



# Full wwPDB NMR Structure Validation Report ⓘ

Jun 5, 2023 – 11:47 AM EDT

PDB ID : 2M7L  
BMRB ID : 19195  
Title : Alfa-actinin from parasite Entamoeba histolytica  
Authors : Persson, C.K.; Mayzel, M.L.; Karlsson, B.G.; Backman, L.  
Deposited on : 2013-04-26

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 : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
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) : 2.33

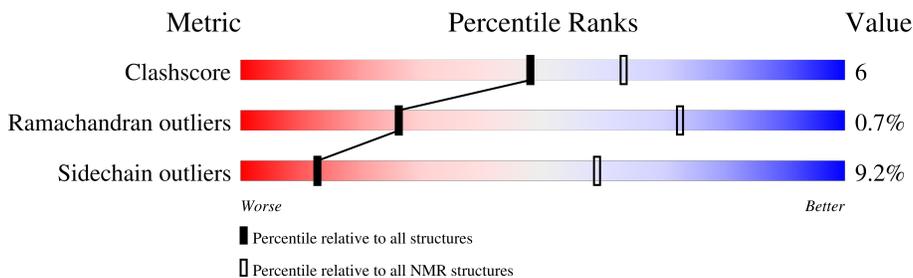
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 87%.

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            | 158937                      | 12864                     |
| Ramachandran outliers | 154571                      | 11451                     |
| Sidechain outliers    | 154315                      | 11428                     |

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     | 144    | 77% 8% • 13%     |

## 2 Ensemble composition and analysis i

This entry contains 12 models. Model 7 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:5-A:83 (79)                   | 1.44              | 7            |
| 2                                    | A:92-A:130, A:134-A:140<br>(46) | 0.90              | 11           |

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 1 single-model cluster was found.

| Cluster number        | Models                |
|-----------------------|-----------------------|
| 1                     | 1, 2, 5, 7, 9, 10, 11 |
| 2                     | 3, 6, 8, 12           |
| Single-model clusters | 4                     |

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2143 atoms, of which 1027 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Calponin homology domain protein, putative.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|-------|
|     |       |          | Total | C   | H    | N   | O   | S |       |
| 1   | A     | 144      | 2143  | 690 | 1027 | 179 | 241 | 6 | 0     |

There are 2 discrepancies between the modelled and reference sequences:

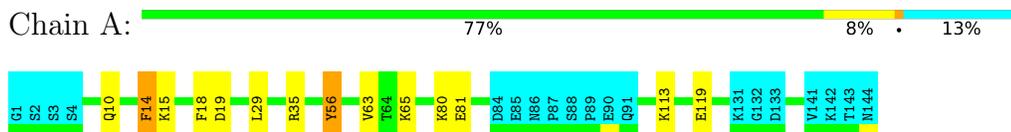
| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 1       | GLY      | -      | expression tag | UNP C4LWU6 |
| A     | 2       | SER      | -      | expression tag | UNP C4LWU6 |

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

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

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

- Molecule 1: Calponin homology domain protein, putative

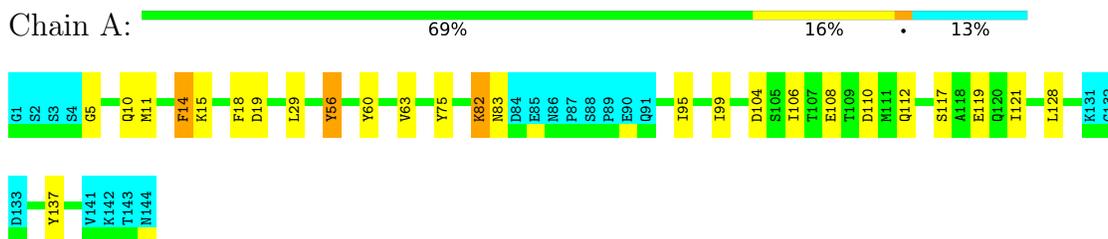


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section [4.1](#) above.

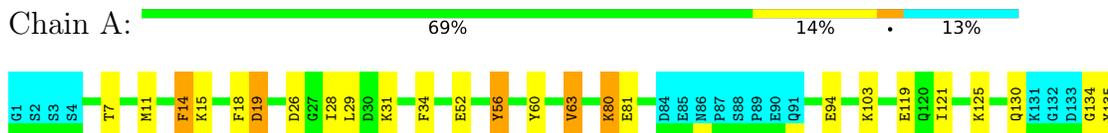
#### 4.2.1 Score per residue for model 1

- Molecule 1: Calponin homology domain protein, putative



#### 4.2.2 Score per residue for model 2

- Molecule 1: Calponin homology domain protein, putative





### 4.2.3 Score per residue for model 3

- Molecule 1: Calponin homology domain protein, putative



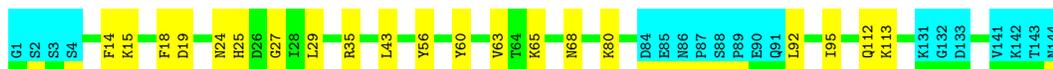
### 4.2.4 Score per residue for model 4

- Molecule 1: Calponin homology domain protein, putative



### 4.2.5 Score per residue for model 5

- Molecule 1: Calponin homology domain protein, putative



### 4.2.6 Score per residue for model 6

- Molecule 1: Calponin homology domain protein, putative

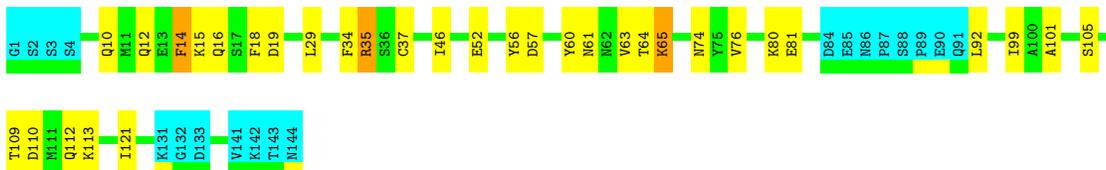




#### 4.2.7 Score per residue for model 7 (medoid)

- Molecule 1: Calponin homology domain protein, putative

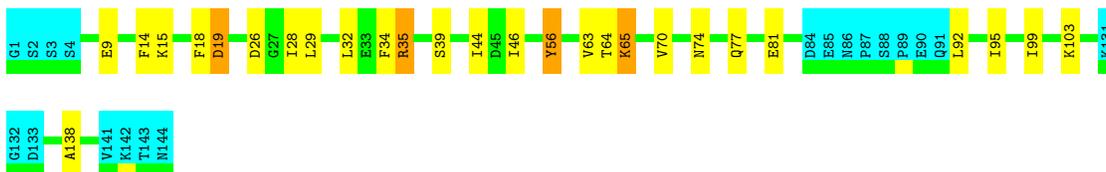
Chain A: 64% 21% 13%



#### 4.2.8 Score per residue for model 8

- Molecule 1: Calponin homology domain protein, putative

Chain A: 68% 16% 13%



#### 4.2.9 Score per residue for model 9

- Molecule 1: Calponin homology domain protein, putative

Chain A: 69% 14% 13%



#### 4.2.10 Score per residue for model 10

- Molecule 1: Calponin homology domain protein, putative

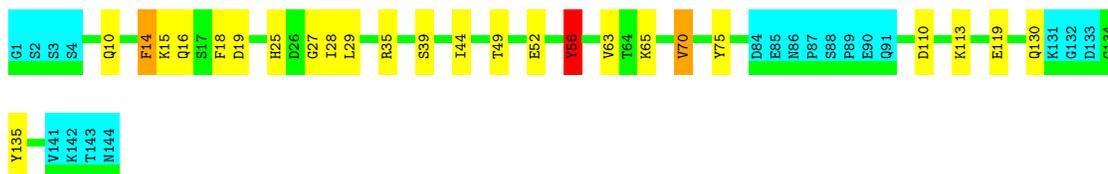
Chain A: 66% 19% 13%



#### 4.2.11 Score per residue for model 11

- Molecule 1: Calponin homology domain protein, putative

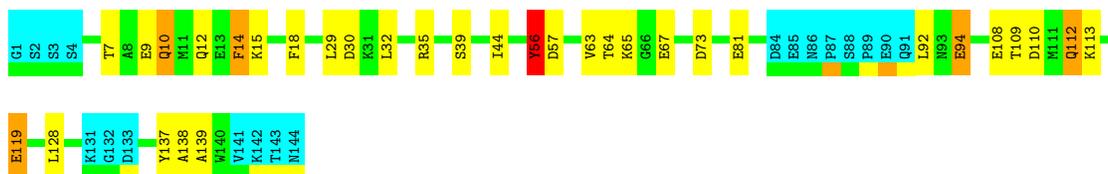
Chain A: 69% 15% 13%



#### 4.2.12 Score per residue for model 12

- Molecule 1: Calponin homology domain protein, putative

Chain A: 64% 19% 13%



## 5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 12 were deposited, based on the following criterion: *target function*.

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

| Software name | Classification     | Version |
|---------------|--------------------|---------|
| CYANA         | structure solution | 2.2     |
| 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                       | 1542           |
| Number of shifts mapped to atoms             | 1542           |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 87%            |

## 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     | 0.84±0.02    | 0±0/997 ( 0.0± 0.0%) | 0.74±0.02   | 0±1/1344 ( 0.0± 0.0%) |
| All | All   | 0.84         | 0/11964 ( 0.0%)      | 0.74        | 4/16128 ( 0.0%)       |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | Chirality | Planarity |
|-----|-------|-----------|-----------|
| 1   | A     | 0.0±0.0   | 0.2±0.4   |
| All | All   | 0         | 2         |

There are no bond-length outliers.

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

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|-----------|-------|-------------|----------|--------|-------|
|     |       |     |      |           |       |             |          | Worst  | Total |
| 1   | A     | 56  | TYR  | CB-CG-CD1 | 7.58  | 125.55      | 121.00   | 8      | 3     |
| 1   | A     | 56  | TYR  | CB-CG-CD2 | -6.37 | 117.18      | 121.00   | 8      | 1     |

There are no chirality outliers.

All unique planar outliers are listed below.

| Mol | Chain | Res | Type | Group     | Models (Total) |
|-----|-------|-----|------|-----------|----------------|
| 1   | A     | 35  | ARG  | Sidechain | 2              |

### 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     | 979   | 906      | 906      | 12±3    |
| All | All   | 11748 | 10872    | 10872    | 143     |

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 6.

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

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:67:GLU:HB3   | 1:A:74:ASN:ND2   | 0.69     | 2.03        | 10     | 1     |
| 1:A:110:ASP:HA   | 1:A:113:LYS:NZ   | 0.66     | 2.05        | 12     | 2     |
| 1:A:15:LYS:O     | 1:A:19:ASP:HB2   | 0.63     | 1.93        | 3      | 7     |
| 1:A:109:THR:O    | 1:A:113:LYS:HB2  | 0.62     | 1.94        | 10     | 3     |
| 1:A:18:PHE:CZ    | 1:A:27:GLY:HA2   | 0.61     | 2.30        | 11     | 4     |
| 1:A:15:LYS:HA    | 1:A:18:PHE:CE2   | 0.61     | 2.31        | 7      | 8     |
| 1:A:18:PHE:HB2   | 1:A:29:LEU:HD12  | 0.60     | 1.73        | 9      | 3     |
| 1:A:32:LEU:O     | 1:A:35:ARG:HB3   | 0.58     | 1.99        | 3      | 6     |
| 1:A:56:TYR:CE1   | 1:A:60:TYR:HB2   | 0.55     | 2.37        | 7      | 2     |
| 1:A:39:SER:HA    | 1:A:44:ILE:O     | 0.55     | 2.01        | 6      | 4     |
| 1:A:130:GLN:HG2  | 1:A:135:TYR:CE1  | 0.54     | 2.37        | 11     | 1     |
| 1:A:10:GLN:HG2   | 1:A:14:PHE:HB3   | 0.54     | 1.79        | 11     | 4     |
| 1:A:35:ARG:HA    | 1:A:56:TYR:CE2   | 0.54     | 2.38        | 7      | 3     |
| 1:A:128:LEU:HD23 | 1:A:137:TYR:HA   | 0.53     | 1.80        | 1      | 2     |
| 1:A:130:GLN:HA   | 1:A:134:GLY:O    | 0.53     | 2.03        | 6      | 3     |
| 1:A:112:GLN:HA   | 1:A:121:ILE:HD13 | 0.53     | 1.81        | 7      | 1     |
| 1:A:130:GLN:HB3  | 1:A:135:TYR:CE2  | 0.52     | 2.39        | 2      | 1     |
| 1:A:29:LEU:HD22  | 1:A:34:PHE:HB2   | 0.52     | 1.80        | 4      | 1     |
| 1:A:11:MET:HA    | 1:A:14:PHE:CE2   | 0.52     | 2.40        | 4      | 2     |
| 1:A:18:PHE:HB2   | 1:A:29:LEU:CD1   | 0.51     | 2.35        | 2      | 1     |
| 1:A:35:ARG:HA    | 1:A:56:TYR:CD2   | 0.51     | 2.41        | 5      | 2     |
| 1:A:64:THR:HB    | 1:A:67:GLU:O     | 0.50     | 2.07        | 12     | 1     |
| 1:A:76:VAL:O     | 1:A:80:LYS:HG2   | 0.50     | 2.07        | 7      | 1     |
| 1:A:29:LEU:HD13  | 1:A:34:PHE:CD1   | 0.50     | 2.41        | 7      | 5     |
| 1:A:108:GLU:HA   | 1:A:111:MET:SD   | 0.50     | 2.47        | 3      | 1     |
| 1:A:109:THR:O    | 1:A:113:LYS:HD2  | 0.49     | 2.08        | 4      | 1     |
| 1:A:77:GLN:O     | 1:A:81:GLU:HB2   | 0.49     | 2.08        | 3      | 3     |
| 1:A:128:LEU:CD2  | 1:A:137:TYR:HA   | 0.48     | 2.39        | 12     | 1     |
| 1:A:64:THR:HA    | 1:A:74:ASN:OD1   | 0.48     | 2.09        | 10     | 2     |
| 1:A:73:ASP:O     | 1:A:77:GLN:HG2   | 0.48     | 2.09        | 10     | 1     |
| 1:A:18:PHE:CE1   | 1:A:27:GLY:HA2   | 0.47     | 2.44        | 11     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:65:LYS:H     | 1:A:65:LYS:HD3   | 0.47     | 1.68        | 9      | 2     |
| 1:A:34:PHE:HA    | 1:A:37:CYS:SG    | 0.47     | 2.49        | 7      | 1     |
| 1:A:117:SER:O    | 1:A:121:ILE:HG12 | 0.47     | 2.10        | 1      | 1     |
| 1:A:67:GLU:CD    | 1:A:71:SER:HB3   | 0.47     | 2.30        | 10     | 1     |
| 1:A:95:ILE:O     | 1:A:99:ILE:HG12  | 0.46     | 2.10        | 4      | 1     |
| 1:A:119:GLU:CD   | 1:A:119:GLU:H    | 0.46     | 2.13        | 12     | 2     |
| 1:A:26:ASP:OD1   | 1:A:28:ILE:HG12  | 0.46     | 2.10        | 2      | 3     |
| 1:A:18:PHE:HB3   | 1:A:75:TYR:CE2   | 0.46     | 2.45        | 11     | 2     |
| 1:A:33:GLU:HA    | 1:A:33:GLU:OE1   | 0.46     | 2.11        | 4      | 1     |
| 1:A:15:LYS:HA    | 1:A:18:PHE:CD2   | 0.46     | 2.46        | 4      | 1     |
| 1:A:110:ASP:HA   | 1:A:113:LYS:HZ2  | 0.45     | 1.68        | 12     | 2     |
| 1:A:12:GLN:O     | 1:A:16:GLN:HG2   | 0.45     | 2.11        | 7      | 1     |
| 1:A:121:ILE:O    | 1:A:125:LYS:HG3  | 0.45     | 2.11        | 2      | 1     |
| 1:A:29:LEU:HB3   | 1:A:70:VAL:HG23  | 0.44     | 1.89        | 9      | 1     |
| 1:A:78:TYR:O     | 1:A:82:LYS:HB2   | 0.44     | 2.12        | 4      | 1     |
| 1:A:95:ILE:O     | 1:A:99:ILE:HG13  | 0.44     | 2.12        | 1      | 4     |
| 1:A:28:ILE:HG22  | 1:A:71:SER:HA    | 0.43     | 1.89        | 4      | 1     |
| 1:A:22:ASP:OD1   | 1:A:29:LEU:HA    | 0.43     | 2.14        | 3      | 1     |
| 1:A:19:ASP:OD1   | 1:A:25:HIS:HB2   | 0.43     | 2.13        | 4      | 1     |
| 1:A:29:LEU:HB2   | 1:A:70:VAL:HG23  | 0.43     | 1.90        | 11     | 1     |
| 1:A:64:THR:HA    | 1:A:74:ASN:ND2   | 0.43     | 2.27        | 8      | 1     |
| 1:A:106:ILE:HG13 | 1:A:110:ASP:CB   | 0.43     | 2.44        | 1      | 1     |
| 1:A:99:ILE:CG2   | 1:A:110:ASP:HB3  | 0.42     | 2.44        | 7      | 1     |
| 1:A:44:ILE:HG23  | 1:A:45:ASP:O     | 0.42     | 2.14        | 9      | 1     |
| 1:A:52:GLU:H     | 1:A:52:GLU:CD    | 0.42     | 2.16        | 10     | 1     |
| 1:A:57:ASP:O     | 1:A:61:ASN:HB2   | 0.42     | 2.13        | 10     | 1     |
| 1:A:31:LYS:HG2   | 1:A:56:TYR:OH    | 0.42     | 2.15        | 6      | 2     |
| 1:A:63:VAL:O     | 1:A:65:LYS:HE2   | 0.42     | 2.15        | 5      | 1     |
| 1:A:109:THR:HA   | 1:A:113:LYS:HG2  | 0.42     | 1.90        | 7      | 1     |
| 1:A:9:GLU:CD     | 1:A:9:GLU:H      | 0.42     | 2.18        | 8      | 1     |
| 1:A:16:GLN:O     | 1:A:19:ASP:HB3   | 0.42     | 2.14        | 9      | 1     |
| 1:A:129:PRO:O    | 1:A:135:TYR:HA   | 0.42     | 2.14        | 10     | 1     |
| 1:A:56:TYR:CD1   | 1:A:60:TYR:HB2   | 0.42     | 2.50        | 1      | 1     |
| 1:A:80:LYS:HZ3   | 1:A:81:GLU:CD    | 0.42     | 2.18        | 9      | 2     |
| 1:A:78:TYR:O     | 1:A:81:GLU:HB3   | 0.42     | 2.15        | 3      | 1     |
| 1:A:113:LYS:HD3  | 1:A:114:ALA:N    | 0.42     | 2.30        | 4      | 1     |
| 1:A:65:LYS:HD3   | 1:A:65:LYS:N     | 0.41     | 2.30        | 8      | 1     |
| 1:A:56:TYR:C     | 1:A:56:TYR:CD1   | 0.41     | 2.93        | 11     | 2     |
| 1:A:10:GLN:O     | 1:A:14:PHE:HD2   | 0.41     | 1.97        | 12     | 1     |
| 1:A:108:GLU:HG3  | 1:A:112:GLN:HG3  | 0.41     | 1.90        | 12     | 1     |
| 1:A:44:ILE:HG13  | 1:A:44:ILE:O     | 0.41     | 2.16        | 4      | 1     |

