:A:VAL:N | 1        | 40.03         |
| (1,222) | 1:150:A:PRO:N | 1:150:A:PRO:CA | 1:150:A:PRO:C | 1:151:A:VAL:N | 7        | 39.99         |
| (1,222) | 1:150:A:PRO:N | 1:150:A:PRO:CA | 1:150:A:PRO:C | 1:151:A:VAL:N | 2        | 39.91         |
| (1,222) | 1:150:A:PRO:N | 1:150:A:PRO:CA | 1:150:A:PRO:C | 1:151:A:VAL:N | 10       | 39.81         |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,222) | 1:150:A:PRO:N | 1:150:A:PRO:CA | 1:150:A:PRO:C  | 1:151:A:VAL:N | 6        | 39.66         |
| (1,226) | 1:152:A:ALA:N | 1:152:A:ALA:CA | 1:152:A:ALA:C  | 1:153:A:ILE:N | 3        | 37.22         |
| (1,226) | 1:152:A:ALA:N | 1:152:A:ALA:CA | 1:152:A:ALA:C  | 1:153:A:ILE:N | 8        | 36.78         |
| (1,226) | 1:152:A:ALA:N | 1:152:A:ALA:CA | 1:152:A:ALA:C  | 1:153:A:ILE:N | 2        | 36.68         |
| (1,14)  | 1:28:A:HIS:N  | 1:28:A:HIS:CA  | 1:28:A:HIS:C   | 1:29:A:LEU:N  | 2        | 36.14         |
| (1,226) | 1:152:A:ALA:N | 1:152:A:ALA:CA | 1:152:A:ALA:C  | 1:153:A:ILE:N | 4        | 36.0          |
| (1,157) | 1:112:A:VAL:C | 1:113:A:LEU:N  | 1:113:A:LEU:CA | 1:113:A:LEU:C | 7        | 35.94         |
| (1,14)  | 1:28:A:HIS:N  | 1:28:A:HIS:CA  | 1:28:A:HIS:C   | 1:29:A:LEU:N  | 10       | 35.94         |
| (1,14)  | 1:28:A:HIS:N  | 1:28:A:HIS:CA  | 1:28:A:HIS:C   | 1:29:A:LEU:N  | 5        | 35.91         |
| (1,14)  | 1:28:A:HIS:N  | 1:28:A:HIS:CA  | 1:28:A:HIS:C   | 1:29:A:LEU:N  | 8        | 35.91         |
| (1,14)  | 1:28:A:HIS:N  | 1:28:A:HIS:CA  | 1:28:A:HIS:C   | 1:29:A:LEU:N  | 7        | 35.86         |
| (1,14)  | 1:28:A:HIS:N  | 1:28:A:HIS:CA  | 1:28:A:HIS:C   | 1:29:A:LEU:N  | 9        | 35.86         |
| (1,157) | 1:112:A:VAL:C | 1:113:A:LEU:N  | 1:113:A:LEU:CA | 1:113:A:LEU:C | 6        | 35.84         |
| (1,14)  | 1:28:A:HIS:N  | 1:28:A:HIS:CA  | 1:28:A:HIS:C   | 1:29:A:LEU:N  | 4        | 35.75         |
| (1,157) | 1:112:A:VAL:C | 1:113:A:LEU:N  | 1:113:A:LEU:CA | 1:113:A:LEU:C | 3        | 35.72         |
| (1,157) | 1:112:A:VAL:C | 1:113:A:LEU:N  | 1:113:A:LEU:CA | 1:113:A:LEU:C | 10       | 35.67         |
| (1,157) | 1:112:A:VAL:C | 1:113:A:LEU:N  | 1:113:A:LEU:CA | 1:113:A:LEU:C | 8        | 35.61         |
| (1,14)  | 1:28:A:HIS:N  | 1:28:A:HIS:CA  | 1:28:A:HIS:C   | 1:29:A:LEU:N  | 6        | 35.61         |
| (1,14)  | 1:28:A:HIS:N  | 1:28:A:HIS:CA  | 1:28:A:HIS:C   | 1:29:A:LEU:N  | 1        | 35.54         |
| (1,157) | 1:112:A:VAL:C | 1:113:A:LEU:N  | 1:113:A:LEU:CA | 1:113:A:LEU:C | 4        | 35.53         |
| (1,14)  | 1:28:A:HIS:N  | 1:28:A:HIS:CA  | 1:28:A:HIS:C   | 1:29:A:LEU:N  | 3        | 35.51         |
| (1,226) | 1:152:A:ALA:N | 1:152:A:ALA:CA | 1:152:A:ALA:C  | 1:153:A:ILE:N | 9        | 35.48         |
| (1,226) | 1:152:A:ALA:N | 1:152:A:ALA:CA | 1:152:A:ALA:C  | 1:153:A:ILE:N | 7        | 35.46         |
| (1,226) | 1:152:A:ALA:N | 1:152:A:ALA:CA | 1:152:A:ALA:C  | 1:153:A:ILE:N | 1        | 35.36         |
| (1,157) | 1:112:A:VAL:C | 1:113:A:LEU:N  | 1:113:A:LEU:CA | 1:113:A:LEU:C | 9        | 35.33         |
| (1,226) | 1:152:A:ALA:N | 1:152:A:ALA:CA | 1:152:A:ALA:C  | 1:153:A:ILE:N | 5        | 35.31         |
| (1,157) | 1:112:A:VAL:C | 1:113:A:LEU:N  | 1:113:A:LEU:CA | 1:113:A:LEU:C | 2        | 35.27         |
| (1,157) | 1:112:A:VAL:C | 1:113:A:LEU:N  | 1:113:A:LEU:CA | 1:113:A:LEU:C | 5        | 35.11         |
| (1,157) | 1:112:A:VAL:C | 1:113:A:LEU:N  | 1:113:A:LEU:CA | 1:113:A:LEU:C | 1        | 32.8          |
| (1,9)   | 1:25:A:VAL:C  | 1:26:A:GLU:N   | 1:26:A:GLU:CA  | 1:26:A:GLU:C  | 10       | 21.35         |
| (1,9)   | 1:25:A:VAL:C  | 1:26:A:GLU:N   | 1:26:A:GLU:CA  | 1:26:A:GLU:C  | 3        | 17.55         |
| (1,9)   | 1:25:A:VAL:C  | 1:26:A:GLU:N   | 1:26:A:GLU:CA  | 1:26:A:GLU:C  | 7        | 17.31         |
| (1,9)   | 1:25:A:VAL:C  | 1:26:A:GLU:N   | 1:26:A:GLU:CA  | 1:26:A:GLU:C  | 9        | 16.44         |
| (1,9)   | 1:25:A:VAL:C  | 1:26:A:GLU:N   | 1:26:A:GLU:CA  | 1:26:A:GLU:C  | 5        | 14.64         |
| (1,9)   | 1:25:A:VAL:C  | 1:26:A:GLU:N   | 1:26:A:GLU:CA  | 1:26:A:GLU:C  | 6        | 14.52         |
| (1,9)   | 1:25:A:VAL:C  | 1:26:A:GLU:N   | 1:26:A:GLU:CA  | 1:26:A:GLU:C  | 2        | 14.31         |
| (1,9)   | 1:25:A:VAL:C  | 1:26:A:GLU:N   | 1:26:A:GLU:CA  | 1:26:A:GLU:C  | 8        | 14.13         |
| (1,9)   | 1:25:A:VAL:C  | 1:26:A:GLU:N   | 1:26:A:GLU:CA  | 1:26:A:GLU:C  | 1        | 14.1          |
| (1,9)   | 1:25:A:VAL:C  | 1:26:A:GLU:N   | 1:26:A:GLU:CA  | 1:26:A:GLU:C  | 4        | 13.45         |
| (1,121) | 1:91:A:ALA:C  | 1:92:A:LEU:N   | 1:92:A:LEU:CA  | 1:92:A:LEU:C  | 9        | 10.53         |
| (1,121) | 1:91:A:ALA:C  | 1:92:A:LEU:N   | 1:92:A:LEU:CA  | 1:92:A:LEU:C  | 2        | 9.99          |
| (1,120) | 1:91:A:ALA:N  | 1:91:A:ALA:CA  | 1:91:A:ALA:C   | 1:92:A:LEU:N  | 2        | 8.38          |
| (1,116) | 1:89:A:SER:N  | 1:89:A:SER:CA  | 1:89:A:SER:C   | 1:90:A:THR:N  | 9        | 7.98          |
| (1,116) | 1:89:A:SER:N  | 1:89:A:SER:CA  | 1:89:A:SER:C   | 1:90:A:THR:N  | 2        | 7.67          |
| (1,196) | 1:134:A:TRP:N | 1:134:A:TRP:CA | 1:134:A:TRP:C  | 1:135:A:VAL:N | 7        | 7.66          |
| (1,120) | 1:91:A:ALA:N  | 1:91:A:ALA:CA  | 1:91:A:ALA:C   | 1:92:A:LEU:N  | 9        | 7.49          |
| (1,5)   | 1:23:A:ILE:C  | 1:24:A:ASP:N   | 1:24:A:ASP:CA  | 1:24:A:ASP:C  | 10       | 7.44          |
| (1,78)  | 1:69:A:GLN:N  | 1:69:A:GLN:CA  | 1:69:A:GLN:C   | 1:70:A:LEU:N  | 9        | 7.04          |
| (1,24)  | 1:33:A:THR:N  | 1:33:A:THR:CA  | 1:33:A:THR:C   | 1:34:A:PRO:N  | 10       | 6.85          |
| (1,196) | 1:134:A:TRP:N | 1:134:A:TRP:CA | 1:134:A:TRP:C  | 1:135:A:VAL:N | 1        | 6.81          |
| (1,93)  | 1:76:A:TYR:C  | 1:77:A:LEU:N   | 1:77:A:LEU:CA  | 1:77:A:LEU:C  | 10       | 6.56          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,24)  | 1:33:A:THR:N  | 1:33:A:THR:CA  | 1:33:A:THR:C   | 1:34:A:PRO:N  | 9        | 6.32          |
| (1,78)  | 1:69:A:GLN:N  | 1:69:A:GLN:CA  | 1:69:A:GLN:C   | 1:70:A:LEU:N  | 10       | 6.28          |
| (1,196) | 1:134:A:TRP:N | 1:134:A:TRP:CA | 1:134:A:TRP:C  | 1:135:A:VAL:N | 5        | 6.26          |
| (1,196) | 1:134:A:TRP:N | 1:134:A:TRP:CA | 1:134:A:TRP:C  | 1:135:A:VAL:N | 6        | 6.22          |
| (1,117) | 1:89:A:SER:C  | 1:90:A:THR:N   | 1:90:A:THR:CA  | 1:90:A:THR:C  | 9        | 6.2           |
| (1,204) | 1:138:A:GLU:N | 1:138:A:GLU:CA | 1:138:A:GLU:C  | 1:139:A:PRO:N | 7        | 6.05          |
| (1,196) | 1:134:A:TRP:N | 1:134:A:TRP:CA | 1:134:A:TRP:C  | 1:135:A:VAL:N | 8        | 6.05          |
| (1,196) | 1:134:A:TRP:N | 1:134:A:TRP:CA | 1:134:A:TRP:C  | 1:135:A:VAL:N | 4        | 6.04          |
| (1,204) | 1:138:A:GLU:N | 1:138:A:GLU:CA | 1:138:A:GLU:C  | 1:139:A:PRO:N | 3        | 6.03          |
| (1,196) | 1:134:A:TRP:N | 1:134:A:TRP:CA | 1:134:A:TRP:C  | 1:135:A:VAL:N | 10       | 6.01          |
| (1,204) | 1:138:A:GLU:N | 1:138:A:GLU:CA | 1:138:A:GLU:C  | 1:139:A:PRO:N | 8        | 5.88          |
| (1,24)  | 1:33:A:THR:N  | 1:33:A:THR:CA  | 1:33:A:THR:C   | 1:34:A:PRO:N  | 1        | 5.87          |
| (1,204) | 1:138:A:GLU:N | 1:138:A:GLU:CA | 1:138:A:GLU:C  | 1:139:A:PRO:N | 4        | 5.78          |
| (1,223) | 1:150:A:PRO:C | 1:151:A:VAL:N  | 1:151:A:VAL:CA | 1:151:A:VAL:C | 8        | 5.73          |
| (1,24)  | 1:33:A:THR:N  | 1:33:A:THR:CA  | 1:33:A:THR:C   | 1:34:A:PRO:N  | 5        | 5.72          |
| (1,204) | 1:138:A:GLU:N | 1:138:A:GLU:CA | 1:138:A:GLU:C  | 1:139:A:PRO:N | 9        | 5.64          |
| (1,204) | 1:138:A:GLU:N | 1:138:A:GLU:CA | 1:138:A:GLU:C  | 1:139:A:PRO:N | 10       | 5.63          |
| (1,200) | 1:136:A:PRO:N | 1:136:A:PRO:CA | 1:136:A:PRO:C  | 1:137:A:GLY:N | 7        | 5.56          |
| (1,196) | 1:134:A:TRP:N | 1:134:A:TRP:CA | 1:134:A:TRP:C  | 1:135:A:VAL:N | 2        | 5.56          |
| (1,24)  | 1:33:A:THR:N  | 1:33:A:THR:CA  | 1:33:A:THR:C   | 1:34:A:PRO:N  | 3        | 5.55          |
| (1,204) | 1:138:A:GLU:N | 1:138:A:GLU:CA | 1:138:A:GLU:C  | 1:139:A:PRO:N | 6        | 5.31          |
| (1,196) | 1:134:A:TRP:N | 1:134:A:TRP:CA | 1:134:A:TRP:C  | 1:135:A:VAL:N | 3        | 5.21          |
| (1,204) | 1:138:A:GLU:N | 1:138:A:GLU:CA | 1:138:A:GLU:C  | 1:139:A:PRO:N | 1        | 5.13          |
| (1,79)  | 1:69:A:GLN:C  | 1:70:A:LEU:N   | 1:70:A:LEU:CA  | 1:70:A:LEU:C  | 9        | 5.11          |
| (1,204) | 1:138:A:GLU:N | 1:138:A:GLU:CA | 1:138:A:GLU:C  | 1:139:A:PRO:N | 2        | 5.1           |
| (1,196) | 1:134:A:TRP:N | 1:134:A:TRP:CA | 1:134:A:TRP:C  | 1:135:A:VAL:N | 9        | 5.09          |
| (1,223) | 1:150:A:PRO:C | 1:151:A:VAL:N  | 1:151:A:VAL:CA | 1:151:A:VAL:C | 3        | 5.05          |
| (1,204) | 1:138:A:GLU:N | 1:138:A:GLU:CA | 1:138:A:GLU:C  | 1:139:A:PRO:N | 5        | 4.96          |
| (1,52)  | 1:56:A:ASN:N  | 1:56:A:ASN:CA  | 1:56:A:ASN:C   | 1:57:A:ASP:N  | 6        | 4.93          |
| (1,24)  | 1:33:A:THR:N  | 1:33:A:THR:CA  | 1:33:A:THR:C   | 1:34:A:PRO:N  | 6        | 4.91          |
| (1,117) | 1:89:A:SER:C  | 1:90:A:THR:N   | 1:90:A:THR:CA  | 1:90:A:THR:C  | 2        | 4.86          |
| (1,223) | 1:150:A:PRO:C | 1:151:A:VAL:N  | 1:151:A:VAL:CA | 1:151:A:VAL:C | 4        | 4.85          |
| (1,223) | 1:150:A:PRO:C | 1:151:A:VAL:N  | 1:151:A:VAL:CA | 1:151:A:VAL:C | 7        | 4.84          |
| (1,82)  | 1:71:A:LYS:N  | 1:71:A:LYS:CA  | 1:71:A:LYS:C   | 1:72:A:PRO:N  | 5        | 4.79          |
| (1,12)  | 1:27:A:SER:N  | 1:27:A:SER:CA  | 1:27:A:SER:C   | 1:28:A:HIS:N  | 3        | 4.75          |