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| Atom-1         | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|----------------|-----------------|----------|-------------|--------|-------|
|                |                 |          |             | Worst  | Total |
| 1:A:29:LEU:HB3 | 1:A:70:VAL:CG2  | 0.41     | 2.46        | 8      | 1     |
| 1:A:109:THR:O  | 1:A:113:LYS:HG3 | 0.41     | 2.15        | 12     | 1     |
| 1:A:64:THR:HA  | 1:A:74:ASN:HD22 | 0.41     | 1.76        | 6      | 1     |
| 1:A:49:THR:HA  | 1:A:52:GLU:OE1  | 0.41     | 2.16        | 11     | 1     |
| 1:A:39:SER:HA  | 1:A:44:ILE:CG2  | 0.41     | 2.46        | 9      | 1     |
| 1:A:92:LEU:O   | 1:A:96:PHE:HB2  | 0.41     | 2.15        | 10     | 1     |
| 1:A:39:SER:HB3 | 1:A:44:ILE:HD13 | 0.40     | 1.92        | 9      | 1     |
| 1:A:60:TYR:HA  | 1:A:63:VAL:CG1  | 0.40     | 2.46        | 2      | 1     |
| 1:A:15:LYS:HA  | 1:A:18:PHE:CZ   | 0.40     | 2.52        | 1      | 1     |
| 1:A:10:GLN:O   | 1:A:14:PHE:HB3  | 0.40     | 2.16        | 3      | 1     |
| 1:A:112:GLN:HA | 1:A:121:ILE:CD1 | 0.40     | 2.45        | 7      | 1     |
| 1:A:119:GLU:H  | 1:A:119:GLU:CD  | 0.40     | 2.20        | 11     | 1     |

## 6.3 Torsion angles [i](#)

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

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

| Mol | Chain | Analysed        | Favoured      | Allowed     | Outliers   | Percentiles |    |
|-----|-------|-----------------|---------------|-------------|------------|-------------|----|
| 1   | A     | 125/144 (87%)   | 114±2 (91±2%) | 11±2 (8±2%) | 1±1 (1±1%) | 26          | 73 |
| All | All   | 1500/1728 (87%) | 1362 (91%)    | 127 (8%)    | 11 (1%)    | 26          | 73 |

All 6 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     | 46  | ILE  | 3              |
| 1   | A     | 50  | GLY  | 2              |
| 1   | A     | 101 | ALA  | 2              |
| 1   | A     | 53  | ASP  | 2              |
| 1   | A     | 5   | GLY  | 1              |
| 1   | A     | 25  | HIS  | 1              |

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

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

| Mol | Chain | Analysed        | Rotameric    | Outliers    | Percentiles |
|-----|-------|-----------------|--------------|-------------|-------------|
| 1   | A     | 103/120 (86%)   | 94±3 (91±3%) | 10±3 (9±3%) | 13 59       |
| All | All   | 1236/1440 (86%) | 1122 (91%)   | 114 (9%)    | 13 59       |

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     | 14  | PHE  | 12             |
| 1   | A     | 63  | VAL  | 9              |
| 1   | A     | 19  | ASP  | 7              |
| 1   | A     | 56  | TYR  | 7              |
| 1   | A     | 29  | LEU  | 6              |
| 1   | A     | 65  | LYS  | 6              |
| 1   | A     | 112 | GLN  | 4              |
| 1   | A     | 119 | GLU  | 4              |
| 1   | A     | 80  | LYS  | 4              |
| 1   | A     | 113 | LYS  | 4              |
| 1   | A     | 52  | GLU  | 3              |
| 1   | A     | 25  | HIS  | 3              |
| 1   | A     | 24  | ASN  | 3              |
| 1   | A     | 57  | ASP  | 3              |
| 1   | A     | 108 | GLU  | 2              |
| 1   | A     | 7   | THR  | 2              |
| 1   | A     | 103 | LYS  | 2              |
| 1   | A     | 10  | GLN  | 2              |
| 1   | A     | 35  | ARG  | 2              |
| 1   | A     | 94  | GLU  | 2              |
| 1   | A     | 81  | GLU  | 2              |
| 1   | A     | 70  | VAL  | 2              |
| 1   | A     | 11  | MET  | 1              |
| 1   | A     | 82  | LYS  | 1              |
| 1   | A     | 83  | ASN  | 1              |
| 1   | A     | 104 | ASP  | 1              |
| 1   | A     | 74  | ASN  | 1              |
| 1   | A     | 43  | LEU  | 1              |
| 1   | A     | 68  | ASN  | 1              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 95  | ILE  | 1              |
| 1   | A     | 22  | ASP  | 1              |
| 1   | A     | 77  | GLN  | 1              |
| 1   | A     | 107 | THR  | 1              |
| 1   | A     | 61  | ASN  | 1              |
| 1   | A     | 92  | LEU  | 1              |
| 1   | A     | 105 | SER  | 1              |
| 1   | A     | 15  | LYS  | 1              |
| 1   | A     | 67  | GLU  | 1              |
| 1   | A     | 127 | ASN  | 1              |
| 1   | A     | 16  | GLN  | 1              |
| 1   | A     | 28  | ILE  | 1              |
| 1   | A     | 9   | GLU  | 1              |
| 1   | A     | 12  | GLN  | 1              |
| 1   | A     | 30  | ASP  | 1              |
| 1   | A     | 73  | ASP  | 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 monosaccharides 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 [i](#)

The completeness of assignment taking into account all chemical shift lists is 87% for the well-defined parts and 85% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

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

#### 7.1.1 Bookkeeping [i](#)

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                  | 1542 |
| Number of shifts mapped to atoms        | 1542 |
| Number of unparsed shifts               | 0    |
| Number of shifts with mapping errors    | 0    |
| Number of shifts with mapping warnings  | 0    |
| Number of shift outliers (ShiftChecker) | 1    |

#### 7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action        |
|------------------------|----------|---------------------------------|-------------------------|
| $^{13}\text{C}_\alpha$ | 142      | $-0.19 \pm 0.11$                | None needed (< 0.5 ppm) |
| $^{13}\text{C}_\beta$  | 130      | $0.27 \pm 0.09$                 | None needed (< 0.5 ppm) |
| $^{13}\text{C}'$       | 104      | $-0.28 \pm 0.11$                | None needed (< 0.5 ppm) |
| $^{15}\text{N}$        | 136      | $-0.12 \pm 0.31$                | None needed (< 0.5 ppm) |

#### 7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 87%, i.e. 1402 atoms were assigned a chemical shift out of a possible 1608. 0 out of 11 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total         | $^1\text{H}$  | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|---------------|---------------|-----------------|-----------------|
| Backbone  | 598/634 (94%) | 255/260 (98%) | 221/250 (88%)   | 122/124 (98%)   |
| Sidechain | 698/822 (85%) | 473/528 (90%) | 225/267 (84%)   | 0/27 (0%)       |

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|          | <b>Total</b>    | <b><sup>1</sup>H</b> | <b><sup>13</sup>C</b> | <b><sup>15</sup>N</b> |
|----------|-----------------|----------------------|-----------------------|-----------------------|
| Aromatic | 106/152 (70%)   | 65/73 (89%)          | 41/77 (53%)           | 0/2 (0%)              |
| Overall  | 1402/1608 (87%) | 793/861 (92%)        | 487/594 (82%)         | 122/153 (80%)         |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 85%, i.e. 1542 atoms were assigned a chemical shift out of a possible 1819. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | <b>Total</b>    | <b><sup>1</sup>H</b> | <b><sup>13</sup>C</b> | <b><sup>15</sup>N</b> |
|-----------|-----------------|----------------------|-----------------------|-----------------------|
| Backbone  | 664/727 (91%)   | 282/298 (95%)        | 246/288 (85%)         | 136/141 (96%)         |
| Sidechain | 772/940 (82%)   | 522/601 (87%)        | 250/307 (81%)         | 0/32 (0%)             |
| Aromatic  | 106/152 (70%)   | 65/73 (89%)          | 41/77 (53%)           | 0/2 (0%)              |
| Overall   | 1542/1819 (85%) | 869/972 (89%)        | 537/672 (80%)         | 136/175 (78%)         |

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

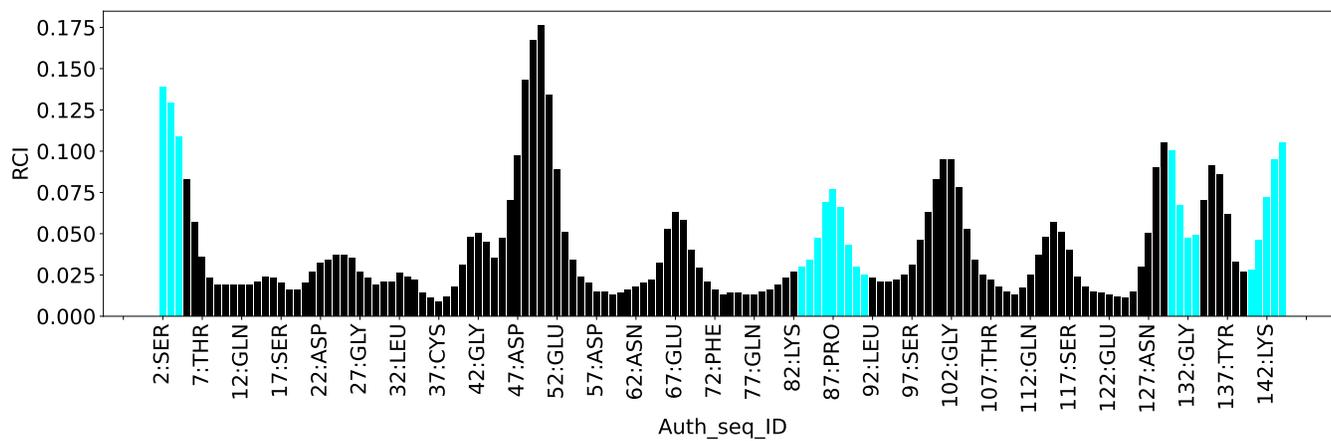
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

| List Id | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|---------|-------|-----|------|------|------------|---------------------|---------|
| 1       | A     | 35  | ARG  | HG3  | 0.11       | 0.15 – 2.94         | -5.2    |

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

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

Random coil index (RCI) for chain A:



## 8 NMR restraints analysis

### 8.1 Conformationally restricting restraints

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

| Description  | Value |
|--|-------|
| Total distance restraints                                | 3223  |
| Intra-residue ( $ i-j =0$ )                              | 1546  |
| Sequential ( $ i-j =1$ )                                 | 602   |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 435   |
| Long range ( $ i-j \geq 5$ )                             | 440   |
| Inter-chain  | 0     |
| Hydrogen bond restraints                                 | 200   |
| Disulfide bond restraints                                | 0     |
| Total dihedral-angle restraints                          | 0     |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 22.4  |
| Number of long range restraints per residue <sup>1</sup> | 3.2   |

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

### 8.2 Residual restraint violations

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

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

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

| Bins (Å)         | Average number of violations per model | Max (Å) |
|------------------|--|---------|
| 0.1-0.2 (Small)  | 36.7                                   | 0.2     |
| 0.2-0.5 (Medium) | 40.9                                   | 0.5     |
| >0.5 (Large)     | 32.8                                   | 2.53    |

### 8.2.2 Average number of dihedral-angle violations per model

Dihedral-angle violations less than  $1^\circ$  are not included in the calculation. There are no dihedral-angle violations

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

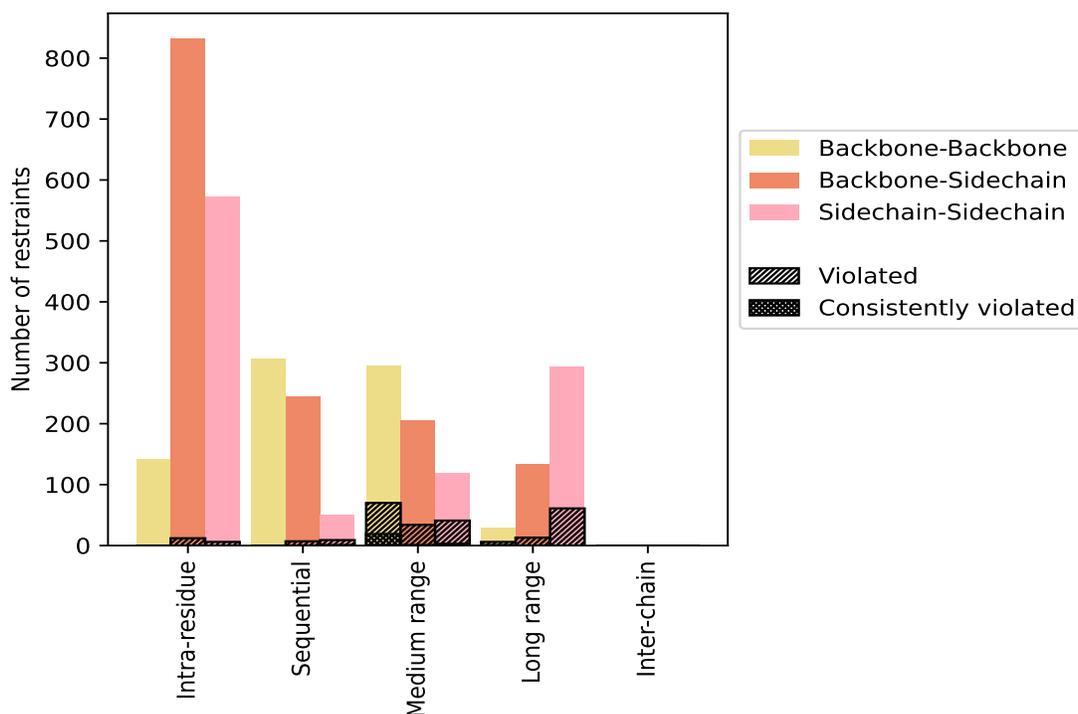
### 9.1 Summary of distance violations [i](#)