| (1,223) | 1:150:A:PRO:C | 1:151:A:VAL:N  | 1:151:A:VAL:CA | 1:151:A:VAL:C | 5        | 4.71          |
| (1,122) | 1:92:A:LEU:N  | 1:92:A:LEU:CA  | 1:92:A:LEU:C   | 1:93:A:GLY:N  | 7        | 4.7           |
| (1,24)  | 1:33:A:THR:N  | 1:33:A:THR:CA  | 1:33:A:THR:C   | 1:34:A:PRO:N  | 8        | 4.66          |
| (1,223) | 1:150:A:PRO:C | 1:151:A:VAL:N  | 1:151:A:VAL:CA | 1:151:A:VAL:C | 1        | 4.64          |
| (1,92)  | 1:76:A:TYR:N  | 1:76:A:TYR:CA  | 1:76:A:TYR:C   | 1:77:A:LEU:N  | 10       | 4.64          |
| (1,113) | 1:86:A:GLU:C  | 1:87:A:THR:N   | 1:87:A:THR:CA  | 1:87:A:THR:C  | 9        | 4.61          |
| (1,24)  | 1:33:A:THR:N  | 1:33:A:THR:CA  | 1:33:A:THR:C   | 1:34:A:PRO:N  | 7        | 4.61          |
| (1,83)  | 1:71:A:LYS:C  | 1:72:A:PRO:N   | 1:72:A:PRO:CA  | 1:72:A:PRO:C  | 5        | 4.57          |
| (1,24)  | 1:33:A:THR:N  | 1:33:A:THR:CA  | 1:33:A:THR:C   | 1:34:A:PRO:N  | 4        | 4.51          |
| (1,7)   | 1:24:A:ASP:C  | 1:25:A:VAL:N   | 1:25:A:VAL:CA  | 1:25:A:VAL:C  | 1        | 4.51          |
| (1,124) | 1:95:A:PHE:N  | 1:95:A:PHE:CA  | 1:95:A:PHE:C   | 1:96:A:SER:N  | 7        | 4.5           |
| (1,81)  | 1:70:A:LEU:C  | 1:71:A:LYS:N   | 1:71:A:LYS:CA  | 1:71:A:LYS:C  | 8        | 4.48          |
| (1,160) | 1:114:A:ASP:N | 1:114:A:ASP:CA | 1:114:A:ASP:C  | 1:115:A:LYS:N | 6        | 4.44          |
| (1,96)  | 1:78:A:GLN:N  | 1:78:A:GLN:CA  | 1:78:A:GLN:C   | 1:79:A:ILE:N  | 9        | 4.44          |
| (1,7)   | 1:24:A:ASP:C  | 1:25:A:VAL:N   | 1:25:A:VAL:CA  | 1:25:A:VAL:C  | 3        | 4.39          |
| (1,223) | 1:150:A:PRO:C | 1:151:A:VAL:N  | 1:151:A:VAL:CA | 1:151:A:VAL:C | 10       | 4.38          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,96)  | 1:78:A:GLN:N  | 1:78:A:GLN:CA  | 1:78:A:GLN:C   | 1:79:A:ILE:N  | 6        | 4.37          |
| (1,7)   | 1:24:A:ASP:C  | 1:25:A:VAL:N   | 1:25:A:VAL:CA  | 1:25:A:VAL:C  | 7        | 4.36          |
| (1,7)   | 1:24:A:ASP:C  | 1:25:A:VAL:N   | 1:25:A:VAL:CA  | 1:25:A:VAL:C  | 9        | 4.33          |
| (1,223) | 1:150:A:PRO:C | 1:151:A:VAL:N  | 1:151:A:VAL:CA | 1:151:A:VAL:C | 9        | 4.3           |
| (1,259) | 1:169:A:ASP:C | 1:170:A:SER:N  | 1:170:A:SER:CA | 1:170:A:SER:C | 2        | 4.27          |
| (1,176) | 1:122:A:TYR:N | 1:122:A:TYR:CA | 1:122:A:TYR:C  | 1:123:A:PRO:N | 1        | 4.23          |
| (1,7)   | 1:24:A:ASP:C  | 1:25:A:VAL:N   | 1:25:A:VAL:CA  | 1:25:A:VAL:C  | 8        | 4.21          |
| (1,12)  | 1:27:A:SER:N  | 1:27:A:SER:CA  | 1:27:A:SER:C   | 1:28:A:HIS:N  | 1        | 4.17          |
| (1,7)   | 1:24:A:ASP:C  | 1:25:A:VAL:N   | 1:25:A:VAL:CA  | 1:25:A:VAL:C  | 2        | 4.17          |
| (1,105) | 1:82:A:THR:C  | 1:83:A:SER:N   | 1:83:A:SER:CA  | 1:83:A:SER:C  | 2        | 4.14          |
| (1,96)  | 1:78:A:GLN:N  | 1:78:A:GLN:CA  | 1:78:A:GLN:C   | 1:79:A:ILE:N  | 1        | 4.13          |
| (1,44)  | 1:50:A:TRP:N  | 1:50:A:TRP:CA  | 1:50:A:TRP:C   | 1:51:A:ILE:N  | 7        | 4.13          |
| (1,13)  | 1:27:A:SER:C  | 1:28:A:HIS:N   | 1:28:A:HIS:CA  | 1:28:A:HIS:C  | 3        | 4.06          |
| (1,7)   | 1:24:A:ASP:C  | 1:25:A:VAL:N   | 1:25:A:VAL:CA  | 1:25:A:VAL:C  | 4        | 4.02          |
| (1,12)  | 1:27:A:SER:N  | 1:27:A:SER:CA  | 1:27:A:SER:C   | 1:28:A:HIS:N  | 7        | 3.99          |
| (1,69)  | 1:64:A:LEU:C  | 1:65:A:ALA:N   | 1:65:A:ALA:CA  | 1:65:A:ALA:C  | 2        | 3.98          |
| (1,53)  | 1:56:A:ASN:C  | 1:57:A:ASP:N   | 1:57:A:ASP:CA  | 1:57:A:ASP:C  | 3        | 3.98          |
| (1,223) | 1:150:A:PRO:C | 1:151:A:VAL:N  | 1:151:A:VAL:CA | 1:151:A:VAL:C | 6        | 3.91          |
| (1,12)  | 1:27:A:SER:N  | 1:27:A:SER:CA  | 1:27:A:SER:C   | 1:28:A:HIS:N  | 9        | 3.9           |
| (1,249) | 1:163:A:LYS:C | 1:164:A:GLU:N  | 1:164:A:GLU:CA | 1:164:A:GLU:C | 2        | 3.87          |
| (1,223) | 1:150:A:PRO:C | 1:151:A:VAL:N  | 1:151:A:VAL:CA | 1:151:A:VAL:C | 2        | 3.87          |
| (1,12)  | 1:27:A:SER:N  | 1:27:A:SER:CA  | 1:27:A:SER:C   | 1:28:A:HIS:N  | 10       | 3.81          |
| (1,96)  | 1:78:A:GLN:N  | 1:78:A:GLN:CA  | 1:78:A:GLN:C   | 1:79:A:ILE:N  | 5        | 3.8           |
| (1,125) | 1:95:A:PHE:C  | 1:96:A:SER:N   | 1:96:A:SER:CA  | 1:96:A:SER:C  | 7        | 3.77          |
| (1,82)  | 1:71:A:LYS:N  | 1:71:A:LYS:CA  | 1:71:A:LYS:C   | 1:72:A:PRO:N  | 3        | 3.77          |
| (1,44)  | 1:50:A:TRP:N  | 1:50:A:TRP:CA  | 1:50:A:TRP:C   | 1:51:A:ILE:N  | 4        | 3.77          |
| (1,7)   | 1:24:A:ASP:C  | 1:25:A:VAL:N   | 1:25:A:VAL:CA  | 1:25:A:VAL:C  | 5        | 3.75          |
| (1,206) | 1:141:A:LYS:N | 1:141:A:LYS:CA | 1:141:A:LYS:C  | 1:142:A:ILE:N | 7        | 3.72          |
| (1,24)  | 1:33:A:THR:N  | 1:33:A:THR:CA  | 1:33:A:THR:C   | 1:34:A:PRO:N  | 2        | 3.68          |
| (1,96)  | 1:78:A:GLN:N  | 1:78:A:GLN:CA  | 1:78:A:GLN:C   | 1:79:A:ILE:N  | 2        | 3.66          |
| (1,7)   | 1:24:A:ASP:C  | 1:25:A:VAL:N   | 1:25:A:VAL:CA  | 1:25:A:VAL:C  | 10       | 3.66          |
| (1,124) | 1:95:A:PHE:N  | 1:95:A:PHE:CA  | 1:95:A:PHE:C   | 1:96:A:SER:N  | 6        | 3.65          |
| (1,26)  | 1:34:A:PRO:N  | 1:34:A:PRO:CA  | 1:34:A:PRO:C   | 1:35:A:ALA:N  | 7        | 3.63          |
| (1,12)  | 1:27:A:SER:N  | 1:27:A:SER:CA  | 1:27:A:SER:C   | 1:28:A:HIS:N  | 5        | 3.61          |
| (1,45)  | 1:50:A:TRP:C  | 1:51:A:ILE:N   | 1:51:A:ILE:CA  | 1:51:A:ILE:C  | 7        | 3.59          |
| (1,44)  | 1:50:A:TRP:N  | 1:50:A:TRP:CA  | 1:50:A:TRP:C   | 1:51:A:ILE:N  | 6        | 3.52          |
| (1,45)  | 1:50:A:TRP:C  | 1:51:A:ILE:N   | 1:51:A:ILE:CA  | 1:51:A:ILE:C  | 4        | 3.48          |
| (1,253) | 1:165:A:GLY:C | 1:166:A:MET:N  | 1:166:A:MET:CA | 1:166:A:MET:C | 4        | 3.47          |
| (1,124) | 1:95:A:PHE:N  | 1:95:A:PHE:CA  | 1:95:A:PHE:C   | 1:96:A:SER:N  | 3        | 3.47          |
| (1,76)  | 1:68:A:GLU:N  | 1:68:A:GLU:CA  | 1:68:A:GLU:C   | 1:69:A:GLN:N  | 5        | 3.45          |
| (1,12)  | 1:27:A:SER:N  | 1:27:A:SER:CA  | 1:27:A:SER:C   | 1:28:A:HIS:N  | 4        | 3.45          |
| (1,176) | 1:122:A:TYR:N | 1:122:A:TYR:CA | 1:122:A:TYR:C  | 1:123:A:PRO:N | 9        | 3.44          |
| (1,12)  | 1:27:A:SER:N  | 1:27:A:SER:CA  | 1:27:A:SER:C   | 1:28:A:HIS:N  | 8        | 3.43          |
| (1,111) | 1:85:A:TYR:C  | 1:86:A:GLU:N   | 1:86:A:GLU:CA  | 1:86:A:GLU:C  | 2        | 3.41          |
| (1,218) | 1:148:A:THR:N | 1:148:A:THR:CA | 1:148:A:THR:C  | 1:149:A:LYS:N | 4        | 3.37          |
| (1,13)  | 1:27:A:SER:C  | 1:28:A:HIS:N   | 1:28:A:HIS:CA  | 1:28:A:HIS:C  | 10       | 3.36          |
| (1,240) | 1:159:A:PHE:N | 1:159:A:PHE:CA | 1:159:A:PHE:C  | 1:160:A:TYR:N | 1        | 3.35          |
| (1,83)  | 1:71:A:LYS:C  | 1:72:A:PRO:N   | 1:72:A:PRO:CA  | 1:72:A:PRO:C  | 3        | 3.35          |
| (1,78)  | 1:69:A:GLN:N  | 1:69:A:GLN:CA  | 1:69:A:GLN:C   | 1:70:A:LEU:N  | 8        | 3.35          |
| (1,13)  | 1:27:A:SER:C  | 1:28:A:HIS:N   | 1:28:A:HIS:CA  | 1:28:A:HIS:C  | 9        | 3.29          |
| (1,13)  | 1:27:A:SER:C  | 1:28:A:HIS:N   | 1:28:A:HIS:CA  | 1:28:A:HIS:C  | 7        | 3.28          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,93)  | 1:76:A:TYR:C  | 1:77:A:LEU:N   | 1:77:A:LEU:CA  | 1:77:A:LEU:C  | 6        | 3.27          |
| (1,13)  | 1:27:A:SER:C  | 1:28:A:HIS:N   | 1:28:A:HIS:CA  | 1:28:A:HIS:C  | 1        | 3.27          |
| (1,254) | 1:166:A:MET:N | 1:166:A:MET:CA | 1:166:A:MET:C  | 1:167:A:LEU:N | 6        | 3.25          |
| (1,93)  | 1:76:A:TYR:C  | 1:77:A:LEU:N   | 1:77:A:LEU:CA  | 1:77:A:LEU:C  | 2        | 3.23          |
| (1,81)  | 1:70:A:LEU:C  | 1:71:A:LYS:N   | 1:71:A:LYS:CA  | 1:71:A:LYS:C  | 6        | 3.23          |
| (1,106) | 1:83:A:SER:N  | 1:83:A:SER:CA  | 1:83:A:SER:C   | 1:84:A:GLY:N  | 2        | 3.19          |
| (1,254) | 1:166:A:MET:N | 1:166:A:MET:CA | 1:166:A:MET:C  | 1:167:A:LEU:N | 8        | 3.18          |
| (1,253) | 1:165:A:GLY:C | 1:166:A:MET:N  | 1:166:A:MET:CA | 1:166:A:MET:C | 1        | 3.17          |
| (1,176) | 1:122:A:TYR:N | 1:122:A:TYR:CA | 1:122:A:TYR:C  | 1:123:A:PRO:N | 6        | 3.17          |
| (1,207) | 1:141:A:LYS:C | 1:142:A:ILE:N  | 1:142:A:ILE:CA | 1:142:A:ILE:C | 7        | 3.16          |
| (1,93)  | 1:76:A:TYR:C  | 1:77:A:LEU:N   | 1:77:A:LEU:CA  | 1:77:A:LEU:C  | 5        | 3.16          |
| (1,197) | 1:134:A:TRP:C | 1:135:A:VAL:N  | 1:135:A:VAL:CA | 1:135:A:VAL:C | 1        | 3.13          |
| (1,125) | 1:95:A:PHE:C  | 1:96:A:SER:N   | 1:96:A:SER:CA  | 1:96:A:SER:C  | 6        | 3.13          |
| (1,105) | 1:82:A:THR:C  | 1:83:A:SER:N   | 1:83:A:SER:CA  | 1:83:A:SER:C  | 9        | 3.11          |
| (1,69)  | 1:64:A:LEU:C  | 1:65:A:ALA:N   | 1:65:A:ALA:CA  | 1:65:A:ALA:C  | 1        | 3.1           |
| (1,68)  | 1:64:A:LEU:N  | 1:64:A:LEU:CA  | 1:64:A:LEU:C   | 1:65:A:ALA:N  | 2        | 3.1           |
| (1,80)  | 1:70:A:LEU:N  | 1:70:A:LEU:CA  | 1:70:A:LEU:C   | 1:71:A:LYS:N  | 8        | 3.09          |
| (1,12)  | 1:27:A:SER:N  | 1:27:A:SER:CA  | 1:27:A:SER:C   | 1:28:A:HIS:N  | 6        | 3.09          |
| (1,240) | 1:159:A:PHE:N | 1:159:A:PHE:CA | 1:159:A:PHE:C  | 1:160:A:TYR:N | 6        | 3.08          |
| (1,107) | 1:83:A:SER:C  | 1:84:A:GLY:N   | 1:84:A:GLY:CA  | 1:84:A:GLY:C  | 2        | 3.05          |
| (1,45)  | 1:50:A:TRP:C  | 1:51:A:ILE:N   | 1:51:A:ILE:CA  | 1:51:A:ILE:C  | 6        | 3.05          |
| (1,7)   | 1:24:A:ASP:C  | 1:25:A:VAL:N   | 1:25:A:VAL:CA  | 1:25:A:VAL:C  | 6        | 3.04          |
| (1,219) | 1:148:A:THR:C | 1:149:A:LYS:N  | 1:149:A:LYS:CA | 1:149:A:LYS:C | 4        | 3.02          |
| (1,13)  | 1:27:A:SER:C  | 1:28:A:HIS:N   | 1:28:A:HIS:CA  | 1:28:A:HIS:C  | 4        | 3.02          |
| (1,69)  | 1:64:A:LEU:C  | 1:65:A:ALA:N   | 1:65:A:ALA:CA  | 1:65:A:ALA:C  | 7        | 3.01          |
| (1,13)  | 1:27:A:SER:C  | 1:28:A:HIS:N   | 1:28:A:HIS:CA  | 1:28:A:HIS:C  | 6        | 2.97          |
| (1,186) | 1:129:A:THR:N | 1:129:A:THR:CA | 1:129:A:THR:C  | 1:130:A:ASN:N | 6        | 2.95          |
| (1,186) | 1:129:A:THR:N | 1:129:A:THR:CA | 1:129:A:THR:C  | 1:130:A:ASN:N | 9        | 2.94          |
| (1,93)  | 1:76:A:TYR:C  | 1:77:A:LEU:N   | 1:77:A:LEU:CA  | 1:77:A:LEU:C  | 9        | 2.93          |
| (1,85)  | 1:72:A:PRO:C  | 1:73:A:TYR:N   | 1:73:A:TYR:CA  | 1:73:A:TYR:C  | 10       | 2.92          |
| (1,53)  | 1:56:A:ASN:C  | 1:57:A:ASP:N   | 1:57:A:ASP:CA  | 1:57:A:ASP:C  | 10       | 2.92          |
| (1,22)  | 1:32:A:ILE:N  | 1:32:A:ILE:CA  | 1:32:A:ILE:C   | 1:33:A:THR:N  | 5        | 2.9           |
| (1,83)  | 1:71:A:LYS:C  | 1:72:A:PRO:N   | 1:72:A:PRO:CA  | 1:72:A:PRO:C  | 4        | 2.87          |
| (1,125) | 1:95:A:PHE:C  | 1:96:A:SER:N   | 1:96:A:SER:CA  | 1:96:A:SER:C  | 3        | 2.85          |
| (1,75)  | 1:67:A:ALA:C  | 1:68:A:GLU:N   | 1:68:A:GLU:CA  | 1:68:A:GLU:C  | 10       | 2.85          |
| (1,22)  | 1:32:A:ILE:N  | 1:32:A:ILE:CA  | 1:32:A:ILE:C   | 1:33:A:THR:N  | 6        | 2.85          |
| (1,176) | 1:122:A:TYR:N | 1:122:A:TYR:CA | 1:122:A:TYR:C  | 1:123:A:PRO:N | 4        | 2.84          |
| (1,11)  | 1:26:A:GLU:C  | 1:27:A:SER:N   | 1:27:A:SER:CA  | 1:27:A:SER:C  | 10       | 2.84          |
| (1,53)  | 1:56:A:ASN:C  | 1:57:A:ASP:N   | 1:57:A:ASP:CA  | 1:57:A:ASP:C  | 9        | 2.83          |
| (1,253) | 1:165:A:GLY:C | 1:166:A:MET:N  | 1:166:A:MET:CA | 1:166:A:MET:C | 10       | 2.82          |
| (1,105) | 1:82:A:THR:C  | 1:83:A:SER:N   | 1:83:A:SER:CA  | 1:83:A:SER:C  | 3        | 2.82          |
| (1,12)  | 1:27:A:SER:N  | 1:27:A:SER:CA  | 1:27:A:SER:C   | 1:28:A:HIS:N  | 2        | 2.82          |
| (1,86)  | 1:73:A:TYR:N  | 1:73:A:TYR:CA  | 1:73:A:TYR:C   | 1:74:A:PHE:N  | 6        | 2.81          |
| (1,53)  | 1:56:A:ASN:C  | 1:57:A:ASP:N   | 1:57:A:ASP:CA  | 1:57:A:ASP:C  | 8        | 2.81          |
| (1,22)  | 1:32:A:ILE:N  | 1:32:A:ILE:CA  | 1:32:A:ILE:C   | 1:33:A:THR:N  | 1        | 2.8           |
| (1,75)  | 1:67:A:ALA:C  | 1:68:A:GLU:N   | 1:68:A:GLU:CA  | 1:68:A:GLU:C  | 3        | 2.77          |
| (1,11)  | 1:26:A:GLU:C  | 1:27:A:SER:N   | 1:27:A:SER:CA  | 1:27:A:SER:C  | 3        | 2.77          |
| (1,252) | 1:165:A:GLY:N | 1:165:A:GLY:CA | 1:165:A:GLY:C  | 1:166:A:MET:N | 10       | 2.75          |
| (1,53)  | 1:56:A:ASN:C  | 1:57:A:ASP:N   | 1:57:A:ASP:CA  | 1:57:A:ASP:C  | 4        | 2.74          |
| (1,248) | 1:163:A:LYS:N | 1:163:A:LYS:CA | 1:163:A:LYS:C  | 1:164:A:GLU:N | 2        | 2.73          |
| (1,127) | 1:96:A:SER:C  | 1:97:A:GLU:N   | 1:97:A:GLU:CA  | 1:97:A:GLU:C  | 5        | 2.72          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,22)  | 1:32:A:ILE:N  | 1:32:A:ILE:CA  | 1:32:A:ILE:C   | 1:33:A:THR:N  | 9        | 2.72          |
| (1,77)  | 1:68:A:GLU:C  | 1:69:A:GLN:N   | 1:69:A:GLN:CA  | 1:69:A:GLN:C  | 8        | 2.71          |
| (1,160) | 1:114:A:ASP:N | 1:114:A:ASP:CA | 1:114:A:ASP:C  | 1:115:A:LYS:N | 7        | 2.7           |
| (1,13)  | 1:27:A:SER:C  | 1:28:A:HIS:N   | 1:28:A:HIS:CA  | 1:28:A:HIS:C  | 8        | 2.7           |
| (1,26)  | 1:34:A:PRO:N  | 1:34:A:PRO:CA  | 1:34:A:PRO:C   | 1:35:A:ALA:N  | 6        | 2.69          |
| (1,127) | 1:96:A:SER:C  | 1:97:A:GLU:N   | 1:97:A:GLU:CA  | 1:97:A:GLU:C  | 9        | 2.67          |
| (1,197) | 1:134:A:TRP:C | 1:135:A:VAL:N  | 1:135:A:VAL:CA | 1:135:A:VAL:C | 5        | 2.65          |
| (1,197) | 1:134:A:TRP:C | 1:135:A:VAL:N  | 1:135:A:VAL:CA | 1:135:A:VAL:C | 7        | 2.64          |
| (1,186) | 1:129:A:THR:N | 1:129:A:THR:CA | 1:129:A:THR:C  | 1:130:A:ASN:N | 4        | 2.64          |
| (1,172) | 1:120:A:VAL:N | 1:120:A:VAL:CA | 1:120:A:VAL:C  | 1:121:A:LEU:N | 4        | 2.64          |
| (1,240) | 1:159:A:PHE:N | 1:159:A:PHE:CA | 1:159:A:PHE:C  | 1:160:A:TYR:N | 2        | 2.62          |
| (1,176) | 1:122:A:TYR:N | 1:122:A:TYR:CA | 1:122:A:TYR:C  | 1:123:A:PRO:N | 3        | 2.62          |
| (1,53)  | 1:56:A:ASN:C  | 1:57:A:ASP:N   | 1:57:A:ASP:CA  | 1:57:A:ASP:C  | 5        | 2.62          |
| (1,25)  | 1:33:A:THR:C  | 1:34:A:PRO:N   | 1:34:A:PRO:CA  | 1:34:A:PRO:C  | 10       | 2.6           |
| (1,93)  | 1:76:A:TYR:C  | 1:77:A:LEU:N   | 1:77:A:LEU:CA  | 1:77:A:LEU:C  | 1        | 2.59          |
| (1,241) | 1:159:A:PHE:C | 1:160:A:TYR:N  | 1:160:A:TYR:CA | 1:160:A:TYR:C | 1        | 2.58          |
| (1,20)  | 1:31:A:SER:N  | 1:31:A:SER:CA  | 1:31:A:SER:C   | 1:32:A:ILE:N  | 8        | 2.58          |
| (1,213) | 1:144:A:VAL:C | 1:145:A:TYR:N  | 1:145:A:TYR:CA | 1:145:A:TYR:C | 9        | 2.57          |
| (1,75)  | 1:67:A:ALA:C  | 1:68:A:GLU:N   | 1:68:A:GLU:CA  | 1:68:A:GLU:C  | 5        | 2.56          |
| (1,69)  | 1:64:A:LEU:C  | 1:65:A:ALA:N   | 1:65:A:ALA:CA  | 1:65:A:ALA:C  | 6        | 2.56          |
| (1,95)  | 1:77:A:LEU:C  | 1:78:A:GLN:N   | 1:78:A:GLN:CA  | 1:78:A:GLN:C  | 4        | 2.54          |
| (1,79)  | 1:69:A:GLN:C  | 1:70:A:LEU:N   | 1:70:A:LEU:CA  | 1:70:A:LEU:C  | 7        | 2.52          |
| (1,213) | 1:144:A:VAL:C | 1:145:A:TYR:N  | 1:145:A:TYR:CA | 1:145:A:TYR:C | 4        | 2.51          |
| (1,206) | 1:141:A:LYS:N | 1:141:A:LYS:CA | 1:141:A:LYS:C  | 1:142:A:ILE:N | 3        | 2.51          |
| (1,83)  | 1:71:A:LYS:C  | 1:72:A:PRO:N   | 1:72:A:PRO:CA  | 1:72:A:PRO:C  | 2        | 2.51          |
| (1,254) | 1:166:A:MET:N | 1:166:A:MET:CA | 1:166:A:MET:C  | 1:167:A:LEU:N | 7        | 2.5           |
| (1,218) | 1:148:A:THR:N | 1:148:A:THR:CA | 1:148:A:THR:C  | 1:149:A:LYS:N | 5        | 2.5           |
| (1,187) | 1:129:A:THR:C | 1:130:A:ASN:N  | 1:130:A:ASN:CA | 1:130:A:ASN:C | 9        | 2.5           |
| (1,172) | 1:120:A:VAL:N | 1:120:A:VAL:CA | 1:120:A:VAL:C  | 1:121:A:LEU:N | 6        | 2.5           |
| (1,176) | 1:122:A:TYR:N | 1:122:A:TYR:CA | 1:122:A:TYR:C  | 1:123:A:PRO:N | 8        | 2.49          |
| (1,93)  | 1:76:A:TYR:C  | 1:77:A:LEU:N   | 1:77:A:LEU:CA  | 1:77:A:LEU:C  | 7        | 2.48          |
| (1,197) | 1:134:A:TRP:C | 1:135:A:VAL:N  | 1:135:A:VAL:CA | 1:135:A:VAL:C | 6        | 2.47          |
| (1,127) | 1:96:A:SER:C  | 1:97:A:GLU:N   | 1:97:A:GLU:CA  | 1:97:A:GLU:C  | 6        | 2.47          |
| (1,13)  | 1:27:A:SER:C  | 1:28:A:HIS:N   | 1:28:A:HIS:CA  | 1:28:A:HIS:C  | 5        | 2.47          |
| (1,249) | 1:163:A:LYS:C | 1:164:A:GLU:N  | 1:164:A:GLU:CA | 1:164:A:GLU:C | 10       | 2.45          |
| (1,213) | 1:144:A:VAL:C | 1:145:A:TYR:N  | 1:145:A:TYR:CA | 1:145:A:TYR:C | 10       | 2.44          |
| (1,105) | 1:82:A:THR:C  | 1:83:A:SER:N   | 1:83:A:SER:CA  | 1:83:A:SER:C  | 7        | 2.44          |
| (1,87)  | 1:73:A:TYR:C  | 1:74:A:PHE:N   | 1:74:A:PHE:CA  | 1:74:A:PHE:C  | 2        | 2.44          |
| (1,252) | 1:165:A:GLY:N | 1:165:A:GLY:CA | 1:165:A:GLY:C  | 1:166:A:MET:N | 4        | 2.42          |
| (1,186) | 1:129:A:THR:N | 1:129:A:THR:CA | 1:129:A:THR:C  | 1:130:A:ASN:N | 1        | 2.42          |
| (1,105) | 1:82:A:THR:C  | 1:83:A:SER:N   | 1:83:A:SER:CA  | 1:83:A:SER:C  | 4        | 2.42          |
| (1,20)  | 1:31:A:SER:N  | 1:31:A:SER:CA  | 1:31:A:SER:C   | 1:32:A:ILE:N  | 5        | 2.42          |
| (1,120) | 1:91:A:ALA:N  | 1:91:A:ALA:CA  | 1:91:A:ALA:C   | 1:92:A:LEU:N  | 10       | 2.4           |
| (1,83)  | 1:71:A:LYS:C  | 1:72:A:PRO:N   | 1:72:A:PRO:CA  | 1:72:A:PRO:C  | 6        | 2.4           |
| (1,26)  | 1:34:A:PRO:N  | 1:34:A:PRO:CA  | 1:34:A:PRO:C   | 1:35:A:ALA:N  | 5        | 2.4           |
| (1,13)  | 1:27:A:SER:C  | 1:28:A:HIS:N   | 1:28:A:HIS:CA  | 1:28:A:HIS:C  | 2        | 2.4           |
| (1,206) | 1:141:A:LYS:N | 1:141:A:LYS:CA | 1:141:A:LYS:C  | 1:142:A:ILE:N | 6        | 2.39          |
| (1,47)  | 1:51:A:ILE:C  | 1:52:A:LYS:N   | 1:52:A:LYS:CA  | 1:52:A:LYS:C  | 5        | 2.39          |
| (1,42)  | 1:49:A:VAL:N  | 1:49:A:VAL:CA  | 1:49:A:VAL:C   | 1:50:A:TRP:N  | 5        | 2.39          |
| (1,218) | 1:148:A:THR:N | 1:148:A:THR:CA | 1:148:A:THR:C  | 1:149:A:LYS:N | 3        | 2.38          |
| (1,53)  | 1:56:A:ASN:C  | 1:57:A:ASP:N   | 1:57:A:ASP:CA  | 1:57:A:ASP:C  | 7        | 2.38          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,11)  | 1:26:A:GLU:C  | 1:27:A:SER:N   | 1:27:A:SER:CA  | 1:27:A:SER:C  | 6        | 2.38          |
| (1,47)  | 1:51:A:ILE:C  | 1:52:A:LYS:N   | 1:52:A:LYS:CA  | 1:52:A:LYS:C  | 8        | 2.37          |
| (1,11)  | 1:26:A:GLU:C  | 1:27:A:SER:N   | 1:27:A:SER:CA  | 1:27:A:SER:C  | 9        | 2.37          |
| (1,11)  | 1:26:A:GLU:C  | 1:27:A:SER:N   | 1:27:A:SER:CA  | 1:27:A:SER:C  | 7        | 2.36          |
| (1,263) | 1:171:A:LEU:C | 1:172:A:PRO:N  | 1:172:A:PRO:CA | 1:172:A:PRO:C | 10       | 2.34          |
| (1,47)  | 1:51:A:ILE:C  | 1:52:A:LYS:N   | 1:52:A:LYS:CA  | 1:52:A:LYS:C  | 10       | 2.34          |
| (1,8)   | 1:25:A:VAL:N  | 1:25:A:VAL:CA  | 1:25:A:VAL:C   | 1:26:A:GLU:N  | 10       | 2.34          |
| (1,95)  | 1:77:A:LEU:C  | 1:78:A:GLN:N   | 1:78:A:GLN:CA  | 1:78:A:GLN:C  | 10       | 2.33          |
| (1,225) | 1:151:A:VAL:C | 1:152:A:ALA:N  | 1:152:A:ALA:CA | 1:152:A:ALA:C | 2        | 2.32          |
| (1,127) | 1:96:A:SER:C  | 1:97:A:GLU:N   | 1:97:A:GLU:CA  | 1:97:A:GLU:C  | 3        | 2.31          |