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

| Restrains type  | Count       | % <sup>1</sup> | Violated <sup>3</sup> |                |                | Consistently Violated <sup>4</sup> |                |                |
|---|-------------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
|   |             |                | Count                 | % <sup>2</sup> | % <sup>1</sup> | Count                              | % <sup>2</sup> | % <sup>1</sup> |
| <b>Intra-residue (<math> i-j =0</math>)</b>                                 | <b>1546</b> | <b>48.0</b>    | <b>18</b>             | <b>1.2</b>     | <b>0.6</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| Backbone-Backbone   | 142         | 4.4            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain  | 832         | 25.8           | 12                    | 1.4            | 0.4            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain   | 572         | 17.7           | 6                     | 1.0            | 0.2            | 0                                  | 0.0            | 0.0            |
| <b>Sequential (<math> i-j =1</math>)</b>                                    | <b>602</b>  | <b>18.7</b>    | <b>16</b>             | <b>2.7</b>     | <b>0.5</b>     | <b>1</b>                           | <b>0.2</b>     | <b>0.0</b>     |
| Backbone-Backbone   | 307         | 9.5            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain  | 245         | 7.6            | 7                     | 2.9            | 0.2            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain   | 50          | 1.6            | 9                     | 18.0           | 0.3            | 1                                  | 2.0            | 0.0            |
| <b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b> | <b>435</b>  | <b>13.5</b>    | <b>80</b>             | <b>18.4</b>    | <b>2.5</b>     | <b>6</b>                           | <b>1.4</b>     | <b>0.2</b>     |
| Backbone-Backbone   | 111         | 3.4            | 5                     | 4.5            | 0.2            | 2                                  | 1.8            | 0.1            |
| Backbone-Sidechain  | 205         | 6.4            | 34                    | 16.6           | 1.1            | 1                                  | 0.5            | 0.0            |
| Sidechain-Sidechain   | 119         | 3.7            | 41                    | 34.5           | 1.3            | 3                                  | 2.5            | 0.1            |
| <b>Long range (<math> i-j \geq 5</math>)</b>                                | <b>440</b>  | <b>13.7</b>    | <b>74</b>             | <b>16.8</b>    | <b>2.3</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| Backbone-Backbone   | 13          | 0.4            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain  | 134         | 4.2            | 13                    | 9.7            | 0.4            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain   | 293         | 9.1            | 61                    | 20.8           | 1.9            | 0                                  | 0.0            | 0.0            |
| <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>200</b>  | <b>6.2</b>     | <b>71</b>             | <b>35.5</b>    | <b>2.2</b>     | <b>18</b>                          | <b>9.0</b>     | <b>0.6</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>3223</b> | <b>100.0</b>   | <b>259</b>            | <b>8.0</b>     | <b>8.0</b>     | <b>25</b>                          | <b>0.8</b>     | <b>0.8</b>     |
| Backbone-Backbone   | 773         | 24.0           | 76                    | 9.8            | 2.4            | 20                                 | 2.6            | 0.6            |
| Backbone-Sidechain  | 1416        | 43.9           | 66                    | 4.7            | 2.0            | 1                                  | 0.1            | 0.0            |
| Sidechain-Sidechain   | 1034        | 32.1           | 117                   | 11.3           | 3.6            | 4                                  | 0.4            | 0.1            |

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

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



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and 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        | 6                    | 10              | 70              | 29              | 0               | 115   | 0.54     | 2.25    | 0.54                | 0.29       |
| 2        | 5                    | 10              | 61              | 34              | 0               | 110   | 0.53     | 2.48    | 0.5                 | 0.3        |
| 3        | 3                    | 9               | 72              | 30              | 0               | 114   | 0.51     | 2.07    | 0.49                | 0.3        |
| 4        | 3                    | 8               | 64              | 33              | 0               | 108   | 0.43     | 2.53    | 0.46                | 0.24       |
| 5        | 3                    | 9               | 66              | 32              | 0               | 110   | 0.55     | 2.38    | 0.56                | 0.32       |
| 6        | 0                    | 7               | 69              | 29              | 0               | 105   | 0.5      | 2.31    | 0.51                | 0.28       |
| 7        | 6                    | 9               | 73              | 31              | 0               | 119   | 0.52     | 2.19    | 0.52                | 0.28       |
| 8        | 8                    | 4               | 76              | 29              | 0               | 117   | 0.49     | 2.11    | 0.46                | 0.29       |
| 9        | 7                    | 8               | 67              | 21              | 0               | 103   | 0.45     | 2.45    | 0.42                | 0.29       |
| 10       | 2                    | 8               | 68              | 32              | 0               | 110   | 0.44     | 2.07    | 0.46                | 0.26       |
| 11       | 3                    | 7               | 68              | 33              | 0               | 111   | 0.52     | 2.46    | 0.54                | 0.29       |

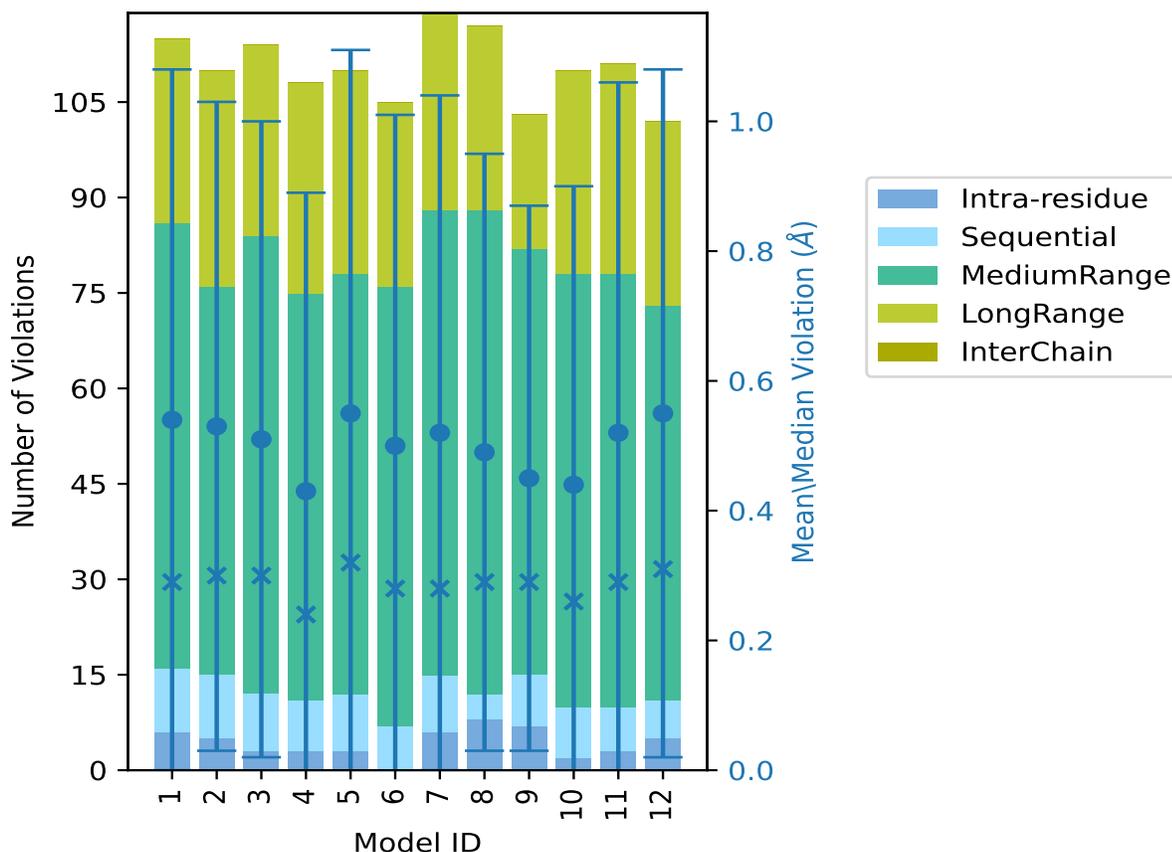
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| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 12       | 5                    | 6               | 62              | 29              | 0               | 102   | 0.55     | 2.28    | 0.53                | 0.31       |

<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

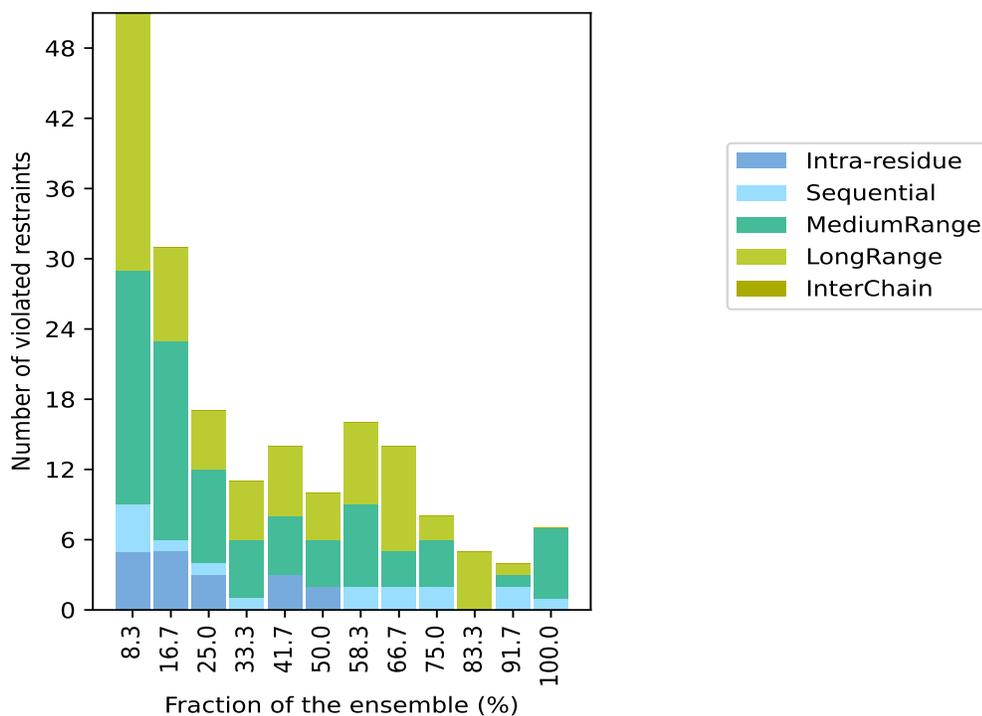
### 9.3 Distance violation statistics for the ensemble [\(i\)](#)

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, 2835(IR:1528, SQ:586, MR:355, LR:366, 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>       | %     |
| 5                             | 4               | 20              | 22              | 0               | 51    | 1                        | 8.3   |
| 5                             | 1               | 17              | 8               | 0               | 31    | 2                        | 16.7  |
| 3                             | 1               | 8               | 5               | 0               | 17    | 3                        | 25.0  |
| 0                             | 1               | 5               | 5               | 0               | 11    | 4                        | 33.3  |
| 3                             | 0               | 5               | 6               | 0               | 14    | 5                        | 41.7  |
| 2                             | 0               | 4               | 4               | 0               | 10    | 6                        | 50.0  |
| 0                             | 2               | 7               | 7               | 0               | 16    | 7                        | 58.3  |
| 0                             | 2               | 3               | 9               | 0               | 14    | 8                        | 66.7  |
| 0                             | 2               | 4               | 2               | 0               | 8     | 9                        | 75.0  |
| 0                             | 0               | 0               | 5               | 0               | 5     | 10                       | 83.3  |
| 0                             | 2               | 1               | 1               | 0               | 4     | 11                       | 91.7  |
| 0                             | 1               | 6               | 0               | 0               | 7     | 12                       | 100.0 |

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

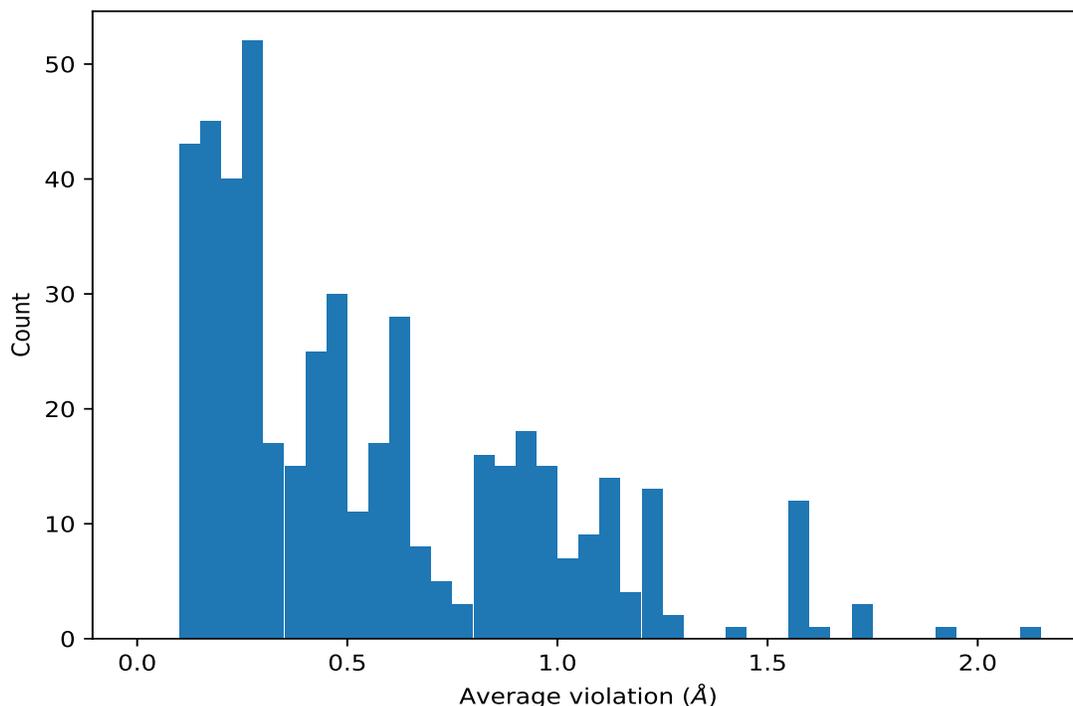
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [\(i\)](#)



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

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

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



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

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

| Key      | Atom-1          | Atom-2         | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|----------------|---------------------|----------|---------------------|------------|
| (2,35)   | 1:A:29:LEU:H    | 1:A:33:GLU:H   | 12                  | 2.1      | 0.26                | 2.1        |
| (1,695)  | 1:A:62:ASN:H    | 1:A:65:LYS:H   | 12                  | 1.92     | 0.36                | 1.98       |
| (1,835)  | 1:A:78:TYR:HB2  | 1:A:75:TYR:HD1 | 12                  | 1.27     | 0.1                 | 1.28       |
| (1,835)  | 1:A:78:TYR:HB2  | 1:A:75:TYR:HD2 | 12                  | 1.27     | 0.1                 | 1.28       |
| (1,1119) | 1:A:70:VAL:HG21 | 1:A:71:SER:HB3 | 12                  | 0.59     | 0.28                | 0.47       |
| (1,1119) | 1:A:70:VAL:HG22 | 1:A:71:SER:HB3 | 12                  | 0.59     | 0.28                | 0.47       |
| (1,1119) | 1:A:70:VAL:HG23 | 1:A:71:SER:HB3 | 12                  | 0.59     | 0.28                | 0.47       |
| (1,2312) | 1:A:14:PHE:HB2  | 1:A:11:MET:HA  | 12                  | 0.51     | 0.03                | 0.51       |
| (1,1000) | 1:A:20:ALA:HB1  | 1:A:17:SER:HB3 | 12                  | 0.39     | 0.18                | 0.3        |