| (1,114) | 1:87:A:THR:N  | 1:87:A:THR:CA  | 1:87:A:THR:C   | 1:88:A:ASN:N  | 2        | 2.31          |
| (1,207) | 1:141:A:LYS:C | 1:142:A:ILE:N  | 1:142:A:ILE:CA | 1:142:A:ILE:C | 3        | 2.3           |
| (1,127) | 1:96:A:SER:C  | 1:97:A:GLU:N   | 1:97:A:GLU:CA  | 1:97:A:GLU:C  | 2        | 2.3           |
| (1,255) | 1:166:A:MET:C | 1:167:A:LEU:N  | 1:167:A:LEU:CA | 1:167:A:LEU:C | 8        | 2.29          |
| (1,237) | 1:157:A:LYS:C | 1:158:A:ALA:N  | 1:158:A:ALA:CA | 1:158:A:ALA:C | 1        | 2.29          |
| (1,237) | 1:157:A:LYS:C | 1:158:A:ALA:N  | 1:158:A:ALA:CA | 1:158:A:ALA:C | 4        | 2.29          |
| (1,75)  | 1:67:A:ALA:C  | 1:68:A:GLU:N   | 1:68:A:GLU:CA  | 1:68:A:GLU:C  | 7        | 2.29          |
| (1,104) | 1:82:A:THR:N  | 1:82:A:THR:CA  | 1:82:A:THR:C   | 1:83:A:SER:N  | 2        | 2.28          |
| (1,253) | 1:165:A:GLY:C | 1:166:A:MET:N  | 1:166:A:MET:CA | 1:166:A:MET:C | 9        | 2.27          |
| (1,213) | 1:144:A:VAL:C | 1:145:A:TYR:N  | 1:145:A:TYR:CA | 1:145:A:TYR:C | 5        | 2.27          |
| (1,52)  | 1:56:A:ASN:N  | 1:56:A:ASN:CA  | 1:56:A:ASN:C   | 1:57:A:ASP:N  | 3        | 2.27          |
| (1,244) | 1:161:A:GLU:N | 1:161:A:GLU:CA | 1:161:A:GLU:C  | 1:162:A:ALA:N | 6        | 2.26          |
| (1,79)  | 1:69:A:GLN:C  | 1:70:A:LEU:N   | 1:70:A:LEU:CA  | 1:70:A:LEU:C  | 2        | 2.26          |
| (1,225) | 1:151:A:VAL:C | 1:152:A:ALA:N  | 1:152:A:ALA:CA | 1:152:A:ALA:C | 4        | 2.25          |
| (1,144) | 1:105:A:ASP:N | 1:105:A:ASP:CA | 1:105:A:ASP:C  | 1:106:A:ASN:N | 8        | 2.25          |
| (1,83)  | 1:71:A:LYS:C  | 1:72:A:PRO:N   | 1:72:A:PRO:CA  | 1:72:A:PRO:C  | 1        | 2.25          |
| (1,26)  | 1:34:A:PRO:N  | 1:34:A:PRO:CA  | 1:34:A:PRO:C   | 1:35:A:ALA:N  | 2        | 2.24          |
| (1,11)  | 1:26:A:GLU:C  | 1:27:A:SER:N   | 1:27:A:SER:CA  | 1:27:A:SER:C  | 5        | 2.23          |
| (1,237) | 1:157:A:LYS:C | 1:158:A:ALA:N  | 1:158:A:ALA:CA | 1:158:A:ALA:C | 7        | 2.22          |
| (1,197) | 1:134:A:TRP:C | 1:135:A:VAL:N  | 1:135:A:VAL:CA | 1:135:A:VAL:C | 10       | 2.21          |
| (1,176) | 1:122:A:TYR:N | 1:122:A:TYR:CA | 1:122:A:TYR:C  | 1:123:A:PRO:N | 2        | 2.21          |
| (1,75)  | 1:67:A:ALA:C  | 1:68:A:GLU:N   | 1:68:A:GLU:CA  | 1:68:A:GLU:C  | 4        | 2.21          |
| (1,82)  | 1:71:A:LYS:N  | 1:71:A:LYS:CA  | 1:71:A:LYS:C   | 1:72:A:PRO:N  | 1        | 2.2           |
| (1,69)  | 1:64:A:LEU:C  | 1:65:A:ALA:N   | 1:65:A:ALA:CA  | 1:65:A:ALA:C  | 3        | 2.2           |
| (1,46)  | 1:51:A:ILE:N  | 1:51:A:ILE:CA  | 1:51:A:ILE:C   | 1:52:A:LYS:N  | 7        | 2.2           |
| (1,68)  | 1:64:A:LEU:N  | 1:64:A:LEU:CA  | 1:64:A:LEU:C   | 1:65:A:ALA:N  | 6        | 2.19          |
| (1,26)  | 1:34:A:PRO:N  | 1:34:A:PRO:CA  | 1:34:A:PRO:C   | 1:35:A:ALA:N  | 8        | 2.19          |
| (1,241) | 1:159:A:PHE:C | 1:160:A:TYR:N  | 1:160:A:TYR:CA | 1:160:A:TYR:C | 2        | 2.18          |
| (1,76)  | 1:68:A:GLU:N  | 1:68:A:GLU:CA  | 1:68:A:GLU:C   | 1:69:A:GLN:N  | 3        | 2.18          |
| (1,264) | 1:172:A:PRO:N | 1:172:A:PRO:CA | 1:172:A:PRO:C  | 1:173:A:VAL:N | 9        | 2.17          |
| (1,241) | 1:159:A:PHE:C | 1:160:A:TYR:N  | 1:160:A:TYR:CA | 1:160:A:TYR:C | 6        | 2.17          |
| (1,206) | 1:141:A:LYS:N | 1:141:A:LYS:CA | 1:141:A:LYS:C  | 1:142:A:ILE:N | 1        | 2.17          |
| (1,160) | 1:114:A:ASP:N | 1:114:A:ASP:CA | 1:114:A:ASP:C  | 1:115:A:LYS:N | 8        | 2.17          |
| (1,112) | 1:86:A:GLU:N  | 1:86:A:GLU:CA  | 1:86:A:GLU:C   | 1:87:A:THR:N  | 9        | 2.17          |
| (1,95)  | 1:77:A:LEU:C  | 1:78:A:GLN:N   | 1:78:A:GLN:CA  | 1:78:A:GLN:C  | 8        | 2.17          |
| (1,23)  | 1:32:A:ILE:C  | 1:33:A:THR:N   | 1:33:A:THR:CA  | 1:33:A:THR:C  | 2        | 2.17          |
| (1,219) | 1:148:A:THR:C | 1:149:A:LYS:N  | 1:149:A:LYS:CA | 1:149:A:LYS:C | 5        | 2.16          |
| (1,203) | 1:137:A:GLY:C | 1:138:A:GLU:N  | 1:138:A:GLU:CA | 1:138:A:GLU:C | 7        | 2.16          |
| (1,127) | 1:96:A:SER:C  | 1:97:A:GLU:N   | 1:97:A:GLU:CA  | 1:97:A:GLU:C  | 1        | 2.16          |
| (1,26)  | 1:34:A:PRO:N  | 1:34:A:PRO:CA  | 1:34:A:PRO:C   | 1:35:A:ALA:N  | 9        | 2.16          |
| (1,11)  | 1:26:A:GLU:C  | 1:27:A:SER:N   | 1:27:A:SER:CA  | 1:27:A:SER:C  | 2        | 2.15          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,237) | 1:157:A:LYS:C | 1:158:A:ALA:N  | 1:158:A:ALA:CA | 1:158:A:ALA:C | 2        | 2.14          |
| (1,82)  | 1:71:A:LYS:N  | 1:71:A:LYS:CA  | 1:71:A:LYS:C   | 1:72:A:PRO:N  | 2        | 2.13          |
| (1,248) | 1:163:A:LYS:N | 1:163:A:LYS:CA | 1:163:A:LYS:C  | 1:164:A:GLU:N | 9        | 2.12          |
| (1,188) | 1:130:A:ASN:N | 1:130:A:ASN:CA | 1:130:A:ASN:C  | 1:131:A:THR:N | 6        | 2.12          |
| (1,144) | 1:105:A:ASP:N | 1:105:A:ASP:CA | 1:105:A:ASP:C  | 1:106:A:ASN:N | 2        | 2.12          |
| (1,69)  | 1:64:A:LEU:C  | 1:65:A:ALA:N   | 1:65:A:ALA:CA  | 1:65:A:ALA:C  | 4        | 2.12          |
| (1,69)  | 1:64:A:LEU:C  | 1:65:A:ALA:N   | 1:65:A:ALA:CA  | 1:65:A:ALA:C  | 5        | 2.12          |
| (1,262) | 1:171:A:LEU:N | 1:171:A:LEU:CA | 1:171:A:LEU:C  | 1:172:A:PRO:N | 2        | 2.11          |
| (1,186) | 1:129:A:THR:N | 1:129:A:THR:CA | 1:129:A:THR:C  | 1:130:A:ASN:N | 3        | 2.11          |
| (1,144) | 1:105:A:ASP:N | 1:105:A:ASP:CA | 1:105:A:ASP:C  | 1:106:A:ASN:N | 3        | 2.11          |
| (1,103) | 1:81:A:ILE:C  | 1:82:A:THR:N   | 1:82:A:THR:CA  | 1:82:A:THR:C  | 9        | 2.11          |
| (1,237) | 1:157:A:LYS:C | 1:158:A:ALA:N  | 1:158:A:ALA:CA | 1:158:A:ALA:C | 8        | 2.1           |
| (1,131) | 1:98:A:THR:C  | 1:99:A:LYS:N   | 1:99:A:LYS:CA  | 1:99:A:LYS:C  | 8        | 2.1           |
| (1,26)  | 1:34:A:PRO:N  | 1:34:A:PRO:CA  | 1:34:A:PRO:C   | 1:35:A:ALA:N  | 3        | 2.1           |
| (1,127) | 1:96:A:SER:C  | 1:97:A:GLU:N   | 1:97:A:GLU:CA  | 1:97:A:GLU:C  | 4        | 2.09          |
| (1,104) | 1:82:A:THR:N  | 1:82:A:THR:CA  | 1:82:A:THR:C   | 1:83:A:SER:N  | 9        | 2.09          |
| (1,11)  | 1:26:A:GLU:C  | 1:27:A:SER:N   | 1:27:A:SER:CA  | 1:27:A:SER:C  | 4        | 2.09          |
| (1,117) | 1:89:A:SER:C  | 1:90:A:THR:N   | 1:90:A:THR:CA  | 1:90:A:THR:C  | 10       | 2.08          |
| (1,46)  | 1:51:A:ILE:N  | 1:51:A:ILE:CA  | 1:51:A:ILE:C   | 1:52:A:LYS:N  | 4        | 2.08          |
| (1,240) | 1:159:A:PHE:N | 1:159:A:PHE:CA | 1:159:A:PHE:C  | 1:160:A:TYR:N | 7        | 2.07          |
| (1,207) | 1:141:A:LYS:C | 1:142:A:ILE:N  | 1:142:A:ILE:CA | 1:142:A:ILE:C | 1        | 2.06          |
| (1,26)  | 1:34:A:PRO:N  | 1:34:A:PRO:CA  | 1:34:A:PRO:C   | 1:35:A:ALA:N  | 4        | 2.06          |
| (1,218) | 1:148:A:THR:N | 1:148:A:THR:CA | 1:148:A:THR:C  | 1:149:A:LYS:N | 1        | 2.05          |
| (1,75)  | 1:67:A:ALA:C  | 1:68:A:GLU:N   | 1:68:A:GLU:CA  | 1:68:A:GLU:C  | 9        | 2.05          |
| (1,26)  | 1:34:A:PRO:N  | 1:34:A:PRO:CA  | 1:34:A:PRO:C   | 1:35:A:ALA:N  | 1        | 2.05          |
| (1,160) | 1:114:A:ASP:N | 1:114:A:ASP:CA | 1:114:A:ASP:C  | 1:115:A:LYS:N | 1        | 2.04          |
| (1,133) | 1:99:A:LYS:C  | 1:100:A:ALA:N  | 1:100:A:ALA:CA | 1:100:A:ALA:C | 7        | 2.04          |
| (1,47)  | 1:51:A:ILE:C  | 1:52:A:LYS:N   | 1:52:A:LYS:CA  | 1:52:A:LYS:C  | 3        | 2.04          |
| (1,187) | 1:129:A:THR:C | 1:130:A:ASN:N  | 1:130:A:ASN:CA | 1:130:A:ASN:C | 4        | 2.03          |
| (1,82)  | 1:71:A:LYS:N  | 1:71:A:LYS:CA  | 1:71:A:LYS:C   | 1:72:A:PRO:N  | 7        | 2.03          |
| (1,227) | 1:152:A:ALA:C | 1:153:A:ILE:N  | 1:153:A:ILE:CA | 1:153:A:ILE:C | 2        | 2.02          |
| (1,144) | 1:105:A:ASP:N | 1:105:A:ASP:CA | 1:105:A:ASP:C  | 1:106:A:ASN:N | 5        | 2.02          |
| (1,75)  | 1:67:A:ALA:C  | 1:68:A:GLU:N   | 1:68:A:GLU:CA  | 1:68:A:GLU:C  | 8        | 2.02          |
| (1,83)  | 1:71:A:LYS:C  | 1:72:A:PRO:N   | 1:72:A:PRO:CA  | 1:72:A:PRO:C  | 9        | 2.01          |
| (1,78)  | 1:69:A:GLN:N  | 1:69:A:GLN:CA  | 1:69:A:GLN:C   | 1:70:A:LEU:N  | 6        | 2.01          |
| (1,53)  | 1:56:A:ASN:C  | 1:57:A:ASP:N   | 1:57:A:ASP:CA  | 1:57:A:ASP:C  | 2        | 2.01          |
| (1,79)  | 1:69:A:GLN:C  | 1:70:A:LEU:N   | 1:70:A:LEU:CA  | 1:70:A:LEU:C  | 10       | 2.0           |
| (1,127) | 1:96:A:SER:C  | 1:97:A:GLU:N   | 1:97:A:GLU:CA  | 1:97:A:GLU:C  | 10       | 1.99          |
| (1,144) | 1:105:A:ASP:N | 1:105:A:ASP:CA | 1:105:A:ASP:C  | 1:106:A:ASN:N | 7        | 1.98          |
| (1,86)  | 1:73:A:TYR:N  | 1:73:A:TYR:CA  | 1:73:A:TYR:C   | 1:74:A:PHE:N  | 2        | 1.98          |
| (1,249) | 1:163:A:LYS:C | 1:164:A:GLU:N  | 1:164:A:GLU:CA | 1:164:A:GLU:C | 5        | 1.97          |
| (1,261) | 1:170:A:SER:C | 1:171:A:LEU:N  | 1:171:A:LEU:CA | 1:171:A:LEU:C | 9        | 1.96          |
| (1,249) | 1:163:A:LYS:C | 1:164:A:GLU:N  | 1:164:A:GLU:CA | 1:164:A:GLU:C | 3        | 1.96          |
| (1,176) | 1:122:A:TYR:N | 1:122:A:TYR:CA | 1:122:A:TYR:C  | 1:123:A:PRO:N | 10       | 1.96          |
| (1,169) | 1:118:A:ILE:C | 1:119:A:ALA:N  | 1:119:A:ALA:CA | 1:119:A:ALA:C | 6        | 1.96          |
| (1,47)  | 1:51:A:ILE:C  | 1:52:A:LYS:N   | 1:52:A:LYS:CA  | 1:52:A:LYS:C  | 9        | 1.96          |
| (1,20)  | 1:31:A:SER:N  | 1:31:A:SER:CA  | 1:31:A:SER:C   | 1:32:A:ILE:N  | 2        | 1.96          |
| (1,3)   | 1:22:A:PRO:C  | 1:23:A:ILE:N   | 1:23:A:ILE:CA  | 1:23:A:ILE:C  | 3        | 1.96          |
| (1,20)  | 1:31:A:SER:N  | 1:31:A:SER:CA  | 1:31:A:SER:C   | 1:32:A:ILE:N  | 9        | 1.95          |