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| Key      | Atom-1         | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1000) | 1:A:20:ALA:HB2 | 1:A:17:SER:HB3  | 12                  | 0.39     | 0.18                | 0.3        |
| (1,1000) | 1:A:20:ALA:HB3 | 1:A:17:SER:HB3  | 12                  | 0.39     | 0.18                | 0.3        |
| (3,101)  | 1:A:7:THR:O    | 1:A:11:MET:N    | 12                  | 0.33     | 0.02                | 0.33       |
| (3,149)  | 1:A:136:ASP:O  | 1:A:139:ALA:N   | 12                  | 0.32     | 0.02                | 0.32       |
| (3,108)  | 1:A:16:GLN:O   | 1:A:20:ALA:N    | 12                  | 0.3      | 0.03                | 0.3        |
| (3,118)  | 1:A:38:LEU:O   | 1:A:44:ILE:N    | 12                  | 0.28     | 0.06                | 0.3        |
| (3,123)  | 1:A:59:ILE:O   | 1:A:63:VAL:N    | 12                  | 0.28     | 0.05                | 0.29       |
| (3,120)  | 1:A:54:ALA:O   | 1:A:58:ALA:N    | 12                  | 0.27     | 0.09                | 0.32       |
| (3,107)  | 1:A:14:PHE:O   | 1:A:18:PHE:N    | 12                  | 0.26     | 0.07                | 0.28       |
| (3,111)  | 1:A:31:LYS:O   | 1:A:35:ARG:N    | 12                  | 0.25     | 0.05                | 0.26       |
| (3,132)  | 1:A:90:GLU:O   | 1:A:93:ASN:N    | 12                  | 0.24     | 0.05                | 0.24       |
| (2,318)  | 1:A:10:GLN:HB3 | 1:A:14:PHE:HZ   | 12                  | 0.24     | 0.02                | 0.24       |
| (3,137)  | 1:A:100:ALA:O  | 1:A:103:LYS:N   | 12                  | 0.23     | 0.05                | 0.22       |
| (3,114)  | 1:A:34:PHE:O   | 1:A:38:LEU:N    | 12                  | 0.23     | 0.07                | 0.26       |
| (3,103)  | 1:A:9:GLU:O    | 1:A:13:GLU:N    | 12                  | 0.2      | 0.05                | 0.2        |
| (3,146)  | 1:A:123:TYR:O  | 1:A:126:ALA:N   | 12                  | 0.19     | 0.03                | 0.19       |
| (3,142)  | 1:A:117:SER:O  | 1:A:120:GLN:N   | 12                  | 0.18     | 0.03                | 0.18       |
| (3,134)  | 1:A:94:GLU:O   | 1:A:97:SER:N    | 12                  | 0.17     | 0.05                | 0.16       |
| (3,135)  | 1:A:95:ILE:O   | 1:A:98:THR:N    | 12                  | 0.16     | 0.02                | 0.16       |
| (3,138)  | 1:A:107:THR:O  | 1:A:110:ASP:N   | 12                  | 0.15     | 0.02                | 0.16       |
| (3,143)  | 1:A:120:GLN:O  | 1:A:123:TYR:N   | 12                  | 0.14     | 0.02                | 0.15       |
| (1,2314) | 1:A:6:VAL:HG21 | 1:A:11:MET:HA   | 11                  | 1.59     | 0.71                | 2.03       |
| (1,2314) | 1:A:6:VAL:HG22 | 1:A:11:MET:HA   | 11                  | 1.59     | 0.71                | 2.03       |
| (1,2314) | 1:A:6:VAL:HG23 | 1:A:11:MET:HA   | 11                  | 1.59     | 0.71                | 2.03       |
| (2,268)  | 1:A:134:GLY:H  | 1:A:130:GLN:H   | 11                  | 1.42     | 0.42                | 1.33       |
| (1,1631) | 1:A:109:THR:HB | 1:A:108:GLU:HG3 | 11                  | 1.13     | 0.58                | 1.49       |
| (1,1510) | 1:A:78:TYR:HB2 | 1:A:79:MET:HE1  | 11                  | 0.61     | 0.4                 | 0.46       |
| (1,1510) | 1:A:78:TYR:HB2 | 1:A:79:MET:HE2  | 11                  | 0.61     | 0.4                 | 0.46       |
| (1,1510) | 1:A:78:TYR:HB2 | 1:A:79:MET:HE3  | 11                  | 0.61     | 0.4                 | 0.46       |
| (3,115)  | 1:A:36:SER:O   | 1:A:40:SER:N    | 11                  | 0.26     | 0.05                | 0.28       |
| (3,144)  | 1:A:120:GLN:O  | 1:A:124:VAL:N   | 11                  | 0.25     | 0.04                | 0.25       |
| (3,113)  | 1:A:33:GLU:O   | 1:A:37:CYS:N    | 11                  | 0.22     | 0.08                | 0.23       |
| (3,136)  | 1:A:95:ILE:O   | 1:A:99:ILE:N    | 11                  | 0.21     | 0.06                | 0.22       |
| (3,102)  | 1:A:9:GLU:O    | 1:A:12:GLN:N    | 11                  | 0.19     | 0.03                | 0.17       |
| (3,141)  | 1:A:113:LYS:O  | 1:A:115:GLY:N   | 11                  | 0.16     | 0.03                | 0.15       |
| (1,1168) | 1:A:6:VAL:HG21 | 1:A:11:MET:HB2  | 10                  | 1.57     | 0.4                 | 1.75       |
| (1,1168) | 1:A:6:VAL:HG21 | 1:A:11:MET:HB3  | 10                  | 1.57     | 0.4                 | 1.75       |
| (1,1168) | 1:A:6:VAL:HG22 | 1:A:11:MET:HB2  | 10                  | 1.57     | 0.4                 | 1.75       |
| (1,1168) | 1:A:6:VAL:HG22 | 1:A:11:MET:HB3  | 10                  | 1.57     | 0.4                 | 1.75       |
| (1,1168) | 1:A:6:VAL:HG23 | 1:A:11:MET:HB2  | 10                  | 1.57     | 0.4                 | 1.75       |
| (1,1168) | 1:A:6:VAL:HG23 | 1:A:11:MET:HB3  | 10                  | 1.57     | 0.4                 | 1.75       |
| (1,1274) | 1:A:6:VAL:HG21 | 1:A:11:MET:HB2  | 10                  | 1.2      | 0.4                 | 1.38       |

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| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1274) | 1:A:6:VAL:HG21   | 1:A:11:MET:HB3  | 10                  | 1.2      | 0.4                 | 1.38       |
| (1,1274) | 1:A:6:VAL:HG22   | 1:A:11:MET:HB2  | 10                  | 1.2      | 0.4                 | 1.38       |
| (1,1274) | 1:A:6:VAL:HG22   | 1:A:11:MET:HB3  | 10                  | 1.2      | 0.4                 | 1.38       |
| (1,1274) | 1:A:6:VAL:HG23   | 1:A:11:MET:HB2  | 10                  | 1.2      | 0.4                 | 1.38       |
| (1,1274) | 1:A:6:VAL:HG23   | 1:A:11:MET:HB3  | 10                  | 1.2      | 0.4                 | 1.38       |
| (1,2253) | 1:A:79:MET:HE1   | 1:A:43:LEU:HD21 | 10                  | 1.14     | 0.74                | 1.38       |
| (1,2253) | 1:A:79:MET:HE1   | 1:A:43:LEU:HD22 | 10                  | 1.14     | 0.74                | 1.38       |
| (1,2253) | 1:A:79:MET:HE1   | 1:A:43:LEU:HD23 | 10                  | 1.14     | 0.74                | 1.38       |
| (1,2253) | 1:A:79:MET:HE2   | 1:A:43:LEU:HD21 | 10                  | 1.14     | 0.74                | 1.38       |
| (1,2253) | 1:A:79:MET:HE2   | 1:A:43:LEU:HD22 | 10                  | 1.14     | 0.74                | 1.38       |
| (1,2253) | 1:A:79:MET:HE2   | 1:A:43:LEU:HD23 | 10                  | 1.14     | 0.74                | 1.38       |
| (1,2253) | 1:A:79:MET:HE3   | 1:A:43:LEU:HD21 | 10                  | 1.14     | 0.74                | 1.38       |
| (1,2253) | 1:A:79:MET:HE3   | 1:A:43:LEU:HD22 | 10                  | 1.14     | 0.74                | 1.38       |
| (1,2253) | 1:A:79:MET:HE3   | 1:A:43:LEU:HD23 | 10                  | 1.14     | 0.74                | 1.38       |
| (1,882)  | 1:A:80:LYS:HE3   | 1:A:6:VAL:HG11  | 10                  | 0.87     | 0.25                | 0.95       |
| (1,882)  | 1:A:80:LYS:HE3   | 1:A:6:VAL:HG12  | 10                  | 0.87     | 0.25                | 0.95       |
| (1,882)  | 1:A:80:LYS:HE3   | 1:A:6:VAL:HG13  | 10                  | 0.87     | 0.25                | 0.95       |
| (1,1847) | 1:A:6:VAL:HG11   | 1:A:80:LYS:HB3  | 10                  | 0.48     | 0.21                | 0.43       |
| (1,1847) | 1:A:6:VAL:HG12   | 1:A:80:LYS:HB3  | 10                  | 0.48     | 0.21                | 0.43       |
| (1,1847) | 1:A:6:VAL:HG13   | 1:A:80:LYS:HB3  | 10                  | 0.48     | 0.21                | 0.43       |
| (3,139)  | 1:A:107:THR:O    | 1:A:111:MET:N   | 10                  | 0.28     | 0.06                | 0.29       |
| (3,119)  | 1:A:45:ASP:O     | 1:A:47:ASP:N    | 10                  | 0.23     | 0.08                | 0.24       |
| (3,131)  | 1:A:89:PRO:O     | 1:A:92:LEU:N    | 10                  | 0.23     | 0.04                | 0.24       |
| (3,106)  | 1:A:13:GLU:O     | 1:A:17:SER:N    | 10                  | 0.23     | 0.06                | 0.23       |
| (3,145)  | 1:A:121:ILE:O    | 1:A:125:LYS:N   | 10                  | 0.23     | 0.06                | 0.24       |
| (3,110)  | 1:A:30:ASP:O     | 1:A:34:PHE:N    | 10                  | 0.22     | 0.06                | 0.2        |
| (3,133)  | 1:A:91:GLN:O     | 1:A:94:GLU:N    | 10                  | 0.21     | 0.07                | 0.2        |
| (3,128)  | 1:A:75:TYR:O     | 1:A:79:MET:N    | 10                  | 0.18     | 0.06                | 0.16       |
| (3,127)  | 1:A:75:TYR:O     | 1:A:78:TYR:N    | 10                  | 0.16     | 0.03                | 0.16       |
| (1,1872) | 1:A:65:LYS:HE3   | 1:A:64:THR:HG21 | 9                   | 1.17     | 0.34                | 1.37       |
| (1,1872) | 1:A:65:LYS:HE3   | 1:A:64:THR:HG22 | 9                   | 1.17     | 0.34                | 1.37       |
| (1,1872) | 1:A:65:LYS:HE3   | 1:A:64:THR:HG23 | 9                   | 1.17     | 0.34                | 1.37       |
| (1,2273) | 1:A:109:THR:HG21 | 1:A:108:GLU:HG3 | 9                   | 0.99     | 0.34                | 1.19       |
| (1,2273) | 1:A:109:THR:HG22 | 1:A:108:GLU:HG3 | 9                   | 0.99     | 0.34                | 1.19       |
| (1,2273) | 1:A:109:THR:HG23 | 1:A:108:GLU:HG3 | 9                   | 0.99     | 0.34                | 1.19       |
| (1,2124) | 1:A:38:LEU:HD11  | 1:A:43:LEU:HD21 | 9                   | 0.89     | 0.51                | 1.01       |
| (1,2124) | 1:A:38:LEU:HD11  | 1:A:43:LEU:HD22 | 9                   | 0.89     | 0.51                | 1.01       |
| (1,2124) | 1:A:38:LEU:HD11  | 1:A:43:LEU:HD23 | 9                   | 0.89     | 0.51                | 1.01       |
| (1,2124) | 1:A:38:LEU:HD12  | 1:A:43:LEU:HD21 | 9                   | 0.89     | 0.51                | 1.01       |
| (1,2124) | 1:A:38:LEU:HD12  | 1:A:43:LEU:HD22 | 9                   | 0.89     | 0.51                | 1.01       |
| (1,2124) | 1:A:38:LEU:HD12  | 1:A:43:LEU:HD23 | 9                   | 0.89     | 0.51                | 1.01       |
| (1,2124) | 1:A:38:LEU:HD13  | 1:A:43:LEU:HD21 | 9                   | 0.89     | 0.51                | 1.01       |

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| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,2124) | 1:A:38:LEU:HD13  | 1:A:43:LEU:HD22 | 9                   | 0.89     | 0.51                | 1.01       |
| (1,2124) | 1:A:38:LEU:HD13  | 1:A:43:LEU:HD23 | 9                   | 0.89     | 0.51                | 1.01       |
| (2,300)  | 1:A:109:THR:HB   | 1:A:112:GLN:HG3 | 9                   | 0.74     | 0.32                | 0.62       |
| (1,2167) | 1:A:81:GLU:HA    | 1:A:84:ASP:HB3  | 9                   | 0.67     | 0.49                | 0.61       |
| (1,2326) | 1:A:74:ASN:HA    | 1:A:77:GLN:HG3  | 9                   | 0.52     | 0.45                | 0.28       |
| (1,1745) | 1:A:80:LYS:HE3   | 1:A:6:VAL:HG11  | 9                   | 0.43     | 0.05                | 0.43       |
| (1,1745) | 1:A:80:LYS:HE3   | 1:A:6:VAL:HG12  | 9                   | 0.43     | 0.05                | 0.43       |
| (1,1745) | 1:A:80:LYS:HE3   | 1:A:6:VAL:HG13  | 9                   | 0.43     | 0.05                | 0.43       |
| (1,1489) | 1:A:20:ALA:HB1   | 1:A:17:SER:HB3  | 9                   | 0.25     | 0.19                | 0.14       |
| (1,1489) | 1:A:20:ALA:HB2   | 1:A:17:SER:HB3  | 9                   | 0.25     | 0.19                | 0.14       |
| (1,1489) | 1:A:20:ALA:HB3   | 1:A:17:SER:HB3  | 9                   | 0.25     | 0.19                | 0.14       |
| (1,1218) | 1:A:6:VAL:HG11   | 1:A:80:LYS:HG3  | 8                   | 1.71     | 0.7                 | 1.96       |
| (1,1218) | 1:A:6:VAL:HG12   | 1:A:80:LYS:HG3  | 8                   | 1.71     | 0.7                 | 1.96       |
| (1,1218) | 1:A:6:VAL:HG13   | 1:A:80:LYS:HG3  | 8                   | 1.71     | 0.7                 | 1.96       |
| (1,2623) | 1:A:56:TYR:HB3   | 1:A:44:ILE:HG12 | 8                   | 1.62     | 0.22                | 1.72       |
| (1,1021) | 1:A:6:VAL:HG11   | 1:A:80:LYS:HG3  | 8                   | 1.58     | 0.7                 | 1.83       |
| (1,1021) | 1:A:6:VAL:HG12   | 1:A:80:LYS:HG3  | 8                   | 1.58     | 0.7                 | 1.83       |
| (1,1021) | 1:A:6:VAL:HG13   | 1:A:80:LYS:HG3  | 8                   | 1.58     | 0.7                 | 1.83       |
| (1,2393) | 1:A:6:VAL:HG11   | 1:A:80:LYS:HD3  | 8                   | 1.0      | 0.54                | 0.9        |
| (1,2393) | 1:A:6:VAL:HG12   | 1:A:80:LYS:HD3  | 8                   | 1.0      | 0.54                | 0.9        |
| (1,2393) | 1:A:6:VAL:HG13   | 1:A:80:LYS:HD3  | 8                   | 1.0      | 0.54                | 0.9        |
| (1,947)  | 1:A:6:VAL:HG11   | 1:A:80:LYS:HD3  | 8                   | 0.99     | 0.54                | 0.9        |
| (1,947)  | 1:A:6:VAL:HG12   | 1:A:80:LYS:HD3  | 8                   | 0.99     | 0.54                | 0.9        |
| (1,947)  | 1:A:6:VAL:HG13   | 1:A:80:LYS:HD3  | 8                   | 0.99     | 0.54                | 0.9        |
| (1,2573) | 1:A:109:THR:HG21 | 1:A:113:LYS:HG2 | 8                   | 0.93     | 0.44                | 1.1        |
| (1,2573) | 1:A:109:THR:HG22 | 1:A:113:LYS:HG2 | 8                   | 0.93     | 0.44                | 1.1        |
| (1,2573) | 1:A:109:THR:HG23 | 1:A:113:LYS:HG2 | 8                   | 0.93     | 0.44                | 1.1        |
| (1,1122) | 1:A:29:LEU:HD11  | 1:A:38:LEU:HD11 | 8                   | 0.83     | 0.3                 | 0.93       |
| (1,1122) | 1:A:29:LEU:HD11  | 1:A:38:LEU:HD12 | 8                   | 0.83     | 0.3                 | 0.93       |
| (1,1122) | 1:A:29:LEU:HD11  | 1:A:38:LEU:HD13 | 8                   | 0.83     | 0.3                 | 0.93       |
| (1,1122) | 1:A:29:LEU:HD12  | 1:A:38:LEU:HD11 | 8                   | 0.83     | 0.3                 | 0.93       |
| (1,1122) | 1:A:29:LEU:HD12  | 1:A:38:LEU:HD12 | 8                   | 0.83     | 0.3                 | 0.93       |
| (1,1122) | 1:A:29:LEU:HD12  | 1:A:38:LEU:HD13 | 8                   | 0.83     | 0.3                 | 0.93       |
| (1,1122) | 1:A:29:LEU:HD13  | 1:A:38:LEU:HD11 | 8                   | 0.83     | 0.3                 | 0.93       |
| (1,1122) | 1:A:29:LEU:HD13  | 1:A:38:LEU:HD12 | 8                   | 0.83     | 0.3                 | 0.93       |
| (1,1122) | 1:A:29:LEU:HD13  | 1:A:38:LEU:HD13 | 8                   | 0.83     | 0.3                 | 0.93       |
| (1,1145) | 1:A:6:VAL:HG21   | 1:A:11:MET:HA   | 8                   | 0.81     | 0.23                | 0.86       |
| (1,1145) | 1:A:6:VAL:HG22   | 1:A:11:MET:HA   | 8                   | 0.81     | 0.23                | 0.86       |
| (1,1145) | 1:A:6:VAL:HG23   | 1:A:11:MET:HA   | 8                   | 0.81     | 0.23                | 0.86       |
| (1,2001) | 1:A:52:GLU:HG2   | 1:A:51:GLY:HA3  | 8                   | 0.68     | 0.23                | 0.66       |
| (1,56)   | 1:A:52:GLU:HA    | 1:A:50:GLY:H    | 8                   | 0.66     | 0.5                 | 0.5        |
| (1,1387) | 1:A:109:THR:HG21 | 1:A:113:LYS:HE3 | 8                   | 0.62     | 0.51                | 0.34       |