| (1,197) | 1:134:A:TRP:C | 1:135:A:VAL:N  | 1:135:A:VAL:CA | 1:135:A:VAL:C | 2        | 1.94          |
| (1,176) | 1:122:A:TYR:N | 1:122:A:TYR:CA | 1:122:A:TYR:C  | 1:123:A:PRO:N | 5        | 1.94          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,103) | 1:81:A:ILE:C  | 1:82:A:THR:N   | 1:82:A:THR:CA  | 1:82:A:THR:C  | 4        | 1.94          |
| (1,103) | 1:81:A:ILE:C  | 1:82:A:THR:N   | 1:82:A:THR:CA  | 1:82:A:THR:C  | 7        | 1.94          |
| (1,197) | 1:134:A:TRP:C | 1:135:A:VAL:N  | 1:135:A:VAL:CA | 1:135:A:VAL:C | 8        | 1.93          |
| (1,189) | 1:130:A:ASN:C | 1:131:A:THR:N  | 1:131:A:THR:CA | 1:131:A:THR:C | 6        | 1.93          |
| (1,187) | 1:129:A:THR:C | 1:130:A:ASN:N  | 1:130:A:ASN:CA | 1:130:A:ASN:C | 3        | 1.93          |
| (1,68)  | 1:64:A:LEU:N  | 1:64:A:LEU:CA  | 1:64:A:LEU:C   | 1:65:A:ALA:N  | 1        | 1.93          |
| (1,8)   | 1:25:A:VAL:N  | 1:25:A:VAL:CA  | 1:25:A:VAL:C   | 1:26:A:GLU:N  | 5        | 1.93          |
| (1,218) | 1:148:A:THR:N | 1:148:A:THR:CA | 1:148:A:THR:C  | 1:149:A:LYS:N | 7        | 1.92          |
| (1,187) | 1:129:A:THR:C | 1:130:A:ASN:N  | 1:130:A:ASN:CA | 1:130:A:ASN:C | 1        | 1.92          |
| (1,176) | 1:122:A:TYR:N | 1:122:A:TYR:CA | 1:122:A:TYR:C  | 1:123:A:PRO:N | 7        | 1.92          |
| (1,82)  | 1:71:A:LYS:N  | 1:71:A:LYS:CA  | 1:71:A:LYS:C   | 1:72:A:PRO:N  | 6        | 1.92          |
| (1,249) | 1:163:A:LYS:C | 1:164:A:GLU:N  | 1:164:A:GLU:CA | 1:164:A:GLU:C | 7        | 1.91          |
| (1,244) | 1:161:A:GLU:N | 1:161:A:GLU:CA | 1:161:A:GLU:C  | 1:162:A:ALA:N | 2        | 1.91          |
| (1,203) | 1:137:A:GLY:C | 1:138:A:GLU:N  | 1:138:A:GLU:CA | 1:138:A:GLU:C | 3        | 1.91          |
| (1,197) | 1:134:A:TRP:C | 1:135:A:VAL:N  | 1:135:A:VAL:CA | 1:135:A:VAL:C | 4        | 1.91          |
| (1,177) | 1:122:A:TYR:C | 1:123:A:PRO:N  | 1:123:A:PRO:CA | 1:123:A:PRO:C | 2        | 1.91          |
| (1,85)  | 1:72:A:PRO:C  | 1:73:A:TYR:N   | 1:73:A:TYR:CA  | 1:73:A:TYR:C  | 8        | 1.91          |
| (1,76)  | 1:68:A:GLU:N  | 1:68:A:GLU:CA  | 1:68:A:GLU:C   | 1:69:A:GLN:N  | 6        | 1.91          |
| (1,8)   | 1:25:A:VAL:N  | 1:25:A:VAL:CA  | 1:25:A:VAL:C   | 1:26:A:GLU:N  | 6        | 1.91          |
| (1,259) | 1:169:A:ASP:C | 1:170:A:SER:N  | 1:170:A:SER:CA | 1:170:A:SER:C | 8        | 1.9           |
| (1,225) | 1:151:A:VAL:C | 1:152:A:ALA:N  | 1:152:A:ALA:CA | 1:152:A:ALA:C | 5        | 1.9           |
| (1,113) | 1:86:A:GLU:C  | 1:87:A:THR:N   | 1:87:A:THR:CA  | 1:87:A:THR:C  | 2        | 1.9           |
| (1,83)  | 1:71:A:LYS:C  | 1:72:A:PRO:N   | 1:72:A:PRO:CA  | 1:72:A:PRO:C  | 7        | 1.9           |
| (1,79)  | 1:69:A:GLN:C  | 1:70:A:LEU:N   | 1:70:A:LEU:CA  | 1:70:A:LEU:C  | 1        | 1.9           |
| (1,52)  | 1:56:A:ASN:N  | 1:56:A:ASN:CA  | 1:56:A:ASN:C   | 1:57:A:ASP:N  | 4        | 1.9           |
| (1,249) | 1:163:A:LYS:C | 1:164:A:GLU:N  | 1:164:A:GLU:CA | 1:164:A:GLU:C | 8        | 1.89          |
| (1,244) | 1:161:A:GLU:N | 1:161:A:GLU:CA | 1:161:A:GLU:C  | 1:162:A:ALA:N | 9        | 1.89          |
| (1,237) | 1:157:A:LYS:C | 1:158:A:ALA:N  | 1:158:A:ALA:CA | 1:158:A:ALA:C | 3        | 1.89          |
| (1,219) | 1:148:A:THR:C | 1:149:A:LYS:N  | 1:149:A:LYS:CA | 1:149:A:LYS:C | 3        | 1.89          |
| (1,207) | 1:141:A:LYS:C | 1:142:A:ILE:N  | 1:142:A:ILE:CA | 1:142:A:ILE:C | 9        | 1.89          |
| (1,131) | 1:98:A:THR:C  | 1:99:A:LYS:N   | 1:99:A:LYS:CA  | 1:99:A:LYS:C  | 4        | 1.88          |
| (1,106) | 1:83:A:SER:N  | 1:83:A:SER:CA  | 1:83:A:SER:C   | 1:84:A:GLY:N  | 3        | 1.88          |
| (1,263) | 1:171:A:LEU:C | 1:172:A:PRO:N  | 1:172:A:PRO:CA | 1:172:A:PRO:C | 4        | 1.87          |
| (1,144) | 1:105:A:ASP:N | 1:105:A:ASP:CA | 1:105:A:ASP:C  | 1:106:A:ASN:N | 9        | 1.87          |
| (1,244) | 1:161:A:GLU:N | 1:161:A:GLU:CA | 1:161:A:GLU:C  | 1:162:A:ALA:N | 5        | 1.86          |
| (1,144) | 1:105:A:ASP:N | 1:105:A:ASP:CA | 1:105:A:ASP:C  | 1:106:A:ASN:N | 6        | 1.86          |
| (1,103) | 1:81:A:ILE:C  | 1:82:A:THR:N   | 1:82:A:THR:CA  | 1:82:A:THR:C  | 8        | 1.86          |
| (1,81)  | 1:70:A:LEU:C  | 1:71:A:LYS:N   | 1:71:A:LYS:CA  | 1:71:A:LYS:C  | 2        | 1.86          |
| (1,160) | 1:114:A:ASP:N | 1:114:A:ASP:CA | 1:114:A:ASP:C  | 1:115:A:LYS:N | 2        | 1.85          |
| (1,47)  | 1:51:A:ILE:C  | 1:52:A:LYS:N   | 1:52:A:LYS:CA  | 1:52:A:LYS:C  | 1        | 1.85          |
| (1,206) | 1:141:A:LYS:N | 1:141:A:LYS:CA | 1:141:A:LYS:C  | 1:142:A:ILE:N | 10       | 1.84          |
| (1,97)  | 1:78:A:GLN:C  | 1:79:A:ILE:N   | 1:79:A:ILE:CA  | 1:79:A:ILE:C  | 4        | 1.84          |
| (1,263) | 1:171:A:LEU:C | 1:172:A:PRO:N  | 1:172:A:PRO:CA | 1:172:A:PRO:C | 5        | 1.83          |
| (1,255) | 1:166:A:MET:C | 1:167:A:LEU:N  | 1:167:A:LEU:CA | 1:167:A:LEU:C | 7        | 1.83          |
| (1,47)  | 1:51:A:ILE:C  | 1:52:A:LYS:N   | 1:52:A:LYS:CA  | 1:52:A:LYS:C  | 2        | 1.83          |
| (1,203) | 1:137:A:GLY:C | 1:138:A:GLU:N  | 1:138:A:GLU:CA | 1:138:A:GLU:C | 4        | 1.81          |
| (1,127) | 1:96:A:SER:C  | 1:97:A:GLU:N   | 1:97:A:GLU:CA  | 1:97:A:GLU:C  | 7        | 1.81          |
| (1,11)  | 1:26:A:GLU:C  | 1:27:A:SER:N   | 1:27:A:SER:CA  | 1:27:A:SER:C  | 8        | 1.81          |
| (1,263) | 1:171:A:LEU:C | 1:172:A:PRO:N  | 1:172:A:PRO:CA | 1:172:A:PRO:C | 2        | 1.8           |
| (1,263) | 1:171:A:LEU:C | 1:172:A:PRO:N  | 1:172:A:PRO:CA | 1:172:A:PRO:C | 3        | 1.8           |
| (1,255) | 1:166:A:MET:C | 1:167:A:LEU:N  | 1:167:A:LEU:CA | 1:167:A:LEU:C | 2        | 1.8           |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,219) | 1:148:A:THR:C | 1:149:A:LYS:N  | 1:149:A:LYS:CA | 1:149:A:LYS:C | 7        | 1.8           |
| (1,237) | 1:157:A:LYS:C | 1:158:A:ALA:N  | 1:158:A:ALA:CA | 1:158:A:ALA:C | 9        | 1.79          |
| (1,212) | 1:144:A:VAL:N | 1:144:A:VAL:CA | 1:144:A:VAL:C  | 1:145:A:TYR:N | 10       | 1.79          |
| (1,144) | 1:105:A:ASP:N | 1:105:A:ASP:CA | 1:105:A:ASP:C  | 1:106:A:ASN:N | 1        | 1.78          |
| (1,68)  | 1:64:A:LEU:N  | 1:64:A:LEU:CA  | 1:64:A:LEU:C   | 1:65:A:ALA:N  | 7        | 1.78          |
| (1,52)  | 1:56:A:ASN:N  | 1:56:A:ASN:CA  | 1:56:A:ASN:C   | 1:57:A:ASP:N  | 2        | 1.78          |
| (1,249) | 1:163:A:LYS:C | 1:164:A:GLU:N  | 1:164:A:GLU:CA | 1:164:A:GLU:C | 6        | 1.77          |
| (1,240) | 1:159:A:PHE:N | 1:159:A:PHE:CA | 1:159:A:PHE:C  | 1:160:A:TYR:N | 8        | 1.77          |
| (1,244) | 1:161:A:GLU:N | 1:161:A:GLU:CA | 1:161:A:GLU:C  | 1:162:A:ALA:N | 1        | 1.76          |
| (1,237) | 1:157:A:LYS:C | 1:158:A:ALA:N  | 1:158:A:ALA:CA | 1:158:A:ALA:C | 5        | 1.76          |
| (1,237) | 1:157:A:LYS:C | 1:158:A:ALA:N  | 1:158:A:ALA:CA | 1:158:A:ALA:C | 6        | 1.76          |
| (1,203) | 1:137:A:GLY:C | 1:138:A:GLU:N  | 1:138:A:GLU:CA | 1:138:A:GLU:C | 10       | 1.76          |
| (1,25)  | 1:33:A:THR:C  | 1:34:A:PRO:N   | 1:34:A:PRO:CA  | 1:34:A:PRO:C  | 2        | 1.76          |
| (1,255) | 1:166:A:MET:C | 1:167:A:LEU:N  | 1:167:A:LEU:CA | 1:167:A:LEU:C | 4        | 1.75          |
| (1,240) | 1:159:A:PHE:N | 1:159:A:PHE:CA | 1:159:A:PHE:C  | 1:160:A:TYR:N | 3        | 1.75          |
| (1,240) | 1:159:A:PHE:N | 1:159:A:PHE:CA | 1:159:A:PHE:C  | 1:160:A:TYR:N | 5        | 1.75          |
| (1,118) | 1:90:A:THR:N  | 1:90:A:THR:CA  | 1:90:A:THR:C   | 1:91:A:ALA:N  | 9        | 1.75          |
| (1,81)  | 1:70:A:LEU:C  | 1:71:A:LYS:N   | 1:71:A:LYS:CA  | 1:71:A:LYS:C  | 1        | 1.75          |
| (1,81)  | 1:70:A:LEU:C  | 1:71:A:LYS:N   | 1:71:A:LYS:CA  | 1:71:A:LYS:C  | 7        | 1.75          |
| (1,263) | 1:171:A:LEU:C | 1:172:A:PRO:N  | 1:172:A:PRO:CA | 1:172:A:PRO:C | 8        | 1.74          |
| (1,237) | 1:157:A:LYS:C | 1:158:A:ALA:N  | 1:158:A:ALA:CA | 1:158:A:ALA:C | 10       | 1.74          |
| (1,206) | 1:141:A:LYS:N | 1:141:A:LYS:CA | 1:141:A:LYS:C  | 1:142:A:ILE:N | 9        | 1.74          |
| (1,97)  | 1:78:A:GLN:C  | 1:79:A:ILE:N   | 1:79:A:ILE:CA  | 1:79:A:ILE:C  | 8        | 1.74          |
| (1,122) | 1:92:A:LEU:N  | 1:92:A:LEU:CA  | 1:92:A:LEU:C   | 1:93:A:GLY:N  | 10       | 1.73          |
| (1,97)  | 1:78:A:GLN:C  | 1:79:A:ILE:N   | 1:79:A:ILE:CA  | 1:79:A:ILE:C  | 10       | 1.72          |
| (1,52)  | 1:56:A:ASN:N  | 1:56:A:ASN:CA  | 1:56:A:ASN:C   | 1:57:A:ASP:N  | 8        | 1.72          |
| (1,217) | 1:147:A:GLU:C | 1:148:A:THR:N  | 1:148:A:THR:CA | 1:148:A:THR:C | 8        | 1.71          |
| (1,206) | 1:141:A:LYS:N | 1:141:A:LYS:CA | 1:141:A:LYS:C  | 1:142:A:ILE:N | 2        | 1.71          |
| (1,114) | 1:87:A:THR:N  | 1:87:A:THR:CA  | 1:87:A:THR:C   | 1:88:A:ASN:N  | 7        | 1.71          |
| (1,207) | 1:141:A:LYS:C | 1:142:A:ILE:N  | 1:142:A:ILE:CA | 1:142:A:ILE:C | 10       | 1.7           |
| (1,203) | 1:137:A:GLY:C | 1:138:A:GLU:N  | 1:138:A:GLU:CA | 1:138:A:GLU:C | 8        | 1.7           |
| (1,203) | 1:137:A:GLY:C | 1:138:A:GLU:N  | 1:138:A:GLU:CA | 1:138:A:GLU:C | 9        | 1.7           |
| (1,184) | 1:127:A:GLY:N | 1:127:A:GLY:CA | 1:127:A:GLY:C  | 1:128:A:TYR:N | 3        | 1.7           |
| (1,197) | 1:134:A:TRP:C | 1:135:A:VAL:N  | 1:135:A:VAL:CA | 1:135:A:VAL:C | 9        | 1.69          |
| (1,188) | 1:130:A:ASN:N | 1:130:A:ASN:CA | 1:130:A:ASN:C  | 1:131:A:THR:N | 4        | 1.69          |
| (1,172) | 1:120:A:VAL:N | 1:120:A:VAL:CA | 1:120:A:VAL:C  | 1:121:A:LEU:N | 3        | 1.69          |