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| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1387) | 1:A:109:THR:HG22 | 1:A:113:LYS:HE3 | 8                   | 0.62     | 0.51                | 0.34       |
| (1,1387) | 1:A:109:THR:HG23 | 1:A:113:LYS:HE3 | 8                   | 0.62     | 0.51                | 0.34       |
| (1,850)  | 1:A:109:THR:HA   | 1:A:108:GLU:HG3 | 8                   | 0.56     | 0.2                 | 0.48       |
| (3,124)  | 1:A:29:LEU:O     | 1:A:70:VAL:N    | 8                   | 0.22     | 0.07                | 0.22       |
| (3,130)  | 1:A:79:MET:O     | 1:A:83:ASN:N    | 8                   | 0.21     | 0.06                | 0.2        |
| (3,117)  | 1:A:38:LEU:O     | 1:A:43:LEU:N    | 8                   | 0.18     | 0.04                | 0.17       |
| (3,116)  | 1:A:37:CYS:O     | 1:A:41:MET:N    | 8                   | 0.16     | 0.04                | 0.14       |
| (1,1493) | 1:A:14:PHE:HE1   | 1:A:79:MET:HE1  | 8                   | 0.13     | 0.02                | 0.12       |
| (1,1493) | 1:A:14:PHE:HE1   | 1:A:79:MET:HE2  | 8                   | 0.13     | 0.02                | 0.12       |
| (1,1493) | 1:A:14:PHE:HE1   | 1:A:79:MET:HE3  | 8                   | 0.13     | 0.02                | 0.12       |
| (1,1493) | 1:A:14:PHE:HE2   | 1:A:79:MET:HE1  | 8                   | 0.13     | 0.02                | 0.12       |
| (1,1493) | 1:A:14:PHE:HE2   | 1:A:79:MET:HE2  | 8                   | 0.13     | 0.02                | 0.12       |
| (1,1493) | 1:A:14:PHE:HE2   | 1:A:79:MET:HE3  | 8                   | 0.13     | 0.02                | 0.12       |
| (1,1276) | 1:A:28:ILE:HA    | 1:A:14:PHE:HZ   | 8                   | 0.13     | 0.02                | 0.13       |
| (3,85)   | 1:A:120:GLN:O    | 1:A:123:TYR:H   | 8                   | 0.12     | 0.01                | 0.11       |
| (1,827)  | 1:A:6:VAL:HG21   | 1:A:10:GLN:HG3  | 7                   | 1.14     | 0.13                | 1.16       |
| (1,827)  | 1:A:6:VAL:HG22   | 1:A:10:GLN:HG3  | 7                   | 1.14     | 0.13                | 1.16       |
| (1,827)  | 1:A:6:VAL:HG23   | 1:A:10:GLN:HG3  | 7                   | 1.14     | 0.13                | 1.16       |
| (1,1890) | 1:A:79:MET:HE1   | 1:A:38:LEU:HD11 | 7                   | 1.07     | 0.15                | 1.13       |
| (1,1890) | 1:A:79:MET:HE1   | 1:A:38:LEU:HD12 | 7                   | 1.07     | 0.15                | 1.13       |
| (1,1890) | 1:A:79:MET:HE1   | 1:A:38:LEU:HD13 | 7                   | 1.07     | 0.15                | 1.13       |
| (1,1890) | 1:A:79:MET:HE2   | 1:A:38:LEU:HD11 | 7                   | 1.07     | 0.15                | 1.13       |
| (1,1890) | 1:A:79:MET:HE2   | 1:A:38:LEU:HD12 | 7                   | 1.07     | 0.15                | 1.13       |
| (1,1890) | 1:A:79:MET:HE2   | 1:A:38:LEU:HD13 | 7                   | 1.07     | 0.15                | 1.13       |
| (1,1890) | 1:A:79:MET:HE3   | 1:A:38:LEU:HD11 | 7                   | 1.07     | 0.15                | 1.13       |
| (1,1890) | 1:A:79:MET:HE3   | 1:A:38:LEU:HD12 | 7                   | 1.07     | 0.15                | 1.13       |
| (1,1890) | 1:A:79:MET:HE3   | 1:A:38:LEU:HD13 | 7                   | 1.07     | 0.15                | 1.13       |
| (1,1565) | 1:A:38:LEU:HD11  | 1:A:43:LEU:HD21 | 7                   | 0.97     | 0.41                | 1.09       |
| (1,1565) | 1:A:38:LEU:HD11  | 1:A:43:LEU:HD22 | 7                   | 0.97     | 0.41                | 1.09       |
| (1,1565) | 1:A:38:LEU:HD11  | 1:A:43:LEU:HD23 | 7                   | 0.97     | 0.41                | 1.09       |
| (1,1565) | 1:A:38:LEU:HD12  | 1:A:43:LEU:HD21 | 7                   | 0.97     | 0.41                | 1.09       |
| (1,1565) | 1:A:38:LEU:HD12  | 1:A:43:LEU:HD22 | 7                   | 0.97     | 0.41                | 1.09       |
| (1,1565) | 1:A:38:LEU:HD12  | 1:A:43:LEU:HD23 | 7                   | 0.97     | 0.41                | 1.09       |
| (1,1565) | 1:A:38:LEU:HD13  | 1:A:43:LEU:HD21 | 7                   | 0.97     | 0.41                | 1.09       |
| (1,1565) | 1:A:38:LEU:HD13  | 1:A:43:LEU:HD22 | 7                   | 0.97     | 0.41                | 1.09       |
| (1,1565) | 1:A:38:LEU:HD13  | 1:A:43:LEU:HD23 | 7                   | 0.97     | 0.41                | 1.09       |
| (1,813)  | 1:A:10:GLN:HB2   | 1:A:6:VAL:HG21  | 7                   | 0.93     | 0.12                | 0.97       |
| (1,813)  | 1:A:10:GLN:HB2   | 1:A:6:VAL:HG22  | 7                   | 0.93     | 0.12                | 0.97       |
| (1,813)  | 1:A:10:GLN:HB2   | 1:A:6:VAL:HG23  | 7                   | 0.93     | 0.12                | 0.97       |
| (1,1016) | 1:A:6:VAL:HG21   | 1:A:11:MET:HG3  | 7                   | 0.85     | 0.16                | 0.91       |
| (1,1016) | 1:A:6:VAL:HG22   | 1:A:11:MET:HG3  | 7                   | 0.85     | 0.16                | 0.91       |
| (1,1016) | 1:A:6:VAL:HG23   | 1:A:11:MET:HG3  | 7                   | 0.85     | 0.16                | 0.91       |

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| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1379) | 1:A:141:VAL:HG11 | 1:A:140:TRP:HA  | 7                   | 0.76     | 0.03                | 0.75       |
| (1,1379) | 1:A:141:VAL:HG12 | 1:A:140:TRP:HA  | 7                   | 0.76     | 0.03                | 0.75       |
| (1,1379) | 1:A:141:VAL:HG13 | 1:A:140:TRP:HA  | 7                   | 0.76     | 0.03                | 0.75       |
| (1,1499) | 1:A:99:ILE:HG21  | 1:A:103:LYS:HE2 | 7                   | 0.73     | 0.44                | 0.79       |
| (1,1499) | 1:A:99:ILE:HG22  | 1:A:103:LYS:HE2 | 7                   | 0.73     | 0.44                | 0.79       |
| (1,1499) | 1:A:99:ILE:HG23  | 1:A:103:LYS:HE2 | 7                   | 0.73     | 0.44                | 0.79       |
| (1,1067) | 1:A:10:GLN:HB3   | 1:A:6:VAL:HG21  | 7                   | 0.61     | 0.02                | 0.6        |
| (1,1067) | 1:A:10:GLN:HB3   | 1:A:6:VAL:HG22  | 7                   | 0.61     | 0.02                | 0.6        |
| (1,1067) | 1:A:10:GLN:HB3   | 1:A:6:VAL:HG23  | 7                   | 0.61     | 0.02                | 0.6        |
| (1,1081) | 1:A:6:VAL:HG21   | 1:A:11:MET:HG2  | 7                   | 0.52     | 0.32                | 0.39       |
| (1,1081) | 1:A:6:VAL:HG22   | 1:A:11:MET:HG2  | 7                   | 0.52     | 0.32                | 0.39       |
| (1,1081) | 1:A:6:VAL:HG23   | 1:A:11:MET:HG2  | 7                   | 0.52     | 0.32                | 0.39       |
| (1,2138) | 1:A:6:VAL:HG11   | 1:A:5:GLY:HA3   | 7                   | 0.52     | 0.16                | 0.55       |
| (1,2138) | 1:A:6:VAL:HG12   | 1:A:5:GLY:HA3   | 7                   | 0.52     | 0.16                | 0.55       |
| (1,2138) | 1:A:6:VAL:HG13   | 1:A:5:GLY:HA3   | 7                   | 0.52     | 0.16                | 0.55       |
| (1,1762) | 1:A:6:VAL:HG21   | 1:A:14:PHE:HE1  | 7                   | 0.45     | 0.09                | 0.47       |
| (1,1762) | 1:A:6:VAL:HG21   | 1:A:14:PHE:HE2  | 7                   | 0.45     | 0.09                | 0.47       |
| (1,1762) | 1:A:6:VAL:HG22   | 1:A:14:PHE:HE1  | 7                   | 0.45     | 0.09                | 0.47       |
| (1,1762) | 1:A:6:VAL:HG22   | 1:A:14:PHE:HE2  | 7                   | 0.45     | 0.09                | 0.47       |
| (1,1762) | 1:A:6:VAL:HG23   | 1:A:14:PHE:HE1  | 7                   | 0.45     | 0.09                | 0.47       |
| (1,1762) | 1:A:6:VAL:HG23   | 1:A:14:PHE:HE2  | 7                   | 0.45     | 0.09                | 0.47       |
| (1,2431) | 1:A:6:VAL:HG21   | 1:A:10:GLN:HG2  | 7                   | 0.43     | 0.12                | 0.39       |
| (1,2431) | 1:A:6:VAL:HG22   | 1:A:10:GLN:HG2  | 7                   | 0.43     | 0.12                | 0.39       |
| (1,2431) | 1:A:6:VAL:HG23   | 1:A:10:GLN:HG2  | 7                   | 0.43     | 0.12                | 0.39       |
| (1,2024) | 1:A:10:GLN:HB3   | 1:A:6:VAL:HG21  | 7                   | 0.43     | 0.02                | 0.42       |
| (1,2024) | 1:A:10:GLN:HB3   | 1:A:6:VAL:HG22  | 7                   | 0.43     | 0.02                | 0.42       |
| (1,2024) | 1:A:10:GLN:HB3   | 1:A:6:VAL:HG23  | 7                   | 0.43     | 0.02                | 0.42       |
| (1,2408) | 1:A:6:VAL:HG21   | 1:A:14:PHE:HD1  | 7                   | 0.4      | 0.1                 | 0.41       |
| (1,2408) | 1:A:6:VAL:HG21   | 1:A:14:PHE:HD2  | 7                   | 0.4      | 0.1                 | 0.41       |
| (1,2408) | 1:A:6:VAL:HG22   | 1:A:14:PHE:HD1  | 7                   | 0.4      | 0.1                 | 0.41       |
| (1,2408) | 1:A:6:VAL:HG22   | 1:A:14:PHE:HD2  | 7                   | 0.4      | 0.1                 | 0.41       |
| (1,2408) | 1:A:6:VAL:HG23   | 1:A:14:PHE:HD1  | 7                   | 0.4      | 0.1                 | 0.41       |
| (1,2408) | 1:A:6:VAL:HG23   | 1:A:14:PHE:HD2  | 7                   | 0.4      | 0.1                 | 0.41       |
| (1,2054) | 1:A:69:GLY:HA3   | 1:A:28:ILE:HB   | 7                   | 0.27     | 0.08                | 0.25       |
| (1,2370) | 1:A:141:VAL:HG11 | 1:A:138:ALA:HA  | 7                   | 0.25     | 0.09                | 0.24       |
| (1,2370) | 1:A:141:VAL:HG12 | 1:A:138:ALA:HA  | 7                   | 0.25     | 0.09                | 0.24       |
| (1,2370) | 1:A:141:VAL:HG13 | 1:A:138:ALA:HA  | 7                   | 0.25     | 0.09                | 0.24       |
| (3,147)  | 1:A:123:TYR:O    | 1:A:127:ASN:N   | 7                   | 0.2      | 0.07                | 0.17       |
| (3,105)  | 1:A:13:GLU:O     | 1:A:16:GLN:N    | 7                   | 0.15     | 0.03                | 0.14       |
| (1,1724) | 1:A:56:TYR:HE1   | 1:A:38:LEU:HD21 | 6                   | 1.24     | 0.87                | 1.19       |
| (1,1724) | 1:A:56:TYR:HE1   | 1:A:38:LEU:HD22 | 6                   | 1.24     | 0.87                | 1.19       |
| (1,1724) | 1:A:56:TYR:HE1   | 1:A:38:LEU:HD23 | 6                   | 1.24     | 0.87                | 1.19       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1724) | 1:A:56:TYR:HE2  | 1:A:38:LEU:HD21 | 6                   | 1.24     | 0.87                | 1.19       |
| (1,1724) | 1:A:56:TYR:HE2  | 1:A:38:LEU:HD22 | 6                   | 1.24     | 0.87                | 1.19       |
| (1,1724) | 1:A:56:TYR:HE2  | 1:A:38:LEU:HD23 | 6                   | 1.24     | 0.87                | 1.19       |
| (2,335)  | 1:A:71:SER:HB3  | 1:A:28:ILE:HG12 | 6                   | 1.03     | 0.51                | 1.03       |
| (1,1900) | 1:A:41:MET:HE1  | 1:A:43:LEU:HD21 | 6                   | 0.94     | 0.18                | 0.9        |
| (1,1900) | 1:A:41:MET:HE1  | 1:A:43:LEU:HD22 | 6                   | 0.94     | 0.18                | 0.9        |
| (1,1900) | 1:A:41:MET:HE1  | 1:A:43:LEU:HD23 | 6                   | 0.94     | 0.18                | 0.9        |
| (1,1900) | 1:A:41:MET:HE2  | 1:A:43:LEU:HD21 | 6                   | 0.94     | 0.18                | 0.9        |
| (1,1900) | 1:A:41:MET:HE2  | 1:A:43:LEU:HD22 | 6                   | 0.94     | 0.18                | 0.9        |
| (1,1900) | 1:A:41:MET:HE2  | 1:A:43:LEU:HD23 | 6                   | 0.94     | 0.18                | 0.9        |
| (1,1900) | 1:A:41:MET:HE3  | 1:A:43:LEU:HD21 | 6                   | 0.94     | 0.18                | 0.9        |
| (1,1900) | 1:A:41:MET:HE3  | 1:A:43:LEU:HD22 | 6                   | 0.94     | 0.18                | 0.9        |
| (1,1900) | 1:A:41:MET:HE3  | 1:A:43:LEU:HD23 | 6                   | 0.94     | 0.18                | 0.9        |
| (1,2642) | 1:A:81:GLU:HA   | 1:A:84:ASP:HB3  | 6                   | 0.8      | 0.38                | 0.82       |
| (1,2641) | 1:A:122:GLU:HB2 | 1:A:126:ALA:HB1 | 6                   | 0.66     | 0.37                | 0.6        |
| (1,2641) | 1:A:122:GLU:HB2 | 1:A:126:ALA:HB2 | 6                   | 0.66     | 0.37                | 0.6        |
| (1,2641) | 1:A:122:GLU:HB2 | 1:A:126:ALA:HB3 | 6                   | 0.66     | 0.37                | 0.6        |
| (1,1983) | 1:A:126:ALA:HB1 | 1:A:122:GLU:HG3 | 6                   | 0.46     | 0.02                | 0.46       |
| (1,1983) | 1:A:126:ALA:HB2 | 1:A:122:GLU:HG3 | 6                   | 0.46     | 0.02                | 0.46       |
| (1,1983) | 1:A:126:ALA:HB3 | 1:A:122:GLU:HG3 | 6                   | 0.46     | 0.02                | 0.46       |
| (1,1336) | 1:A:38:LEU:HA   | 1:A:43:LEU:HD21 | 6                   | 0.45     | 0.15                | 0.42       |
| (1,1336) | 1:A:38:LEU:HA   | 1:A:43:LEU:HD22 | 6                   | 0.45     | 0.15                | 0.42       |
| (1,1336) | 1:A:38:LEU:HA   | 1:A:43:LEU:HD23 | 6                   | 0.45     | 0.15                | 0.42       |
| (1,1781) | 1:A:43:LEU:HD11 | 1:A:43:LEU:HA   | 6                   | 0.26     | 0.02                | 0.25       |
| (1,1781) | 1:A:43:LEU:HD12 | 1:A:43:LEU:HA   | 6                   | 0.26     | 0.02                | 0.25       |
| (1,1781) | 1:A:43:LEU:HD13 | 1:A:43:LEU:HA   | 6                   | 0.26     | 0.02                | 0.25       |
| (1,952)  | 1:A:29:LEU:HD21 | 1:A:70:VAL:HB   | 6                   | 0.16     | 0.03                | 0.14       |
| (1,952)  | 1:A:29:LEU:HD22 | 1:A:70:VAL:HB   | 6                   | 0.16     | 0.03                | 0.14       |
| (1,952)  | 1:A:29:LEU:HD23 | 1:A:70:VAL:HB   | 6                   | 0.16     | 0.03                | 0.14       |
| (3,53)   | 1:A:75:TYR:O    | 1:A:78:TYR:H    | 6                   | 0.15     | 0.02                | 0.16       |
| (1,2639) | 1:A:43:LEU:HD11 | 1:A:43:LEU:HA   | 6                   | 0.13     | 0.02                | 0.12       |
| (1,2639) | 1:A:43:LEU:HD12 | 1:A:43:LEU:HA   | 6                   | 0.13     | 0.02                | 0.12       |
| (1,2639) | 1:A:43:LEU:HD13 | 1:A:43:LEU:HA   | 6                   | 0.13     | 0.02                | 0.12       |
| (3,9)    | 1:A:13:GLU:O    | 1:A:16:GLN:H    | 6                   | 0.13     | 0.01                | 0.13       |
| (1,2083) | 1:A:89:PRO:HA   | 1:A:92:LEU:HD21 | 5                   | 1.04     | 0.7                 | 0.92       |
| (1,2083) | 1:A:89:PRO:HA   | 1:A:92:LEU:HD22 | 5                   | 1.04     | 0.7                 | 0.92       |
| (1,2083) | 1:A:89:PRO:HA   | 1:A:92:LEU:HD23 | 5                   | 1.04     | 0.7                 | 0.92       |
| (1,1447) | 1:A:89:PRO:HA   | 1:A:92:LEU:HD21 | 5                   | 0.9      | 0.7                 | 0.78       |
| (1,1447) | 1:A:89:PRO:HA   | 1:A:92:LEU:HD22 | 5                   | 0.9      | 0.7                 | 0.78       |
| (1,1447) | 1:A:89:PRO:HA   | 1:A:92:LEU:HD23 | 5                   | 0.9      | 0.7                 | 0.78       |
| (1,2331) | 1:A:6:VAL:HB    | 1:A:11:MET:HG2  | 5                   | 0.65     | 0.07                | 0.62       |
| (1,1829) | 1:A:103:LYS:HE2 | 1:A:101:ALA:HB1 | 5                   | 0.64     | 0.4                 | 0.57       |

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| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1829) | 1:A:103:LYS:HE2  | 1:A:101:ALA:HB2 | 5                   | 0.64     | 0.4                 | 0.57       |
| (1,1829) | 1:A:103:LYS:HE2  | 1:A:101:ALA:HB3 | 5                   | 0.64     | 0.4                 | 0.57       |
| (1,1259) | 1:A:38:LEU:HD21  | 1:A:59:ILE:HG21 | 5                   | 0.55     | 0.13                | 0.56       |
| (1,1259) | 1:A:38:LEU:HD21  | 1:A:59:ILE:HG22 | 5                   | 0.55     | 0.13                | 0.56       |
| (1,1259) | 1:A:38:LEU:HD21  | 1:A:59:ILE:HG23 | 5                   | 0.55     | 0.13                | 0.56       |
| (1,1259) | 1:A:38:LEU:HD22  | 1:A:59:ILE:HG21 | 5                   | 0.55     | 0.13                | 0.56       |
| (1,1259) | 1:A:38:LEU:HD22  | 1:A:59:ILE:HG22 | 5                   | 0.55     | 0.13                | 0.56       |
| (1,1259) | 1:A:38:LEU:HD22  | 1:A:59:ILE:HG23 | 5                   | 0.55     | 0.13                | 0.56       |
| (1,1259) | 1:A:38:LEU:HD23  | 1:A:59:ILE:HG21 | 5                   | 0.55     | 0.13                | 0.56       |
| (1,1259) | 1:A:38:LEU:HD23  | 1:A:59:ILE:HG22 | 5                   | 0.55     | 0.13                | 0.56       |
| (1,1259) | 1:A:38:LEU:HD23  | 1:A:59:ILE:HG23 | 5                   | 0.55     | 0.13                | 0.56       |
| (1,2462) | 1:A:65:LYS:HE3   | 1:A:65:LYS:HA   | 5                   | 0.53     | 0.09                | 0.53       |
| (1,2653) | 1:A:61:ASN:HB3   | 1:A:58:ALA:HB1  | 5                   | 0.47     | 0.19                | 0.58       |
| (1,2653) | 1:A:61:ASN:HB3   | 1:A:58:ALA:HB2  | 5                   | 0.47     | 0.19                | 0.58       |
| (1,2653) | 1:A:61:ASN:HB3   | 1:A:58:ALA:HB3  | 5                   | 0.47     | 0.19                | 0.58       |
| (1,2327) | 1:A:113:LYS:HB3  | 1:A:113:LYS:HE3 | 5                   | 0.43     | 0.3                 | 0.33       |
| (1,1978) | 1:A:38:LEU:HA    | 1:A:43:LEU:HD21 | 5                   | 0.29     | 0.14                | 0.25       |
| (1,1978) | 1:A:38:LEU:HA    | 1:A:43:LEU:HD22 | 5                   | 0.29     | 0.14                | 0.25       |
| (1,1978) | 1:A:38:LEU:HA    | 1:A:43:LEU:HD23 | 5                   | 0.29     | 0.14                | 0.25       |
| (1,1439) | 1:A:141:VAL:HG11 | 1:A:137:TYR:HE1 | 5                   | 0.28     | 0.05                | 0.3        |
| (1,1439) | 1:A:141:VAL:HG11 | 1:A:137:TYR:HE2 | 5                   | 0.28     | 0.05                | 0.3        |
| (1,1439) | 1:A:141:VAL:HG12 | 1:A:137:TYR:HE1 | 5                   | 0.28     | 0.05                | 0.3        |
| (1,1439) | 1:A:141:VAL:HG12 | 1:A:137:TYR:HE2 | 5                   | 0.28     | 0.05                | 0.3        |
| (1,1439) | 1:A:141:VAL:HG13 | 1:A:137:TYR:HE1 | 5                   | 0.28     | 0.05                | 0.3        |
| (1,1439) | 1:A:141:VAL:HG13 | 1:A:137:TYR:HE2 | 5                   | 0.28     | 0.05                | 0.3        |
| (1,2212) | 1:A:35:ARG:HD2   | 1:A:56:TYR:HE1  | 5                   | 0.26     | 0.04                | 0.25       |
| (1,2212) | 1:A:35:ARG:HD2   | 1:A:56:TYR:HE2  | 5                   | 0.26     | 0.04                | 0.25       |
| (1,1491) | 1:A:65:LYS:HE3   | 1:A:65:LYS:HB2  | 5                   | 0.25     | 0.05                | 0.26       |
| (1,2164) | 1:A:121:ILE:HG21 | 1:A:108:GLU:HB3 | 5                   | 0.21     | 0.01                | 0.21       |
| (1,2164) | 1:A:121:ILE:HG22 | 1:A:108:GLU:HB3 | 5                   | 0.21     | 0.01                | 0.21       |
| (1,2164) | 1:A:121:ILE:HG23 | 1:A:108:GLU:HB3 | 5                   | 0.21     | 0.01                | 0.21       |
| (3,109)  | 1:A:29:LEU:N     | 1:A:70:VAL:O    | 5                   | 0.2      | 0.06                | 0.19       |
| (3,126)  | 1:A:73:ASP:O     | 1:A:77:GLN:N    | 5                   | 0.18     | 0.04                | 0.19       |
| (2,267)  | 1:A:63:VAL:HG11  | 1:A:69:GLY:H    | 5                   | 0.16     | 0.03                | 0.14       |
| (2,267)  | 1:A:63:VAL:HG12  | 1:A:69:GLY:H    | 5                   | 0.16     | 0.03                | 0.14       |
| (2,267)  | 1:A:63:VAL:HG13  | 1:A:69:GLY:H    | 5                   | 0.16     | 0.03                | 0.14       |
| (3,59)   | 1:A:79:MET:O     | 1:A:83:ASN:H    | 5                   | 0.14     | 0.02                | 0.15       |
| (3,81)   | 1:A:113:LYS:O    | 1:A:115:GLY:H   | 5                   | 0.13     | 0.02                | 0.12       |
| (1,2118) | 1:A:89:PRO:HA    | 1:A:92:LEU:HB2  | 4                   | 1.19     | 0.63                | 1.5        |
| (1,1149) | 1:A:82:LYS:HA    | 1:A:85:GLU:HG3  | 4                   | 0.56     | 0.34                | 0.47       |
| (1,542)  | 1:A:108:GLU:HG2  | 1:A:113:LYS:H   | 4                   | 0.5      | 0.04                | 0.49       |
| (1,2543) | 1:A:59:ILE:HD11  | 1:A:55:GLN:HG3  | 4                   | 0.46     | 0.17                | 0.4        |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2543) | 1:A:59:ILE:HD12  | 1:A:55:GLN:HG3   | 4                   | 0.46     | 0.17                | 0.4        |
| (1,2543) | 1:A:59:ILE:HD13  | 1:A:55:GLN:HG3   | 4                   | 0.46     | 0.17                | 0.4        |
| (1,1334) | 1:A:38:LEU:HD11  | 1:A:43:LEU:HB3   | 4                   | 0.4      | 0.04                | 0.4        |
| (1,1334) | 1:A:38:LEU:HD12  | 1:A:43:LEU:HB3   | 4                   | 0.4      | 0.04                | 0.4        |
| (1,1334) | 1:A:38:LEU:HD13  | 1:A:43:LEU:HB3   | 4                   | 0.4      | 0.04                | 0.4        |
| (1,2436) | 1:A:6:VAL:HG11   | 1:A:80:LYS:HB3   | 4                   | 0.35     | 0.12                | 0.4        |
| (1,2436) | 1:A:6:VAL:HG12   | 1:A:80:LYS:HB3   | 4                   | 0.35     | 0.12                | 0.4        |
| (1,2436) | 1:A:6:VAL:HG13   | 1:A:80:LYS:HB3   | 4                   | 0.35     | 0.12                | 0.4        |
| (1,2602) | 1:A:141:VAL:HG11 | 1:A:137:TYR:HD1  | 4                   | 0.29     | 0.18                | 0.22       |
| (1,2602) | 1:A:141:VAL:HG11 | 1:A:137:TYR:HD2  | 4                   | 0.29     | 0.18                | 0.22       |
| (1,2602) | 1:A:141:VAL:HG12 | 1:A:137:TYR:HD1  | 4                   | 0.29     | 0.18                | 0.22       |
| (1,2602) | 1:A:141:VAL:HG12 | 1:A:137:TYR:HD2  | 4                   | 0.29     | 0.18                | 0.22       |
| (1,2602) | 1:A:141:VAL:HG13 | 1:A:137:TYR:HD1  | 4                   | 0.29     | 0.18                | 0.22       |
| (1,2602) | 1:A:141:VAL:HG13 | 1:A:137:TYR:HD2  | 4                   | 0.29     | 0.18                | 0.22       |
| (1,2444) | 1:A:121:ILE:HD11 | 1:A:112:GLN:HG2  | 4                   | 0.26     | 0.02                | 0.26       |
| (1,2444) | 1:A:121:ILE:HD12 | 1:A:112:GLN:HG2  | 4                   | 0.26     | 0.02                | 0.26       |
| (1,2444) | 1:A:121:ILE:HD13 | 1:A:112:GLN:HG2  | 4                   | 0.26     | 0.02                | 0.26       |
| (1,2290) | 1:A:40:SER:HB3   | 1:A:37:CYS:HA    | 4                   | 0.24     | 0.11                | 0.2        |
| (3,150)  | 1:A:138:ALA:O    | 1:A:142:LYS:N    | 4                   | 0.18     | 0.07                | 0.16       |
| (3,37)   | 1:A:45:ASP:O     | 1:A:47:ASP:H     | 4                   | 0.16     | 0.05                | 0.16       |
| (3,148)  | 1:A:124:VAL:O    | 1:A:128:LEU:N    | 4                   | 0.16     | 0.03                | 0.16       |
| (1,2174) | 1:A:99:ILE:HG21  | 1:A:100:ALA:HB1  | 4                   | 0.15     | 0.04                | 0.15       |
| (1,2174) | 1:A:99:ILE:HG21  | 1:A:100:ALA:HB2  | 4                   | 0.15     | 0.04                | 0.15       |
| (1,2174) | 1:A:99:ILE:HG21  | 1:A:100:ALA:HB3  | 4                   | 0.15     | 0.04                | 0.15       |
| (1,2174) | 1:A:99:ILE:HG22  | 1:A:100:ALA:HB1  | 4                   | 0.15     | 0.04                | 0.15       |
| (1,2174) | 1:A:99:ILE:HG22  | 1:A:100:ALA:HB2  | 4                   | 0.15     | 0.04                | 0.15       |
| (1,2174) | 1:A:99:ILE:HG22  | 1:A:100:ALA:HB3  | 4                   | 0.15     | 0.04                | 0.15       |
| (1,2174) | 1:A:99:ILE:HG23  | 1:A:100:ALA:HB1  | 4                   | 0.15     | 0.04                | 0.15       |
| (1,2174) | 1:A:99:ILE:HG23  | 1:A:100:ALA:HB2  | 4                   | 0.15     | 0.04                | 0.15       |
| (1,2174) | 1:A:99:ILE:HG23  | 1:A:100:ALA:HB3  | 4                   | 0.15     | 0.04                | 0.15       |
| (3,97)   | 1:A:136:ASP:O    | 1:A:139:ALA:H    | 4                   | 0.15     | 0.02                | 0.15       |
| (3,23)   | 1:A:33:GLU:O     | 1:A:36:SER:H     | 4                   | 0.13     | 0.02                | 0.12       |
| (3,65)   | 1:A:91:GLN:O     | 1:A:94:GLU:H     | 4                   | 0.12     | 0.01                | 0.12       |
| (1,1186) | 1:A:135:TYR:HB3  | 1:A:106:ILE:HG12 | 4                   | 0.12     | 0.01                | 0.11       |
| (1,2564) | 1:A:89:PRO:HA    | 1:A:92:LEU:HB2   | 3                   | 1.14     | 0.11                | 1.19       |
| (2,359)  | 1:A:109:THR:HA   | 1:A:113:LYS:HD3  | 3                   | 0.66     | 0.44                | 0.49       |
| (1,1712) | 1:A:106:ILE:HA   | 1:A:103:LYS:HE3  | 3                   | 0.64     | 0.27                | 0.56       |
| (1,2267) | 1:A:92:LEU:HD21  | 1:A:123:TYR:HE1  | 3                   | 0.64     | 0.3                 | 0.46       |
| (1,2267) | 1:A:92:LEU:HD21  | 1:A:123:TYR:HE2  | 3                   | 0.64     | 0.3                 | 0.46       |
| (1,2267) | 1:A:92:LEU:HD22  | 1:A:123:TYR:HE1  | 3                   | 0.64     | 0.3                 | 0.46       |
| (1,2267) | 1:A:92:LEU:HD22  | 1:A:123:TYR:HE2  | 3                   | 0.64     | 0.3                 | 0.46       |