| (1,144) | 1:105:A:ASP:N | 1:105:A:ASP:CA | 1:105:A:ASP:C  | 1:106:A:ASN:N | 10       | 1.69          |
| (1,114) | 1:87:A:THR:N  | 1:87:A:THR:CA  | 1:87:A:THR:C   | 1:88:A:ASN:N  | 10       | 1.69          |
| (1,84)  | 1:72:A:PRO:N  | 1:72:A:PRO:CA  | 1:72:A:PRO:C   | 1:73:A:TYR:N  | 6        | 1.69          |
| (1,20)  | 1:31:A:SER:N  | 1:31:A:SER:CA  | 1:31:A:SER:C   | 1:32:A:ILE:N  | 6        | 1.69          |
| (1,75)  | 1:67:A:ALA:C  | 1:68:A:GLU:N   | 1:68:A:GLU:CA  | 1:68:A:GLU:C  | 6        | 1.68          |
| (1,249) | 1:163:A:LYS:C | 1:164:A:GLU:N  | 1:164:A:GLU:CA | 1:164:A:GLU:C | 9        | 1.67          |
| (1,81)  | 1:70:A:LEU:C  | 1:71:A:LYS:N   | 1:71:A:LYS:CA  | 1:71:A:LYS:C  | 9        | 1.67          |
| (1,255) | 1:166:A:MET:C | 1:167:A:LEU:N  | 1:167:A:LEU:CA | 1:167:A:LEU:C | 3        | 1.66          |
| (1,207) | 1:141:A:LYS:C | 1:142:A:ILE:N  | 1:142:A:ILE:CA | 1:142:A:ILE:C | 6        | 1.66          |
| (1,259) | 1:169:A:ASP:C | 1:170:A:SER:N  | 1:170:A:SER:CA | 1:170:A:SER:C | 4        | 1.65          |
| (1,219) | 1:148:A:THR:C | 1:149:A:LYS:N  | 1:149:A:LYS:CA | 1:149:A:LYS:C | 1        | 1.65          |
| (1,59)  | 1:59:A:LYS:C  | 1:60:A:LEU:N   | 1:60:A:LEU:CA  | 1:60:A:LEU:C  | 3        | 1.65          |
| (1,225) | 1:151:A:VAL:C | 1:152:A:ALA:N  | 1:152:A:ALA:CA | 1:152:A:ALA:C | 7        | 1.64          |
| (1,212) | 1:144:A:VAL:N | 1:144:A:VAL:CA | 1:144:A:VAL:C  | 1:145:A:TYR:N | 4        | 1.63          |
| (1,188) | 1:130:A:ASN:N | 1:130:A:ASN:CA | 1:130:A:ASN:C  | 1:131:A:THR:N | 1        | 1.62          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,46)  | 1:51:A:ILE:N  | 1:51:A:ILE:CA  | 1:51:A:ILE:C   | 1:52:A:LYS:N  | 6        | 1.62          |
| (1,258) | 1:168:A:PHE:N | 1:168:A:PHE:CA | 1:168:A:PHE:C  | 1:169:A:ASP:N | 2        | 1.61          |
| (1,161) | 1:114:A:ASP:C | 1:115:A:LYS:N  | 1:115:A:LYS:CA | 1:115:A:LYS:C | 9        | 1.61          |
| (1,53)  | 1:56:A:ASN:C  | 1:57:A:ASP:N   | 1:57:A:ASP:CA  | 1:57:A:ASP:C  | 1        | 1.61          |
| (1,52)  | 1:56:A:ASN:N  | 1:56:A:ASN:CA  | 1:56:A:ASN:C   | 1:57:A:ASP:N  | 9        | 1.61          |
| (1,52)  | 1:56:A:ASN:N  | 1:56:A:ASN:CA  | 1:56:A:ASN:C   | 1:57:A:ASP:N  | 10       | 1.61          |
| (1,103) | 1:81:A:ILE:C  | 1:82:A:THR:N   | 1:82:A:THR:CA  | 1:82:A:THR:C  | 3        | 1.6           |
| (1,92)  | 1:76:A:TYR:N  | 1:76:A:TYR:CA  | 1:76:A:TYR:C   | 1:77:A:LEU:N  | 2        | 1.6           |
| (1,8)   | 1:25:A:VAL:N  | 1:25:A:VAL:CA  | 1:25:A:VAL:C   | 1:26:A:GLU:N  | 3        | 1.6           |
| (1,263) | 1:171:A:LEU:C | 1:172:A:PRO:N  | 1:172:A:PRO:CA | 1:172:A:PRO:C | 9        | 1.59          |
| (1,255) | 1:166:A:MET:C | 1:167:A:LEU:N  | 1:167:A:LEU:CA | 1:167:A:LEU:C | 6        | 1.59          |
| (1,183) | 1:126:A:THR:C | 1:127:A:GLY:N  | 1:127:A:GLY:CA | 1:127:A:GLY:C | 8        | 1.59          |
| (1,172) | 1:120:A:VAL:N | 1:120:A:VAL:CA | 1:120:A:VAL:C  | 1:121:A:LEU:N | 9        | 1.59          |
| (1,95)  | 1:77:A:LEU:C  | 1:78:A:GLN:N   | 1:78:A:GLN:CA  | 1:78:A:GLN:C  | 7        | 1.59          |
| (1,26)  | 1:34:A:PRO:N  | 1:34:A:PRO:CA  | 1:34:A:PRO:C   | 1:35:A:ALA:N  | 10       | 1.59          |
| (1,20)  | 1:31:A:SER:N  | 1:31:A:SER:CA  | 1:31:A:SER:C   | 1:32:A:ILE:N  | 1        | 1.59          |
| (1,248) | 1:163:A:LYS:N | 1:163:A:LYS:CA | 1:163:A:LYS:C  | 1:164:A:GLU:N | 6        | 1.58          |
| (1,165) | 1:116:A:GLU:C | 1:117:A:ASP:N  | 1:117:A:ASP:CA | 1:117:A:ASP:C | 4        | 1.58          |
| (1,127) | 1:96:A:SER:C  | 1:97:A:GLU:N   | 1:97:A:GLU:CA  | 1:97:A:GLU:C  | 8        | 1.58          |
| (1,74)  | 1:67:A:ALA:N  | 1:67:A:ALA:CA  | 1:67:A:ALA:C   | 1:68:A:GLU:N  | 4        | 1.58          |
| (1,206) | 1:141:A:LYS:N | 1:141:A:LYS:CA | 1:141:A:LYS:C  | 1:142:A:ILE:N | 4        | 1.57          |
| (1,147) | 1:107:A:PRO:C | 1:108:A:SER:N  | 1:108:A:SER:CA | 1:108:A:SER:C | 7        | 1.56          |
| (1,126) | 1:96:A:SER:N  | 1:96:A:SER:CA  | 1:96:A:SER:C   | 1:97:A:GLU:N  | 9        | 1.56          |
| (1,213) | 1:144:A:VAL:C | 1:145:A:TYR:N  | 1:145:A:TYR:CA | 1:145:A:TYR:C | 8        | 1.55          |
| (1,183) | 1:126:A:THR:C | 1:127:A:GLY:N  | 1:127:A:GLY:CA | 1:127:A:GLY:C | 4        | 1.55          |
| (1,128) | 1:97:A:GLU:N  | 1:97:A:GLU:CA  | 1:97:A:GLU:C   | 1:98:A:THR:N  | 7        | 1.55          |
| (1,248) | 1:163:A:LYS:N | 1:163:A:LYS:CA | 1:163:A:LYS:C  | 1:164:A:GLU:N | 3        | 1.54          |
| (1,244) | 1:161:A:GLU:N | 1:161:A:GLU:CA | 1:161:A:GLU:C  | 1:162:A:ALA:N | 10       | 1.54          |
| (1,93)  | 1:76:A:TYR:C  | 1:77:A:LEU:N   | 1:77:A:LEU:CA  | 1:77:A:LEU:C  | 8        | 1.54          |
| (1,203) | 1:137:A:GLY:C | 1:138:A:GLU:N  | 1:138:A:GLU:CA | 1:138:A:GLU:C | 6        | 1.53          |
| (1,182) | 1:126:A:THR:N | 1:126:A:THR:CA | 1:126:A:THR:C  | 1:127:A:GLY:N | 8        | 1.53          |
| (1,148) | 1:108:A:SER:N | 1:108:A:SER:CA | 1:108:A:SER:C  | 1:109:A:ALA:N | 6        | 1.53          |
| (1,248) | 1:163:A:LYS:N | 1:163:A:LYS:CA | 1:163:A:LYS:C  | 1:164:A:GLU:N | 8        | 1.52          |
| (1,160) | 1:114:A:ASP:N | 1:114:A:ASP:CA | 1:114:A:ASP:C  | 1:115:A:LYS:N | 10       | 1.52          |
| (1,103) | 1:81:A:ILE:C  | 1:82:A:THR:N   | 1:82:A:THR:CA  | 1:82:A:THR:C  | 5        | 1.52          |
| (1,97)  | 1:78:A:GLN:C  | 1:79:A:ILE:N   | 1:79:A:ILE:CA  | 1:79:A:ILE:C  | 7        | 1.52          |
| (1,184) | 1:127:A:GLY:N | 1:127:A:GLY:CA | 1:127:A:GLY:C  | 1:128:A:TYR:N | 4        | 1.51          |
| (1,145) | 1:105:A:ASP:C | 1:106:A:ASN:N  | 1:106:A:ASN:CA | 1:106:A:ASN:C | 3        | 1.51          |
| (1,114) | 1:87:A:THR:N  | 1:87:A:THR:CA  | 1:87:A:THR:C   | 1:88:A:ASN:N  | 4        | 1.51          |
| (1,36)  | 1:46:A:TYR:N  | 1:46:A:TYR:CA  | 1:46:A:TYR:C   | 1:47:A:ALA:N  | 6        | 1.51          |
| (1,145) | 1:105:A:ASP:C | 1:106:A:ASN:N  | 1:106:A:ASN:CA | 1:106:A:ASN:C | 5        | 1.5           |
| (1,126) | 1:96:A:SER:N  | 1:96:A:SER:CA  | 1:96:A:SER:C   | 1:97:A:GLU:N  | 2        | 1.5           |
| (1,115) | 1:88:A:ASN:C  | 1:89:A:SER:N   | 1:89:A:SER:CA  | 1:89:A:SER:C  | 9        | 1.5           |
| (1,111) | 1:85:A:TYR:C  | 1:86:A:GLU:N   | 1:86:A:GLU:CA  | 1:86:A:GLU:C  | 9        | 1.5           |
| (1,76)  | 1:68:A:GLU:N  | 1:68:A:GLU:CA  | 1:68:A:GLU:C   | 1:69:A:GLN:N  | 7        | 1.49          |
| (1,68)  | 1:64:A:LEU:N  | 1:64:A:LEU:CA  | 1:64:A:LEU:C   | 1:65:A:ALA:N  | 3        | 1.49          |
| (1,52)  | 1:56:A:ASN:N  | 1:56:A:ASN:CA  | 1:56:A:ASN:C   | 1:57:A:ASP:N  | 5        | 1.49          |
| (1,203) | 1:137:A:GLY:C | 1:138:A:GLU:N  | 1:138:A:GLU:CA | 1:138:A:GLU:C | 5        | 1.48          |
| (1,197) | 1:134:A:TRP:C | 1:135:A:VAL:N  | 1:135:A:VAL:CA | 1:135:A:VAL:C | 3        | 1.48          |
| (1,141) | 1:103:A:SER:C | 1:104:A:LEU:N  | 1:104:A:LEU:CA | 1:104:A:LEU:C | 9        | 1.48          |
| (1,248) | 1:163:A:LYS:N | 1:163:A:LYS:CA | 1:163:A:LYS:C  | 1:164:A:GLU:N | 7        | 1.47          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,183) | 1:126:A:THR:C | 1:127:A:GLY:N  | 1:127:A:GLY:CA | 1:127:A:GLY:C | 1        | 1.47          |
| (1,172) | 1:120:A:VAL:N | 1:120:A:VAL:CA | 1:120:A:VAL:C  | 1:121:A:LEU:N | 1        | 1.47          |
| (1,104) | 1:82:A:THR:N  | 1:82:A:THR:CA  | 1:82:A:THR:C   | 1:83:A:SER:N  | 3        | 1.47          |
| (1,259) | 1:169:A:ASP:C | 1:170:A:SER:N  | 1:170:A:SER:CA | 1:170:A:SER:C | 5        | 1.46          |
| (1,254) | 1:166:A:MET:N | 1:166:A:MET:CA | 1:166:A:MET:C  | 1:167:A:LEU:N | 4        | 1.46          |
| (1,145) | 1:105:A:ASP:C | 1:106:A:ASN:N  | 1:106:A:ASN:CA | 1:106:A:ASN:C | 6        | 1.46          |
| (1,145) | 1:105:A:ASP:C | 1:106:A:ASN:N  | 1:106:A:ASN:CA | 1:106:A:ASN:C | 8        | 1.46          |
| (1,133) | 1:99:A:LYS:C  | 1:100:A:ALA:N  | 1:100:A:ALA:CA | 1:100:A:ALA:C | 6        | 1.46          |
| (1,126) | 1:96:A:SER:N  | 1:96:A:SER:CA  | 1:96:A:SER:C   | 1:97:A:GLU:N  | 5        | 1.46          |
| (1,36)  | 1:46:A:TYR:N  | 1:46:A:TYR:CA  | 1:46:A:TYR:C   | 1:47:A:ALA:N  | 4        | 1.46          |
| (1,20)  | 1:31:A:SER:N  | 1:31:A:SER:CA  | 1:31:A:SER:C   | 1:32:A:ILE:N  | 7        | 1.46          |
| (1,189) | 1:130:A:ASN:C | 1:131:A:THR:N  | 1:131:A:THR:CA | 1:131:A:THR:C | 4        | 1.45          |
| (1,173) | 1:120:A:VAL:C | 1:121:A:LEU:N  | 1:121:A:LEU:CA | 1:121:A:LEU:C | 4        | 1.45          |
| (1,69)  | 1:64:A:LEU:C  | 1:65:A:ALA:N   | 1:65:A:ALA:CA  | 1:65:A:ALA:C  | 10       | 1.45          |
| (1,8)   | 1:25:A:VAL:N  | 1:25:A:VAL:CA  | 1:25:A:VAL:C   | 1:26:A:GLU:N  | 7        | 1.45          |
| (1,255) | 1:166:A:MET:C | 1:167:A:LEU:N  | 1:167:A:LEU:CA | 1:167:A:LEU:C | 5        | 1.44          |
| (1,103) | 1:81:A:ILE:C  | 1:82:A:THR:N   | 1:82:A:THR:CA  | 1:82:A:THR:C  | 1        | 1.44          |
| (1,267) | 1:173:A:VAL:C | 1:174:A:ILE:N  | 1:174:A:ILE:CA | 1:174:A:ILE:C | 6        | 1.43          |
| (1,244) | 1:161:A:GLU:N | 1:161:A:GLU:CA | 1:161:A:GLU:C  | 1:162:A:ALA:N | 3        | 1.43          |
| (1,122) | 1:92:A:LEU:N  | 1:92:A:LEU:CA  | 1:92:A:LEU:C   | 1:93:A:GLY:N  | 8        | 1.43          |
| (1,261) | 1:170:A:SER:C | 1:171:A:LEU:N  | 1:171:A:LEU:CA | 1:171:A:LEU:C | 2        | 1.42          |
| (1,206) | 1:141:A:LYS:N | 1:141:A:LYS:CA | 1:141:A:LYS:C  | 1:142:A:ILE:N | 8        | 1.42          |
| (1,82)  | 1:71:A:LYS:N  | 1:71:A:LYS:CA  | 1:71:A:LYS:C   | 1:72:A:PRO:N  | 4        | 1.42          |
| (1,73)  | 1:66:A:ASN:C  | 1:67:A:ALA:N   | 1:67:A:ALA:CA  | 1:67:A:ALA:C  | 6        | 1.42          |