| (1,2267) | 1:A:92:LEU:HD23  | 1:A:123:TYR:HE1  | 3                   | 0.64     | 0.3                 | 0.46       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,2267) | 1:A:92:LEU:HD23 | 1:A:123:TYR:HE2 | 3                   | 0.64     | 0.3                 | 0.46       |
| (1,2304) | 1:A:43:LEU:HD21 | 1:A:82:LYS:HE2  | 3                   | 0.62     | 0.05                | 0.66       |
| (1,2304) | 1:A:43:LEU:HD22 | 1:A:82:LYS:HE2  | 3                   | 0.62     | 0.05                | 0.66       |
| (1,2304) | 1:A:43:LEU:HD23 | 1:A:82:LYS:HE2  | 3                   | 0.62     | 0.05                | 0.66       |
| (1,1351) | 1:A:80:LYS:HD3  | 1:A:80:LYS:HA   | 3                   | 0.52     | 0.01                | 0.53       |
| (1,2399) | 1:A:103:LYS:HE2 | 1:A:100:ALA:HB1 | 3                   | 0.49     | 0.18                | 0.47       |
| (1,2399) | 1:A:103:LYS:HE2 | 1:A:100:ALA:HB2 | 3                   | 0.49     | 0.18                | 0.47       |
| (1,2399) | 1:A:103:LYS:HE2 | 1:A:100:ALA:HB3 | 3                   | 0.49     | 0.18                | 0.47       |
| (1,2047) | 1:A:43:LEU:HD11 | 1:A:82:LYS:HE3  | 3                   | 0.49     | 0.27                | 0.55       |
| (1,2047) | 1:A:43:LEU:HD12 | 1:A:82:LYS:HE3  | 3                   | 0.49     | 0.27                | 0.55       |
| (1,2047) | 1:A:43:LEU:HD13 | 1:A:82:LYS:HE3  | 3                   | 0.49     | 0.27                | 0.55       |
| (1,2292) | 1:A:113:LYS:HB3 | 1:A:113:LYS:HE3 | 3                   | 0.49     | 0.22                | 0.63       |
| (2,223)  | 1:A:52:GLU:HB3  | 1:A:50:GLY:H    | 3                   | 0.45     | 0.06                | 0.49       |
| (1,1024) | 1:A:15:LYS:HE3  | 1:A:15:LYS:HA   | 3                   | 0.44     | 0.13                | 0.4        |
| (1,1455) | 1:A:10:GLN:HA   | 1:A:13:GLU:HB2  | 3                   | 0.43     | 0.06                | 0.45       |
| (1,1941) | 1:A:44:ILE:HG21 | 1:A:38:LEU:HD21 | 3                   | 0.38     | 0.29                | 0.22       |
| (1,1941) | 1:A:44:ILE:HG21 | 1:A:38:LEU:HD22 | 3                   | 0.38     | 0.29                | 0.22       |
| (1,1941) | 1:A:44:ILE:HG21 | 1:A:38:LEU:HD23 | 3                   | 0.38     | 0.29                | 0.22       |
| (1,1941) | 1:A:44:ILE:HG22 | 1:A:38:LEU:HD21 | 3                   | 0.38     | 0.29                | 0.22       |
| (1,1941) | 1:A:44:ILE:HG22 | 1:A:38:LEU:HD22 | 3                   | 0.38     | 0.29                | 0.22       |
| (1,1941) | 1:A:44:ILE:HG22 | 1:A:38:LEU:HD23 | 3                   | 0.38     | 0.29                | 0.22       |
| (1,1941) | 1:A:44:ILE:HG23 | 1:A:38:LEU:HD21 | 3                   | 0.38     | 0.29                | 0.22       |
| (1,1941) | 1:A:44:ILE:HG23 | 1:A:38:LEU:HD22 | 3                   | 0.38     | 0.29                | 0.22       |
| (1,1941) | 1:A:44:ILE:HG23 | 1:A:38:LEU:HD23 | 3                   | 0.38     | 0.29                | 0.22       |
| (1,2080) | 1:A:38:LEU:HD21 | 1:A:59:ILE:HG21 | 3                   | 0.3      | 0.06                | 0.34       |
| (1,2080) | 1:A:38:LEU:HD21 | 1:A:59:ILE:HG22 | 3                   | 0.3      | 0.06                | 0.34       |
| (1,2080) | 1:A:38:LEU:HD21 | 1:A:59:ILE:HG23 | 3                   | 0.3      | 0.06                | 0.34       |
| (1,2080) | 1:A:38:LEU:HD22 | 1:A:59:ILE:HG21 | 3                   | 0.3      | 0.06                | 0.34       |
| (1,2080) | 1:A:38:LEU:HD22 | 1:A:59:ILE:HG22 | 3                   | 0.3      | 0.06                | 0.34       |
| (1,2080) | 1:A:38:LEU:HD22 | 1:A:59:ILE:HG23 | 3                   | 0.3      | 0.06                | 0.34       |
| (1,2080) | 1:A:38:LEU:HD23 | 1:A:59:ILE:HG21 | 3                   | 0.3      | 0.06                | 0.34       |
| (1,2080) | 1:A:38:LEU:HD23 | 1:A:59:ILE:HG22 | 3                   | 0.3      | 0.06                | 0.34       |
| (1,2080) | 1:A:38:LEU:HD23 | 1:A:59:ILE:HG23 | 3                   | 0.3      | 0.06                | 0.34       |
| (1,1716) | 1:A:40:SER:HB3  | 1:A:37:CYS:HA   | 3                   | 0.24     | 0.1                 | 0.18       |
| (1,2631) | 1:A:10:GLN:HA   | 1:A:13:GLU:HG2  | 3                   | 0.15     | 0.05                | 0.12       |
| (1,1580) | 1:A:44:ILE:HB   | 1:A:43:LEU:HB3  | 3                   | 0.14     | 0.01                | 0.14       |
| (3,77)   | 1:A:107:THR:O   | 1:A:111:MET:H   | 3                   | 0.12     | 0.02                | 0.11       |
| (3,112)  | 1:A:33:GLU:O    | 1:A:36:SER:N    | 3                   | 0.12     | 0.01                | 0.11       |
| (3,1)    | 1:A:7:THR:O     | 1:A:11:MET:H    | 3                   | 0.11     | 0.0                 | 0.11       |
| (2,18)   | 1:A:142:LYS:HB2 | 1:A:144:ASN:H   | 2                   | 1.22     | 0.12                | 1.22       |
| (1,1045) | 1:A:41:MET:HB3  | 1:A:43:LEU:HD21 | 2                   | 0.83     | 0.69                | 0.83       |
| (1,1045) | 1:A:41:MET:HB3  | 1:A:43:LEU:HD22 | 2                   | 0.83     | 0.69                | 0.83       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1045) | 1:A:41:MET:HB3  | 1:A:43:LEU:HD23 | 2                   | 0.83     | 0.69                | 0.83       |
| (1,1407) | 1:A:41:MET:HB3  | 1:A:43:LEU:HG   | 2                   | 0.73     | 0.19                | 0.73       |
| (1,1002) | 1:A:41:MET:HE1  | 1:A:17:SER:HB3  | 2                   | 0.64     | 0.49                | 0.64       |
| (1,1002) | 1:A:41:MET:HE2  | 1:A:17:SER:HB3  | 2                   | 0.64     | 0.49                | 0.64       |
| (1,1002) | 1:A:41:MET:HE3  | 1:A:17:SER:HB3  | 2                   | 0.64     | 0.49                | 0.64       |
| (1,1779) | 1:A:43:LEU:HD11 | 1:A:82:LYS:HE2  | 2                   | 0.63     | 0.23                | 0.63       |
| (1,1779) | 1:A:43:LEU:HD12 | 1:A:82:LYS:HE2  | 2                   | 0.63     | 0.23                | 0.63       |
| (1,1779) | 1:A:43:LEU:HD13 | 1:A:82:LYS:HE2  | 2                   | 0.63     | 0.23                | 0.63       |
| (1,1638) | 1:A:21:PHE:HE1  | 1:A:17:SER:HB3  | 2                   | 0.55     | 0.15                | 0.55       |
| (1,1638) | 1:A:21:PHE:HE2  | 1:A:17:SER:HB3  | 2                   | 0.55     | 0.15                | 0.55       |
| (1,418)  | 1:A:117:SER:H   | 1:A:120:GLN:HB3 | 2                   | 0.55     | 0.4                 | 0.55       |
| (1,2142) | 1:A:79:MET:HA   | 1:A:82:LYS:HB3  | 2                   | 0.46     | 0.29                | 0.46       |
| (1,1741) | 1:A:69:GLY:HA3  | 1:A:60:TYR:HE1  | 2                   | 0.43     | 0.17                | 0.43       |
| (1,1741) | 1:A:69:GLY:HA3  | 1:A:60:TYR:HE2  | 2                   | 0.43     | 0.17                | 0.43       |
| (1,1483) | 1:A:15:LYS:HD2  | 1:A:15:LYS:HA   | 2                   | 0.42     | 0.02                | 0.42       |
| (1,1458) | 1:A:77:GLN:HB3  | 1:A:74:ASN:HA   | 2                   | 0.4      | 0.15                | 0.4        |
| (1,1721) | 1:A:15:LYS:HD2  | 1:A:15:LYS:HA   | 2                   | 0.34     | 0.02                | 0.34       |
| (1,1933) | 1:A:78:TYR:HB3  | 1:A:63:VAL:HA   | 2                   | 0.33     | 0.11                | 0.33       |
| (1,2459) | 1:A:41:MET:HB3  | 1:A:43:LEU:HG   | 2                   | 0.32     | 0.19                | 0.32       |
| (1,494)  | 1:A:10:GLN:HG2  | 1:A:13:GLU:H    | 2                   | 0.3      | 0.03                | 0.3        |
| (1,1814) | 1:A:15:LYS:HD2  | 1:A:15:LYS:HA   | 2                   | 0.3      | 0.02                | 0.3        |
| (1,802)  | 1:A:54:ALA:HB1  | 1:A:57:ASP:HB3  | 2                   | 0.29     | 0.06                | 0.29       |
| (1,802)  | 1:A:54:ALA:HB2  | 1:A:57:ASP:HB3  | 2                   | 0.29     | 0.06                | 0.29       |
| (1,802)  | 1:A:54:ALA:HB3  | 1:A:57:ASP:HB3  | 2                   | 0.29     | 0.06                | 0.29       |
| (1,1539) | 1:A:6:VAL:HG21  | 1:A:11:MET:HE1  | 2                   | 0.28     | 0.13                | 0.28       |
| (1,1539) | 1:A:6:VAL:HG21  | 1:A:11:MET:HE2  | 2                   | 0.28     | 0.13                | 0.28       |
| (1,1539) | 1:A:6:VAL:HG21  | 1:A:11:MET:HE3  | 2                   | 0.28     | 0.13                | 0.28       |
| (1,1539) | 1:A:6:VAL:HG22  | 1:A:11:MET:HE1  | 2                   | 0.28     | 0.13                | 0.28       |
| (1,1539) | 1:A:6:VAL:HG22  | 1:A:11:MET:HE2  | 2                   | 0.28     | 0.13                | 0.28       |
| (1,1539) | 1:A:6:VAL:HG22  | 1:A:11:MET:HE3  | 2                   | 0.28     | 0.13                | 0.28       |
| (1,1539) | 1:A:6:VAL:HG23  | 1:A:11:MET:HE1  | 2                   | 0.28     | 0.13                | 0.28       |
| (1,1539) | 1:A:6:VAL:HG23  | 1:A:11:MET:HE2  | 2                   | 0.28     | 0.13                | 0.28       |
| (1,1539) | 1:A:6:VAL:HG23  | 1:A:11:MET:HE3  | 2                   | 0.28     | 0.13                | 0.28       |
| (1,2324) | 1:A:103:LYS:HB3 | 1:A:103:LYS:HE3 | 2                   | 0.26     | 0.01                | 0.26       |
| (1,1656) | 1:A:8:ALA:HB1   | 1:A:11:MET:HG2  | 2                   | 0.24     | 0.14                | 0.24       |
| (1,1656) | 1:A:8:ALA:HB2   | 1:A:11:MET:HG2  | 2                   | 0.24     | 0.14                | 0.24       |
| (1,1656) | 1:A:8:ALA:HB3   | 1:A:11:MET:HG2  | 2                   | 0.24     | 0.14                | 0.24       |
| (1,2029) | 1:A:116:MET:HG2 | 1:A:114:ALA:HB1 | 2                   | 0.24     | 0.04                | 0.24       |
| (1,2029) | 1:A:116:MET:HG2 | 1:A:114:ALA:HB2 | 2                   | 0.24     | 0.04                | 0.24       |
| (1,2029) | 1:A:116:MET:HG2 | 1:A:114:ALA:HB3 | 2                   | 0.24     | 0.04                | 0.24       |
| (2,184)  | 1:A:92:LEU:HB2  | 1:A:95:ILE:H    | 2                   | 0.24     | 0.04                | 0.24       |
| (1,2300) | 1:A:57:ASP:HB3  | 1:A:54:ALA:HA   | 2                   | 0.24     | 0.05                | 0.24       |