| (1,260) | 1:170:A:SER:N | 1:170:A:SER:CA | 1:170:A:SER:C  | 1:171:A:LEU:N | 2        | 1.41          |
| (1,248) | 1:163:A:LYS:N | 1:163:A:LYS:CA | 1:163:A:LYS:C  | 1:164:A:GLU:N | 1        | 1.41          |
| (1,248) | 1:163:A:LYS:N | 1:163:A:LYS:CA | 1:163:A:LYS:C  | 1:164:A:GLU:N | 5        | 1.41          |
| (1,145) | 1:105:A:ASP:C | 1:106:A:ASN:N  | 1:106:A:ASN:CA | 1:106:A:ASN:C | 9        | 1.41          |
| (1,85)  | 1:72:A:PRO:C  | 1:73:A:TYR:N   | 1:73:A:TYR:CA  | 1:73:A:TYR:C  | 9        | 1.41          |
| (1,203) | 1:137:A:GLY:C | 1:138:A:GLU:N  | 1:138:A:GLU:CA | 1:138:A:GLU:C | 2        | 1.4           |
| (1,202) | 1:137:A:GLY:N | 1:137:A:GLY:CA | 1:137:A:GLY:C  | 1:138:A:GLU:N | 8        | 1.4           |
| (1,198) | 1:135:A:VAL:N | 1:135:A:VAL:CA | 1:135:A:VAL:C  | 1:136:A:PRO:N | 6        | 1.4           |
| (1,165) | 1:116:A:GLU:C | 1:117:A:ASP:N  | 1:117:A:ASP:CA | 1:117:A:ASP:C | 5        | 1.4           |
| (1,145) | 1:105:A:ASP:C | 1:106:A:ASN:N  | 1:106:A:ASN:CA | 1:106:A:ASN:C | 2        | 1.4           |
| (1,116) | 1:89:A:SER:N  | 1:89:A:SER:CA  | 1:89:A:SER:C   | 1:90:A:THR:N  | 10       | 1.4           |
| (1,114) | 1:87:A:THR:N  | 1:87:A:THR:CA  | 1:87:A:THR:C   | 1:88:A:ASN:N  | 9        | 1.4           |
| (1,8)   | 1:25:A:VAL:N  | 1:25:A:VAL:CA  | 1:25:A:VAL:C   | 1:26:A:GLU:N  | 9        | 1.4           |
| (1,261) | 1:170:A:SER:C | 1:171:A:LEU:N  | 1:171:A:LEU:CA | 1:171:A:LEU:C | 6        | 1.39          |
| (1,188) | 1:130:A:ASN:N | 1:130:A:ASN:CA | 1:130:A:ASN:C  | 1:131:A:THR:N | 9        | 1.39          |
| (1,93)  | 1:76:A:TYR:C  | 1:77:A:LEU:N   | 1:77:A:LEU:CA  | 1:77:A:LEU:C  | 3        | 1.39          |
| (1,76)  | 1:68:A:GLU:N  | 1:68:A:GLU:CA  | 1:68:A:GLU:C   | 1:69:A:GLN:N  | 4        | 1.39          |
| (1,62)  | 1:61:A:LYS:N  | 1:61:A:LYS:CA  | 1:61:A:LYS:C   | 1:62:A:VAL:N  | 4        | 1.39          |
| (1,42)  | 1:49:A:VAL:N  | 1:49:A:VAL:CA  | 1:49:A:VAL:C   | 1:50:A:TRP:N  | 8        | 1.39          |
| (1,215) | 1:146:A:ASN:C | 1:147:A:GLU:N  | 1:147:A:GLU:CA | 1:147:A:GLU:C | 10       | 1.38          |
| (1,138) | 1:102:A:ILE:N | 1:102:A:ILE:CA | 1:102:A:ILE:C  | 1:103:A:SER:N | 1        | 1.38          |
| (1,107) | 1:83:A:SER:C  | 1:84:A:GLY:N   | 1:84:A:GLY:CA  | 1:84:A:GLY:C  | 3        | 1.38          |
| (1,49)  | 1:54:A:GLN:C  | 1:55:A:VAL:N   | 1:55:A:VAL:CA  | 1:55:A:VAL:C  | 4        | 1.38          |
| (1,184) | 1:127:A:GLY:N | 1:127:A:GLY:CA | 1:127:A:GLY:C  | 1:128:A:TYR:N | 1        | 1.37          |
| (1,42)  | 1:49:A:VAL:N  | 1:49:A:VAL:CA  | 1:49:A:VAL:C   | 1:50:A:TRP:N  | 4        | 1.37          |
| (1,261) | 1:170:A:SER:C | 1:171:A:LEU:N  | 1:171:A:LEU:CA | 1:171:A:LEU:C | 1        | 1.36          |
| (1,198) | 1:135:A:VAL:N | 1:135:A:VAL:CA | 1:135:A:VAL:C  | 1:136:A:PRO:N | 7        | 1.35          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,182) | 1:126:A:THR:N | 1:126:A:THR:CA | 1:126:A:THR:C  | 1:127:A:GLY:N | 1        | 1.35          |
| (1,182) | 1:126:A:THR:N | 1:126:A:THR:CA | 1:126:A:THR:C  | 1:127:A:GLY:N | 4        | 1.35          |
| (1,180) | 1:124:A:ASP:N | 1:124:A:ASP:CA | 1:124:A:ASP:C  | 1:125:A:LYS:N | 2        | 1.35          |
| (1,68)  | 1:64:A:LEU:N  | 1:64:A:LEU:CA  | 1:64:A:LEU:C   | 1:65:A:ALA:N  | 5        | 1.35          |
| (1,46)  | 1:51:A:ILE:N  | 1:51:A:ILE:CA  | 1:51:A:ILE:C   | 1:52:A:LYS:N  | 5        | 1.35          |
| (1,3)   | 1:22:A:PRO:C  | 1:23:A:ILE:N   | 1:23:A:ILE:CA  | 1:23:A:ILE:C  | 4        | 1.35          |
| (1,267) | 1:173:A:VAL:C | 1:174:A:ILE:N  | 1:174:A:ILE:CA | 1:174:A:ILE:C | 1        | 1.34          |
| (1,240) | 1:159:A:PHE:N | 1:159:A:PHE:CA | 1:159:A:PHE:C  | 1:160:A:TYR:N | 9        | 1.34          |
| (1,198) | 1:135:A:VAL:N | 1:135:A:VAL:CA | 1:135:A:VAL:C  | 1:136:A:PRO:N | 1        | 1.34          |
| (1,146) | 1:106:A:ASN:N | 1:106:A:ASN:CA | 1:106:A:ASN:C  | 1:107:A:PRO:N | 2        | 1.34          |
| (1,105) | 1:82:A:THR:C  | 1:83:A:SER:N   | 1:83:A:SER:CA  | 1:83:A:SER:C  | 8        | 1.34          |
| (1,69)  | 1:64:A:LEU:C  | 1:65:A:ALA:N   | 1:65:A:ALA:CA  | 1:65:A:ALA:C  | 8        | 1.34          |
| (1,68)  | 1:64:A:LEU:N  | 1:64:A:LEU:CA  | 1:64:A:LEU:C   | 1:65:A:ALA:N  | 8        | 1.34          |
| (1,86)  | 1:73:A:TYR:N  | 1:73:A:TYR:CA  | 1:73:A:TYR:C   | 1:74:A:PHE:N  | 8        | 1.33          |
| (1,83)  | 1:71:A:LYS:C  | 1:72:A:PRO:N   | 1:72:A:PRO:CA  | 1:72:A:PRO:C  | 10       | 1.33          |
| (1,60)  | 1:60:A:LEU:N  | 1:60:A:LEU:CA  | 1:60:A:LEU:C   | 1:61:A:LYS:N  | 1        | 1.33          |
| (1,259) | 1:169:A:ASP:C | 1:170:A:SER:N  | 1:170:A:SER:CA | 1:170:A:SER:C | 3        | 1.32          |
| (1,207) | 1:141:A:LYS:C | 1:142:A:ILE:N  | 1:142:A:ILE:CA | 1:142:A:ILE:C | 2        | 1.32          |
| (1,202) | 1:137:A:GLY:N | 1:137:A:GLY:CA | 1:137:A:GLY:C  | 1:138:A:GLU:N | 10       | 1.32          |
| (1,183) | 1:126:A:THR:C | 1:127:A:GLY:N  | 1:127:A:GLY:CA | 1:127:A:GLY:C | 9        | 1.32          |
| (1,103) | 1:81:A:ILE:C  | 1:82:A:THR:N   | 1:82:A:THR:CA  | 1:82:A:THR:C  | 10       | 1.32          |
| (1,97)  | 1:78:A:GLN:C  | 1:79:A:ILE:N   | 1:79:A:ILE:CA  | 1:79:A:ILE:C  | 3        | 1.32          |
| (1,198) | 1:135:A:VAL:N | 1:135:A:VAL:CA | 1:135:A:VAL:C  | 1:136:A:PRO:N | 5        | 1.31          |
| (1,141) | 1:103:A:SER:C | 1:104:A:LEU:N  | 1:104:A:LEU:CA | 1:104:A:LEU:C | 10       | 1.31          |
| (1,256) | 1:167:A:LEU:N | 1:167:A:LEU:CA | 1:167:A:LEU:C  | 1:168:A:PHE:N | 4        | 1.3           |
| (1,225) | 1:151:A:VAL:C | 1:152:A:ALA:N  | 1:152:A:ALA:CA | 1:152:A:ALA:C | 9        | 1.3           |
| (1,133) | 1:99:A:LYS:C  | 1:100:A:ALA:N  | 1:100:A:ALA:CA | 1:100:A:ALA:C | 3        | 1.3           |
| (1,25)  | 1:33:A:THR:C  | 1:34:A:PRO:N   | 1:34:A:PRO:CA  | 1:34:A:PRO:C  | 3        | 1.3           |
| (1,82)  | 1:71:A:LYS:N  | 1:71:A:LYS:CA  | 1:71:A:LYS:C   | 1:72:A:PRO:N  | 9        | 1.29          |
| (1,104) | 1:82:A:THR:N  | 1:82:A:THR:CA  | 1:82:A:THR:C   | 1:83:A:SER:N  | 7        | 1.28          |
| (1,75)  | 1:67:A:ALA:C  | 1:68:A:GLU:N   | 1:68:A:GLU:CA  | 1:68:A:GLU:C  | 1        | 1.28          |
| (1,49)  | 1:54:A:GLN:C  | 1:55:A:VAL:N   | 1:55:A:VAL:CA  | 1:55:A:VAL:C  | 5        | 1.28          |
| (1,11)  | 1:26:A:GLU:C  | 1:27:A:SER:N   | 1:27:A:SER:CA  | 1:27:A:SER:C  | 1        | 1.28          |
| (1,255) | 1:166:A:MET:C | 1:167:A:LEU:N  | 1:167:A:LEU:CA | 1:167:A:LEU:C | 9        | 1.27          |
| (1,240) | 1:159:A:PHE:N | 1:159:A:PHE:CA | 1:159:A:PHE:C  | 1:160:A:TYR:N | 10       | 1.27          |
| (1,189) | 1:130:A:ASN:C | 1:131:A:THR:N  | 1:131:A:THR:CA | 1:131:A:THR:C | 1        | 1.27          |
| (1,105) | 1:82:A:THR:C  | 1:83:A:SER:N   | 1:83:A:SER:CA  | 1:83:A:SER:C  | 6        | 1.27          |
| (1,52)  | 1:56:A:ASN:N  | 1:56:A:ASN:CA  | 1:56:A:ASN:C   | 1:57:A:ASP:N  | 7        | 1.27          |
| (1,284) | 1:182:A:VAL:N | 1:182:A:VAL:CA | 1:182:A:VAL:C  | 1:183:A:GLY:N | 3        | 1.26          |
| (1,207) | 1:141:A:LYS:C | 1:142:A:ILE:N  | 1:142:A:ILE:CA | 1:142:A:ILE:C | 4        | 1.26          |
| (1,58)  | 1:59:A:LYS:N  | 1:59:A:LYS:CA  | 1:59:A:LYS:C   | 1:60:A:LEU:N  | 3        | 1.26          |
| (1,203) | 1:137:A:GLY:C | 1:138:A:GLU:N  | 1:138:A:GLU:CA | 1:138:A:GLU:C | 1        | 1.25          |
| (1,202) | 1:137:A:GLY:N | 1:137:A:GLY:CA | 1:137:A:GLY:C  | 1:138:A:GLU:N | 3        | 1.25          |
| (1,201) | 1:136:A:PRO:C | 1:137:A:GLY:N  | 1:137:A:GLY:CA | 1:137:A:GLY:C | 7        | 1.25          |
| (1,22)  | 1:32:A:ILE:N  | 1:32:A:ILE:CA  | 1:32:A:ILE:C   | 1:33:A:THR:N  | 4        | 1.25          |
| (1,141) | 1:103:A:SER:C | 1:104:A:LEU:N  | 1:104:A:LEU:CA | 1:104:A:LEU:C | 8        | 1.24          |
| (1,106) | 1:83:A:SER:N  | 1:83:A:SER:CA  | 1:83:A:SER:C   | 1:84:A:GLY:N  | 5        | 1.24          |
| (1,85)  | 1:72:A:PRO:C  | 1:73:A:TYR:N   | 1:73:A:TYR:CA  | 1:73:A:TYR:C  | 6        | 1.24          |
| (1,160) | 1:114:A:ASP:N | 1:114:A:ASP:CA | 1:114:A:ASP:C  | 1:115:A:LYS:N | 5        | 1.23          |
| (1,36)  | 1:46:A:TYR:N  | 1:46:A:TYR:CA  | 1:46:A:TYR:C   | 1:47:A:ALA:N  | 8        | 1.23          |
| (1,267) | 1:173:A:VAL:C | 1:174:A:ILE:N  | 1:174:A:ILE:CA | 1:174:A:ILE:C | 9        | 1.22          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,254) | 1:166:A:MET:N | 1:166:A:MET:CA | 1:166:A:MET:C  | 1:167:A:LEU:N | 10       | 1.22          |
| (1,169) | 1:118:A:ILE:C | 1:119:A:ALA:N  | 1:119:A:ALA:CA | 1:119:A:ALA:C | 9        | 1.22          |
| (1,106) | 1:83:A:SER:N  | 1:83:A:SER:CA  | 1:83:A:SER:C   | 1:84:A:GLY:N  | 8        | 1.22          |
| (1,103) | 1:81:A:ILE:C  | 1:82:A:THR:N   | 1:82:A:THR:CA  | 1:82:A:THR:C  | 6        | 1.22          |
| (1,225) | 1:151:A:VAL:C | 1:152:A:ALA:N  | 1:152:A:ALA:CA | 1:152:A:ALA:C | 1        | 1.21          |
| (1,215) | 1:146:A:ASN:C | 1:147:A:GLU:N  | 1:147:A:GLU:CA | 1:147:A:GLU:C | 9        | 1.21          |
| (1,149) | 1:108:A:SER:C | 1:109:A:ALA:N  | 1:109:A:ALA:CA | 1:109:A:ALA:C | 6        | 1.21          |
| (1,133) | 1:99:A:LYS:C  | 1:100:A:ALA:N  | 1:100:A:ALA:CA | 1:100:A:ALA:C | 4        | 1.21          |
| (1,131) | 1:98:A:THR:C  | 1:99:A:LYS:N   | 1:99:A:LYS:CA  | 1:99:A:LYS:C  | 10       | 1.21          |
| (1,104) | 1:82:A:THR:N  | 1:82:A:THR:CA  | 1:82:A:THR:C   | 1:83:A:SER:N  | 4        | 1.21          |
| (1,84)  | 1:72:A:PRO:N  | 1:72:A:PRO:CA  | 1:72:A:PRO:C   | 1:73:A:TYR:N  | 9        | 1.21          |
| (1,36)  | 1:46:A:TYR:N  | 1:46:A:TYR:CA  | 1:46:A:TYR:C   | 1:47:A:ALA:N  | 2        | 1.21          |
| (1,261) | 1:170:A:SER:C | 1:171:A:LEU:N  | 1:171:A:LEU:CA | 1:171:A:LEU:C | 7        | 1.2           |
| (1,254) | 1:166:A:MET:N | 1:166:A:MET:CA | 1:166:A:MET:C  | 1:167:A:LEU:N | 3        | 1.2           |
| (1,186) | 1:129:A:THR:N | 1:129:A:THR:CA | 1:129:A:THR:C  | 1:130:A:ASN:N | 10       | 1.2           |
| (1,49)  | 1:54:A:GLN:C  | 1:55:A:VAL:N   | 1:55:A:VAL:CA  | 1:55:A:VAL:C  | 6        | 1.2           |
| (1,46)  | 1:51:A:ILE:N  | 1:51:A:ILE:CA  | 1:51:A:ILE:C   | 1:52:A:LYS:N  | 1        | 1.2           |
| (1,46)  | 1:51:A:ILE:N  | 1:51:A:ILE:CA  | 1:51:A:ILE:C   | 1:52:A:LYS:N  | 3        | 1.2           |
| (1,8)   | 1:25:A:VAL:N  | 1:25:A:VAL:CA  | 1:25:A:VAL:C   | 1:26:A:GLU:N  | 2        | 1.2           |
| (1,182) | 1:126:A:THR:N | 1:126:A:THR:CA | 1:126:A:THR:C  | 1:127:A:GLY:N | 6        | 1.19          |
| (1,159) | 1:113:A:LEU:C | 1:114:A:ASP:N  | 1:114:A:ASP:CA | 1:114:A:ASP:C | 4        | 1.19          |
| (1,137) | 1:101:A:VAL:C | 1:102:A:ILE:N  | 1:102:A:ILE:CA | 1:102:A:ILE:C | 8        | 1.19          |
| (1,213) | 1:144:A:VAL:C | 1:145:A:TYR:N  | 1:145:A:TYR:CA | 1:145:A:TYR:C | 3        | 1.18          |
| (1,202) | 1:137:A:GLY:N | 1:137:A:GLY:CA | 1:137:A:GLY:C  | 1:138:A:GLU:N | 4        | 1.18          |
| (1,165) | 1:116:A:GLU:C | 1:117:A:ASP:N  | 1:117:A:ASP:CA | 1:117:A:ASP:C | 7        | 1.18          |
| (1,118) | 1:90:A:THR:N  | 1:90:A:THR:CA  | 1:90:A:THR:C   | 1:91:A:ALA:N  | 1        | 1.18          |
| (1,42)  | 1:49:A:VAL:N  | 1:49:A:VAL:CA  | 1:49:A:VAL:C   | 1:50:A:TRP:N  | 2        | 1.18          |
| (1,36)  | 1:46:A:TYR:N  | 1:46:A:TYR:CA  | 1:46:A:TYR:C   | 1:47:A:ALA:N  | 9        | 1.18          |
| (1,195) | 1:133:A:ILE:C | 1:134:A:TRP:N  | 1:134:A:TRP:CA | 1:134:A:TRP:C | 7        | 1.17          |
| (1,114) | 1:87:A:THR:N  | 1:87:A:THR:CA  | 1:87:A:THR:C   | 1:88:A:ASN:N  | 6        | 1.17          |
| (1,73)  | 1:66:A:ASN:C  | 1:67:A:ALA:N   | 1:67:A:ALA:CA  | 1:67:A:ALA:C  | 10       | 1.17          |
| (1,68)  | 1:64:A:LEU:N  | 1:64:A:LEU:CA  | 1:64:A:LEU:C   | 1:65:A:ALA:N  | 10       | 1.17          |
| (1,22)  | 1:32:A:ILE:N  | 1:32:A:ILE:CA  | 1:32:A:ILE:C   | 1:33:A:THR:N  | 3        | 1.17          |
| (1,284) | 1:182:A:VAL:N | 1:182:A:VAL:CA | 1:182:A:VAL:C  | 1:183:A:GLY:N | 5        | 1.16          |
| (1,244) | 1:161:A:GLU:N | 1:161:A:GLU:CA | 1:161:A:GLU:C  | 1:162:A:ALA:N | 7        | 1.16          |
| (1,140) | 1:103:A:SER:N | 1:103:A:SER:CA | 1:103:A:SER:C  | 1:104:A:LEU:N | 4        | 1.16          |
| (1,284) | 1:182:A:VAL:N | 1:182:A:VAL:CA | 1:182:A:VAL:C  | 1:183:A:GLY:N | 4        | 1.15          |
| (1,173) | 1:120:A:VAL:C | 1:121:A:LEU:N  | 1:121:A:LEU:CA | 1:121:A:LEU:C | 6        | 1.15          |
| (1,145) | 1:105:A:ASP:C | 1:106:A:ASN:N  | 1:106:A:ASN:CA | 1:106:A:ASN:C | 10       | 1.15          |
| (1,141) | 1:103:A:SER:C | 1:104:A:LEU:N  | 1:104:A:LEU:CA | 1:104:A:LEU:C | 6        | 1.15          |
| (1,172) | 1:120:A:VAL:N | 1:120:A:VAL:CA | 1:120:A:VAL:C  | 1:121:A:LEU:N | 2        | 1.14          |
| (1,275) | 1:177:A:PHE:C | 1:178:A:GLN:N  | 1:178:A:GLN:CA | 1:178:A:GLN:C | 5        | 1.13          |
| (1,267) | 1:173:A:VAL:C | 1:174:A:ILE:N  | 1:174:A:ILE:CA | 1:174:A:ILE:C | 2        | 1.13          |
| (1,168) | 1:118:A:ILE:N | 1:118:A:ILE:CA | 1:118:A:ILE:C  | 1:119:A:ALA:N | 6        | 1.13          |
| (1,141) | 1:103:A:SER:C | 1:104:A:LEU:N  | 1:104:A:LEU:CA | 1:104:A:LEU:C | 1        | 1.13          |
| (1,119) | 1:90:A:THR:C  | 1:91:A:ALA:N   | 1:91:A:ALA:CA  | 1:91:A:ALA:C  | 1        | 1.13          |
| (1,3)   | 1:22:A:PRO:C  | 1:23:A:ILE:N   | 1:23:A:ILE:CA  | 1:23:A:ILE:C  | 1        | 1.12          |
| (1,240) | 1:159:A:PHE:N | 1:159:A:PHE:CA | 1:159:A:PHE:C  | 1:160:A:TYR:N | 4        | 1.11          |
| (1,49)  | 1:54:A:GLN:C  | 1:55:A:VAL:N   | 1:55:A:VAL:CA  | 1:55:A:VAL:C  | 2        | 1.11          |
| (1,177) | 1:122:A:TYR:C | 1:123:A:PRO:N  | 1:123:A:PRO:CA | 1:123:A:PRO:C | 3        | 1.1           |
| (1,148) | 1:108:A:SER:N | 1:108:A:SER:CA | 1:108:A:SER:C  | 1:109:A:ALA:N | 7        | 1.1           |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,81)  | 1:70:A:LEU:C  | 1:71:A:LYS:N   | 1:71:A:LYS:CA  | 1:71:A:LYS:C  | 10       | 1.1           |
| (1,284) | 1:182:A:VAL:N | 1:182:A:VAL:CA | 1:182:A:VAL:C  | 1:183:A:GLY:N | 10       | 1.09          |
| (1,182) | 1:126:A:THR:N | 1:126:A:THR:CA | 1:126:A:THR:C  | 1:127:A:GLY:N | 9        | 1.09          |
| (1,141) | 1:103:A:SER:C | 1:104:A:LEU:N  | 1:104:A:LEU:CA | 1:104:A:LEU:C | 2        | 1.09          |
| (1,8)   | 1:25:A:VAL:N  | 1:25:A:VAL:CA  | 1:25:A:VAL:C   | 1:26:A:GLU:N  | 8        | 1.09          |
| (1,254) | 1:166:A:MET:N | 1:166:A:MET:CA | 1:166:A:MET:C  | 1:167:A:LEU:N | 2        | 1.08          |
| (1,212) | 1:144:A:VAL:N | 1:144:A:VAL:CA | 1:144:A:VAL:C  | 1:145:A:TYR:N | 9        | 1.08          |
| (1,145) | 1:105:A:ASP:C | 1:106:A:ASN:N  | 1:106:A:ASN:CA | 1:106:A:ASN:C | 7        | 1.08          |
| (1,122) | 1:92:A:LEU:N  | 1:92:A:LEU:CA  | 1:92:A:LEU:C   | 1:93:A:GLY:N  | 3        | 1.08          |
| (1,92)  | 1:76:A:TYR:N  | 1:76:A:TYR:CA  | 1:76:A:TYR:C   | 1:77:A:LEU:N  | 7        | 1.08          |
| (1,91)  | 1:75:A:LYS:C  | 1:76:A:TYR:N   | 1:76:A:TYR:CA  | 1:76:A:TYR:C  | 2        | 1.08          |
| (1,61)  | 1:60:A:LEU:C  | 1:61:A:LYS:N   | 1:61:A:LYS:CA  | 1:61:A:LYS:C  | 5        | 1.08          |
| (1,53)  | 1:56:A:ASN:C  | 1:57:A:ASP:N   | 1:57:A:ASP:CA  | 1:57:A:ASP:C  | 6        | 1.08          |
| (1,141) | 1:103:A:SER:C | 1:104:A:LEU:N  | 1:104:A:LEU:CA | 1:104:A:LEU:C | 3        | 1.07          |
| (1,98)  | 1:79:A:ILE:N  | 1:79:A:ILE:CA  | 1:79:A:ILE:C   | 1:80:A:GLN:N  | 10       | 1.07          |
| (1,79)  | 1:69:A:GLN:C  | 1:70:A:LEU:N   | 1:70:A:LEU:CA  | 1:70:A:LEU:C  | 4        | 1.07          |
| (1,183) | 1:126:A:THR:C | 1:127:A:GLY:N  | 1:127:A:GLY:CA | 1:127:A:GLY:C | 6        | 1.06          |
| (1,73)  | 1:66:A:ASN:C  | 1:67:A:ALA:N   | 1:67:A:ALA:CA  | 1:67:A:ALA:C  | 8        | 1.06          |
| (1,42)  | 1:49:A:VAL:N  | 1:49:A:VAL:CA  | 1:49:A:VAL:C   | 1:50:A:TRP:N  | 1        | 1.06          |
| (1,195) | 1:133:A:ILE:C | 1:134:A:TRP:N  | 1:134:A:TRP:CA | 1:134:A:TRP:C | 6        | 1.05          |
| (1,121) | 1:91:A:ALA:C  | 1:92:A:LEU:N   | 1:92:A:LEU:CA  | 1:92:A:LEU:C  | 10       | 1.05          |
| (1,69)  | 1:64:A:LEU:C  | 1:65:A:ALA:N   | 1:65:A:ALA:CA  | 1:65:A:ALA:C  | 9        | 1.05          |
| (1,65)  | 1:62:A:VAL:C  | 1:63:A:THR:N   | 1:63:A:THR:CA  | 1:63:A:THR:C  | 6        | 1.05          |
| (1,22)  | 1:32:A:ILE:N  | 1:32:A:ILE:CA  | 1:32:A:ILE:C   | 1:33:A:THR:N  | 8        | 1.05          |
| (1,244) | 1:161:A:GLU:N | 1:161:A:GLU:CA | 1:161:A:GLU:C  | 1:162:A:ALA:N | 8        | 1.04          |
| (1,183) | 1:126:A:THR:C | 1:127:A:GLY:N  | 1:127:A:GLY:CA | 1:127:A:GLY:C | 3        | 1.04          |
| (1,179) | 1:123:A:PRO:C | 1:124:A:ASP:N  | 1:124:A:ASP:CA | 1:124:A:ASP:C | 2        | 1.04          |
| (1,141) | 1:103:A:SER:C | 1:104:A:LEU:N  | 1:104:A:LEU:CA | 1:104:A:LEU:C | 5        | 1.04          |
| (1,68)  | 1:64:A:LEU:N  | 1:64:A:LEU:CA  | 1:64:A:LEU:C   | 1:65:A:ALA:N  | 4        | 1.04          |
| (1,36)  | 1:46:A:TYR:N  | 1:46:A:TYR:CA  | 1:46:A:TYR:C   | 1:47:A:ALA:N  | 3        | 1.04          |
| (1,284) | 1:182:A:VAL:N | 1:182:A:VAL:CA | 1:182:A:VAL:C  | 1:183:A:GLY:N | 7        | 1.03          |
| (1,198) | 1:135:A:VAL:N | 1:135:A:VAL:CA | 1:135:A:VAL:C  | 1:136:A:PRO:N | 10       | 1.03          |
| (1,117) | 1:89:A:SER:C  | 1:90:A:THR:N   | 1:90:A:THR:CA  | 1:90:A:THR:C  | 3        | 1.03          |
| (1,103) | 1:81:A:ILE:C  | 1:82:A:THR:N   | 1:82:A:THR:CA  | 1:82:A:THR:C  | 2        | 1.03          |
| (1,71)  | 1:65:A:ALA:C  | 1:66:A:ASN:N   | 1:66:A:ASN:CA  | 1:66:A:ASN:C  | 2        | 1.03          |
| (1,172) | 1:120:A:VAL:N | 1:120:A:VAL:CA | 1:120:A:VAL:C  | 1:121:A:LEU:N | 10       | 1.02          |
| (1,169) | 1:118:A:ILE:C | 1:119:A:ALA:N  | 1:119:A:ALA:CA | 1:119:A:ALA:C | 4        | 1.02          |
| (1,165) | 1:116:A:GLU:C | 1:117:A:ASP:N  | 1:117:A:ASP:CA | 1:117:A:ASP:C | 9        | 1.02          |
| (1,160) | 1:114:A:ASP:N | 1:114:A:ASP:CA | 1:114:A:ASP:C  | 1:115:A:LYS:N | 3        | 1.02          |
| (1,146) | 1:106:A:ASN:N | 1:106:A:ASN:CA | 1:106:A:ASN:C  | 1:107:A:PRO:N | 7        | 1.02          |
| (1,114) | 1:87:A:THR:N  | 1:87:A:THR:CA  | 1:87:A:THR:C   | 1:88:A:ASN:N  | 8        | 1.02          |
| (1,87)  | 1:73:A:TYR:C  | 1:74:A:PHE:N   | 1:74:A:PHE:CA  | 1:74:A:PHE:C  | 7        | 1.02          |
| (1,79)  | 1:69:A:GLN:C  | 1:70:A:LEU:N   | 1:70:A:LEU:CA  | 1:70:A:LEU:C  | 8        | 1.02          |
| (1,257) | 1:167:A:LEU:C | 1:168:A:PHE:N  | 1:168:A:PHE:CA | 1:168:A:PHE:C | 3        | 1.01          |
| (1,182) | 1:126:A:THR:N | 1:126:A:THR:CA | 1:126:A:THR:C  | 1:127:A:GLY:N | 3        | 1.01          |
| (1,110) | 1:85:A:TYR:N  | 1:85:A:TYR:CA  | 1:85:A:TYR:C   | 1:86:A:GLU:N  | 2        | 1.01          |
| (1,105) | 1:82:A:THR:C  | 1:83:A:SER:N   | 1:83:A:SER:CA  | 1:83:A:SER:C  | 1        | 1.01          |
| (1,284) | 1:182:A:VAL:N | 1:182:A:VAL:CA | 1:182:A:VAL:C  | 1:183:A:GLY:N | 2        | 1.0           |
| (1,119) | 1:90:A:THR:C  | 1:91:A:ALA:N   | 1:91:A:ALA:CA  | 1:91:A:ALA:C  | 9        | 1.0           |
| (1,114) | 1:87:A:THR:N  | 1:87:A:THR:CA  | 1:87:A:THR:C   | 1:88:A:ASN:N  | 5        | 1.0           |