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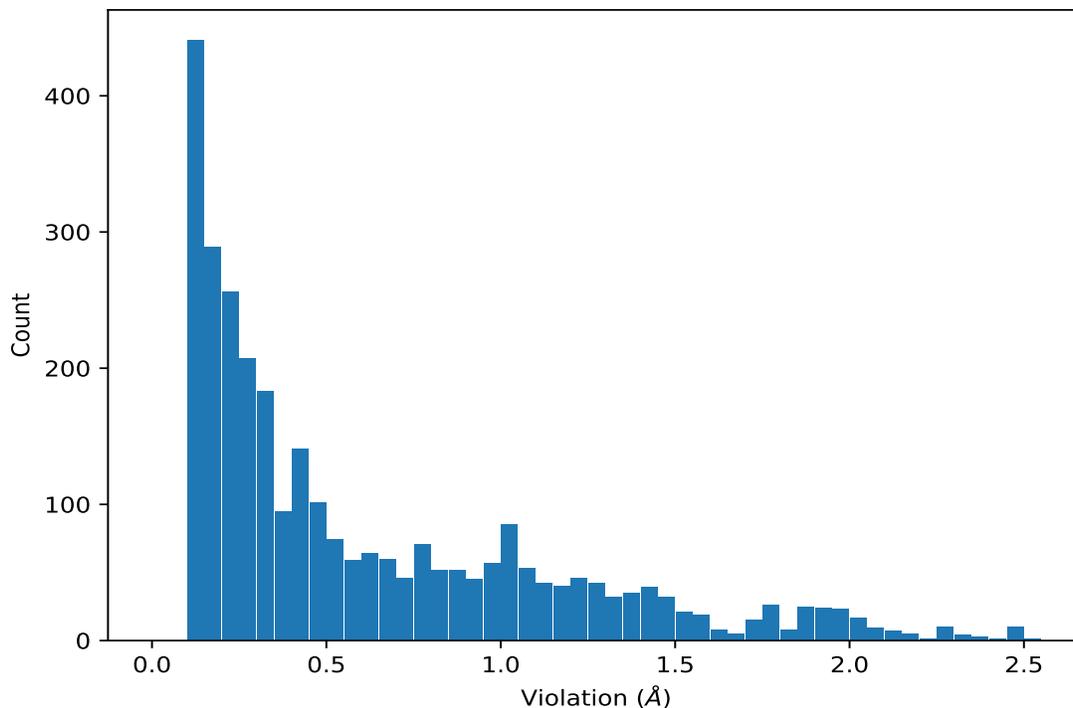
| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1257) | 1:A:41:MET:HE1  | 1:A:38:LEU:HD11 | 2                   | 0.23     | 0.06                | 0.23       |
| (1,1257) | 1:A:41:MET:HE1  | 1:A:38:LEU:HD12 | 2                   | 0.23     | 0.06                | 0.23       |
| (1,1257) | 1:A:41:MET:HE1  | 1:A:38:LEU:HD13 | 2                   | 0.23     | 0.06                | 0.23       |
| (1,1257) | 1:A:41:MET:HE2  | 1:A:38:LEU:HD11 | 2                   | 0.23     | 0.06                | 0.23       |
| (1,1257) | 1:A:41:MET:HE2  | 1:A:38:LEU:HD12 | 2                   | 0.23     | 0.06                | 0.23       |
| (1,1257) | 1:A:41:MET:HE2  | 1:A:38:LEU:HD13 | 2                   | 0.23     | 0.06                | 0.23       |
| (1,1257) | 1:A:41:MET:HE3  | 1:A:38:LEU:HD11 | 2                   | 0.23     | 0.06                | 0.23       |
| (1,1257) | 1:A:41:MET:HE3  | 1:A:38:LEU:HD12 | 2                   | 0.23     | 0.06                | 0.23       |
| (1,1257) | 1:A:41:MET:HE3  | 1:A:38:LEU:HD13 | 2                   | 0.23     | 0.06                | 0.23       |
| (3,129)  | 1:A:76:VAL:O    | 1:A:80:LYS:N    | 2                   | 0.21     | 0.07                | 0.21       |
| (1,1144) | 1:A:44:ILE:HG21 | 1:A:56:TYR:HB3  | 2                   | 0.18     | 0.02                | 0.18       |
| (1,1144) | 1:A:44:ILE:HG22 | 1:A:56:TYR:HB3  | 2                   | 0.18     | 0.02                | 0.18       |
| (1,1144) | 1:A:44:ILE:HG23 | 1:A:56:TYR:HB3  | 2                   | 0.18     | 0.02                | 0.18       |
| (1,1595) | 1:A:78:TYR:HE1  | 1:A:82:LYS:HE3  | 2                   | 0.16     | 0.01                | 0.16       |
| (1,1595) | 1:A:78:TYR:HE2  | 1:A:82:LYS:HE3  | 2                   | 0.16     | 0.01                | 0.16       |
| (1,2182) | 1:A:79:MET:HB2  | 1:A:79:MET:HE1  | 2                   | 0.16     | 0.02                | 0.16       |
| (1,2182) | 1:A:79:MET:HB2  | 1:A:79:MET:HE2  | 2                   | 0.16     | 0.02                | 0.16       |
| (1,2182) | 1:A:79:MET:HB2  | 1:A:79:MET:HE3  | 2                   | 0.16     | 0.02                | 0.16       |
| (1,1138) | 1:A:70:VAL:HG21 | 1:A:74:ASN:HB2  | 2                   | 0.15     | 0.0                 | 0.15       |
| (1,1138) | 1:A:70:VAL:HG22 | 1:A:74:ASN:HB2  | 2                   | 0.15     | 0.0                 | 0.15       |
| (1,1138) | 1:A:70:VAL:HG23 | 1:A:74:ASN:HB2  | 2                   | 0.15     | 0.0                 | 0.15       |
| (1,1653) | 1:A:76:VAL:HG21 | 1:A:75:TYR:HE1  | 2                   | 0.13     | 0.02                | 0.13       |
| (1,1653) | 1:A:76:VAL:HG21 | 1:A:75:TYR:HE2  | 2                   | 0.13     | 0.02                | 0.13       |
| (1,1653) | 1:A:76:VAL:HG22 | 1:A:75:TYR:HE1  | 2                   | 0.13     | 0.02                | 0.13       |
| (1,1653) | 1:A:76:VAL:HG22 | 1:A:75:TYR:HE2  | 2                   | 0.13     | 0.02                | 0.13       |
| (1,1653) | 1:A:76:VAL:HG23 | 1:A:75:TYR:HE1  | 2                   | 0.13     | 0.02                | 0.13       |
| (1,1653) | 1:A:76:VAL:HG23 | 1:A:75:TYR:HE2  | 2                   | 0.13     | 0.02                | 0.13       |
| (1,1468) | 1:A:79:MET:HE1  | 1:A:38:LEU:HD11 | 2                   | 0.12     | 0.02                | 0.12       |
| (1,1468) | 1:A:79:MET:HE1  | 1:A:38:LEU:HD12 | 2                   | 0.12     | 0.02                | 0.12       |
| (1,1468) | 1:A:79:MET:HE1  | 1:A:38:LEU:HD13 | 2                   | 0.12     | 0.02                | 0.12       |
| (1,1468) | 1:A:79:MET:HE2  | 1:A:38:LEU:HD11 | 2                   | 0.12     | 0.02                | 0.12       |
| (1,1468) | 1:A:79:MET:HE2  | 1:A:38:LEU:HD12 | 2                   | 0.12     | 0.02                | 0.12       |
| (1,1468) | 1:A:79:MET:HE2  | 1:A:38:LEU:HD13 | 2                   | 0.12     | 0.02                | 0.12       |
| (1,1468) | 1:A:79:MET:HE3  | 1:A:38:LEU:HD11 | 2                   | 0.12     | 0.02                | 0.12       |
| (1,1468) | 1:A:79:MET:HE3  | 1:A:38:LEU:HD12 | 2                   | 0.12     | 0.02                | 0.12       |
| (1,1468) | 1:A:79:MET:HE3  | 1:A:38:LEU:HD13 | 2                   | 0.12     | 0.02                | 0.12       |
| (3,5)    | 1:A:9:GLU:O     | 1:A:13:GLU:H    | 2                   | 0.12     | 0.01                | 0.12       |
| (3,45)   | 1:A:59:ILE:O    | 1:A:63:VAL:H    | 2                   | 0.12     | 0.01                | 0.12       |
| (1,1395) | 1:A:25:HIS:HB2  | 1:A:18:PHE:HD1  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1395) | 1:A:25:HIS:HB2  | 1:A:18:PHE:HD2  | 2                   | 0.11     | 0.0                 | 0.11       |
| (3,67)   | 1:A:94:GLU:O    | 1:A:97:SER:H    | 2                   | 0.11     | 0.0                 | 0.11       |
| (3,140)  | 1:A:108:GLU:O   | 1:A:112:GLN:N   | 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) |
|----------|----------------|-----------------|----------|---------------|
| (2,35)   | 1:A:29:LEU:H   | 1:A:33:GLU:H    | 4        | 2.53          |
| (2,35)   | 1:A:29:LEU:H   | 1:A:33:GLU:H    | 2        | 2.48          |
| (1,1218) | 1:A:6:VAL:HG11 | 1:A:80:LYS:HG3  | 11       | 2.46          |
| (1,1218) | 1:A:6:VAL:HG12 | 1:A:80:LYS:HG3  | 11       | 2.46          |
| (1,1218) | 1:A:6:VAL:HG13 | 1:A:80:LYS:HG3  | 11       | 2.46          |
| (1,1724) | 1:A:56:TYR:HE1 | 1:A:38:LEU:HD21 | 9        | 2.45          |
| (1,1724) | 1:A:56:TYR:HE1 | 1:A:38:LEU:HD22 | 9        | 2.45          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1724) | 1:A:56:TYR:HE1 | 1:A:38:LEU:HD23 | 9        | 2.45          |
| (1,1724) | 1:A:56:TYR:HE2 | 1:A:38:LEU:HD21 | 9        | 2.45          |
| (1,1724) | 1:A:56:TYR:HE2 | 1:A:38:LEU:HD22 | 9        | 2.45          |
| (1,1724) | 1:A:56:TYR:HE2 | 1:A:38:LEU:HD23 | 9        | 2.45          |
| (1,695)  | 1:A:62:ASN:H   | 1:A:65:LYS:H    | 4        | 2.42          |
| (1,1218) | 1:A:6:VAL:HG11 | 1:A:80:LYS:HG3  | 5        | 2.38          |
| (1,1218) | 1:A:6:VAL:HG12 | 1:A:80:LYS:HG3  | 5        | 2.38          |
| (1,1218) | 1:A:6:VAL:HG13 | 1:A:80:LYS:HG3  | 5        | 2.38          |
| (1,1021) | 1:A:6:VAL:HG11 | 1:A:80:LYS:HG3  | 11       | 2.33          |
| (1,1021) | 1:A:6:VAL:HG12 | 1:A:80:LYS:HG3  | 11       | 2.33          |
| (1,1021) | 1:A:6:VAL:HG13 | 1:A:80:LYS:HG3  | 11       | 2.33          |
| (1,695)  | 1:A:62:ASN:H   | 1:A:65:LYS:H    | 6        | 2.31          |
| (1,1218) | 1:A:6:VAL:HG11 | 1:A:80:LYS:HG3  | 12       | 2.28          |
| (1,1218) | 1:A:6:VAL:HG12 | 1:A:80:LYS:HG3  | 12       | 2.28          |
| (1,1218) | 1:A:6:VAL:HG13 | 1:A:80:LYS:HG3  | 12       | 2.28          |
| (1,2314) | 1:A:6:VAL:HG21 | 1:A:11:MET:HA   | 5        | 2.26          |
| (1,2314) | 1:A:6:VAL:HG22 | 1:A:11:MET:HA   | 5        | 2.26          |
| (1,2314) | 1:A:6:VAL:HG23 | 1:A:11:MET:HA   | 5        | 2.26          |
| (2,35)   | 1:A:29:LEU:H   | 1:A:33:GLU:H    | 1        | 2.25          |
| (1,1021) | 1:A:6:VAL:HG11 | 1:A:80:LYS:HG3  | 5        | 2.25          |
| (1,1021) | 1:A:6:VAL:HG12 | 1:A:80:LYS:HG3  | 5        | 2.25          |
| (1,1021) | 1:A:6:VAL:HG13 | 1:A:80:LYS:HG3  | 5        | 2.25          |
| (2,35)   | 1:A:29:LEU:H   | 1:A:33:GLU:H    | 6        | 2.23          |
| (1,695)  | 1:A:62:ASN:H   | 1:A:65:LYS:H    | 7        | 2.19          |
| (2,35)   | 1:A:29:LEU:H   | 1:A:33:GLU:H    | 12       | 2.16          |
| (1,1021) | 1:A:6:VAL:HG11 | 1:A:80:LYS:HG3  | 12       | 2.15          |
| (1,1021) | 1:A:6:VAL:HG12 | 1:A:80:LYS:HG3  | 12       | 2.15          |
| (1,1021) | 1:A:6:VAL:HG13 | 1:A:80:LYS:HG3  | 12       | 2.15          |
| (2,35)   | 1:A:29:LEU:H   | 1:A:33:GLU:H    | 5        | 2.14          |
| (1,2314) | 1:A:6:VAL:HG21 | 1:A:11:MET:HA   | 6        | 2.14          |
| (1,2314) | 1:A:6:VAL:HG22 | 1:A:11:MET:HA   | 6        | 2.14          |
| (1,2314) | 1:A:6:VAL:HG23 | 1:A:11:MET:HA   | 6        | 2.14          |
| (1,2314) | 1:A:6:VAL:HG21 | 1:A:11:MET:HA   | 8        | 2.11          |
| (1,2314) | 1:A:6:VAL:HG22 | 1:A:11:MET:HA   | 8        | 2.11          |
| (1,2314) | 1:A:6:VAL:HG23 | 1:A:11:MET:HA   | 8        | 2.11          |
| (1,695)  | 1:A:62:ASN:H   | 1:A:65:LYS:H    | 1        | 2.09          |
| (1,2083) | 1:A:89:PRO:HA  | 1:A:92:LEU:HD21 | 12       | 2.08          |
| (1,2083) | 1:A:89:PRO:HA  | 1:A:92:LEU:HD22 | 12       | 2.08          |
| (1,2083) | 1:A:89:PRO:HA  | 1:A:92:LEU:HD23 | 12       | 2.08          |
| (2,35)   | 1:A:29:LEU:H   | 1:A:33:GLU:H    | 3        | 2.07          |
| (1,695)  | 1:A:62:ASN:H   | 1:A:65:LYS:H    | 10       | 2.07          |
| (1,2314) | 1:A:6:VAL:HG21 | 1:A:11:MET:HA   | 11       | 2.05          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,2314) | 1:A:6:VAL:HG22 | 1:A:11:MET:HA   | 11       | 2.05          |
| (1,2314) | 1:A:6:VAL:HG23 | 1:A:11:MET:HA   | 11       | 2.05          |
| (2,35)   | 1:A:29:LEU:H   | 1:A:33:GLU:H    | 10       | 2.04          |
| (1,2314) | 1:A:6:VAL:HG21 | 1:A:11:MET:HA   | 1        | 2.04          |
| (1,2314) | 1:A:6:VAL:HG22 | 1:A:11:MET:HA   | 1        | 2.04          |
| (1,2314) | 1:A:6:VAL:HG23 | 1:A:11:MET:HA   | 1        | 2.04          |
| (1,2314) | 1:A:6:VAL:HG21 | 1:A:11:MET:HA   | 3        | 2.03          |
| (1,2314) | 1:A:6:VAL:HG22 | 1:A:11:MET:HA   | 3        | 2.03          |
| (1,2314) | 1:A:6:VAL:HG23 | 1:A:11:MET:HA   | 3        | 2.03          |
| (1,1218) | 1:A:6:VAL:HG11 | 1:A:80:LYS:HG3  | 1        | 2.02          |
| (1,1218) | 1:A:6:VAL:HG12 | 1:A:80:LYS:HG3  | 1        | 2.02          |
| (1,1218) | 1:A:6:VAL:HG13 | 1:A:80:LYS:HG3  | 1        | 2.02          |
| (1,695)  | 1:A:62:ASN:H   | 1:A:65:LYS:H    | 5        | 2.01          |
| (1,1724) | 1:A:56:TYR:HE1 | 1:A:38:LEU:HD21 | 6        | 2.01          |
| (1,1724) | 1:A:56:TYR:HE1 | 1:A:38:LEU:HD22 | 6        | 2.01          |
| (1,1724) | 1:A:56:TYR:HE1 | 1:A:38:LEU:HD23 | 6        | 2.01          |
| (1,1724) | 1:A:56:TYR:HE2 | 1:A:38:LEU:HD21 | 6        | 2.01          |
| (1,1724) | 1:A:56:TYR:HE2 | 1:A:38:LEU:HD22 | 6        | 2.01          |
| (1,1724) | 1:A:56:TYR:HE2 | 1:A:38:LEU:HD23 | 6        | 2.01          |
| (2,35)   | 1:A:29:LEU:H   | 1:A:33:GLU:H    | 9        | 1.99          |
| (1,2253) | 1:A:79:MET:HE1 | 1:A:43:LEU:HD21 | 1        | 1.99          |
| (1,2253) | 1:A:79:MET:HE1 | 1:A:43:LEU:HD22 | 1        | 1.99          |
| (1,2253) | 1:A:79:MET:HE1 | 1:A:43:LEU:HD23 | 1        | 1.99          |
| (1,2253) | 1:A:79:MET:HE2 | 1:A:43:LEU:HD21 | 1        | 1.99          |
| (1,2253) | 1:A:79:MET:HE2 | 1:A:43:LEU:HD22 | 1        | 1.99          |
| (1,2253) | 1:A:79:MET:HE2 | 1:A:43:LEU:HD23 | 1        | 1.99          |
| (1,2253) | 1:A:79:MET:HE3 | 1:A:43:LEU:HD21 | 1        | 1.99          |
| (1,2253) | 1:A:79:MET:HE3 | 1:A:43:LEU:HD22 | 1        | 1.99          |
| (1,2253) | 1:A:79:MET:HE3 | 1:A:43:LEU:HD23 | 1        | 1.99          |
| (2,35)   | 1:A:29:LEU:H   | 1:A:33:GLU:H    | 7        | 1.96          |
| (1,2253) | 1:A:79:MET:HE1 | 1:A:43:LEU:HD21 | 2        | 1.96          |
| (1,2253) | 1:A:79:MET:HE1 | 1:A:43:LEU:HD22 | 2        | 1.96          |
| (1,2253) | 1:A:79:MET:HE1 | 1:A:43:LEU:HD23 | 2        | 1.96          |
| (1,2253) | 1:A:79:MET:HE2 | 1:A:43:LEU:HD21 | 2        | 1.96          |
| (1,2253) | 1:A:79:MET:HE2 | 1:A:43:LEU:HD22 | 2        | 1.96          |
| (1,2253) | 1:A:79:MET:HE2 | 1:A:43:LEU:HD23 | 2        | 1.96          |
| (1,2253) | 1:A:79:MET:HE3 | 1:A:43:LEU:HD21 | 2        | 1.96          |
| (1,2253) | 1:A:79:MET:HE3 | 1:A:43:LEU:HD22 | 2        | 1.96          |
| (1,2253) | 1:A:79:MET:HE3 | 1:A:43:LEU:HD23 | 2        | 1.96          |
| (1,2393) | 1:A:6:VAL:HG11 | 1:A:80:LYS:HD3  | 11       | 1.95          |
| (1,2393) | 1:A:6:VAL:HG12 | 1:A:80:LYS:HD3  | 11       | 1.95          |
| (1,2393) | 1:A:6:VAL:HG13 | 1:A:80:LYS:HD3  | 11       | 1.95          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,947)  | 1:A:6:VAL:HG11 | 1:A:80:LYS:HD3  | 11       | 1.94          |
| (1,947)  | 1:A:6:VAL:HG12 | 1:A:80:LYS:HD3  | 11       | 1.94          |
| (1,947)  | 1:A:6:VAL:HG13 | 1:A:80:LYS:HD3  | 11       | 1.94          |
| (1,695)  | 1:A:62:ASN:H   | 1:A:65:LYS:H    | 8        | 1.94          |
| (1,1447) | 1:A:89:PRO:HA  | 1:A:92:LEU:HD21 | 12       | 1.94          |
| (1,1447) | 1:A:89:PRO:HA  | 1:A:92:LEU:HD22 | 12       | 1.94          |
| (1,1447) | 1:A:89:PRO:HA  | 1:A:92:LEU:HD23 | 12       | 1.94          |
| (1,1168) | 1:A:6:VAL:HG21 | 1:A:11:MET:HB2  | 5        | 1.93          |
| (1,1168) | 1:A:6:VAL:HG21 | 1:A:11:MET:HB3  | 5        | 1.93          |
| (1,1168) | 1:A:6:VAL:HG22 | 1:A:11:MET:HB2  | 5        | 1.93          |
| (1,1168) | 1:A:6:VAL:HG22 | 1:A:11:MET:HB3  | 5        | 1.93          |
| (1,1168) | 1:A:6:VAL:HG23 | 1:A:11:MET:HB2  | 5        | 1.93          |
| (1,1168) | 1:A:6:VAL:HG23 | 1:A:11:MET:HB3  | 5        | 1.93          |
| (1,1168) | 1:A:6:VAL:HG21 | 1:A:11:MET:HB2  | 6        | 1.91          |
| (1,1168) | 1:A:6:VAL:HG21 | 1:A:11:MET:HB3  | 6        | 1.91          |
| (1,1168) | 1:A:6:VAL:HG22 | 1:A:11:MET:HB2  | 6        | 1.91          |
| (1,1168) | 1:A:6:VAL:HG22 | 1:A:11:MET:HB3  | 6        | 1.91          |
| (1,1168) | 1:A:6:VAL:HG23 | 1:A:11:MET:HB2  | 6        | 1.91          |
| (1,1168) | 1:A:6:VAL:HG23 | 1:A:11:MET:HB3  | 6        | 1.91          |
| (2,268)  | 1:A:134:GLY:H  | 1:A:130:GLN:H   | 6        | 1.9           |
| (2,268)  | 1:A:134:GLY:H  | 1:A:130:GLN:H   | 7        | 1.9           |
| (1,1218) | 1:A:6:VAL:HG11 | 1:A:80:LYS:HG3  | 7        | 1.9           |
| (1,1218) | 1:A:6:VAL:HG12 | 1:A:80:LYS:HG3  | 7        | 1.9           |
| (1,1218) | 1:A:6:VAL:HG13 | 1:A:80:LYS:HG3  | 7        | 1.9           |
| (1,1021) | 1:A:6:VAL:HG11 | 1:A:80:LYS:HG3  | 1        | 1.89          |
| (1,1021) | 1:A:6:VAL:HG12 | 1:A:80:LYS:HG3  | 1        | 1.89          |
| (1,1021) | 1:A:6:VAL:HG13 | 1:A:80:LYS:HG3  | 1        | 1.89          |
| (2,35)   | 1:A:29:LEU:H   | 1:A:33:GLU:H    | 8        | 1.88          |
| (2,268)  | 1:A:134:GLY:H  | 1:A:130:GLN:H   | 1        | 1.88          |
| (1,1168) | 1:A:6:VAL:HG21 | 1:A:11:MET:HB2  | 8        | 1.88          |
| (1,1168) | 1:A:6:VAL:HG21 | 1:A:11:MET:HB3  | 8        | 1.88          |
| (1,1168) | 1:A:6:VAL:HG22 | 1:A:11:MET:HB2  | 8        | 1.88          |
| (1,1168) | 1:A:6:VAL:HG22 | 1:A:11:MET:HB3  | 8        | 1.88          |
| (1,1168) | 1:A:6:VAL:HG23 | 1:A:11:MET:HB2  | 8        | 1.88          |
| (1,1168) | 1:A:6:VAL:HG23 | 1:A:11:MET:HB3  | 8        | 1.88          |
| (2,268)  | 1:A:134:GLY:H  | 1:A:130:GLN:H   | 5        | 1.87          |
| (1,695)  | 1:A:62:ASN:H   | 1:A:65:LYS:H    | 2        | 1.87          |
| (1,2314) | 1:A:6:VAL:HG21 | 1:A:11:MET:HA   | 7        | 1.87          |
| (1,2314) | 1:A:6:VAL:HG22 | 1:A:11:MET:HA   | 7        | 1.87          |
| (1,2314) | 1:A:6:VAL:HG23 | 1:A:11:MET:HA   | 7        | 1.87          |
| (1,2253) | 1:A:79:MET:HE1 | 1:A:43:LEU:HD21 | 3        | 1.86          |
| (1,2253) | 1:A:79:MET:HE1 | 1:A:43:LEU:HD22 | 3        | 1.86          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,2253) | 1:A:79:MET:HE1 | 1:A:43:LEU:HD23 | 3        | 1.86          |
| (1,2253) | 1:A:79:MET:HE2 | 1:A:43:LEU:HD21 | 3        | 1.86          |
| (1,2253) | 1:A:79:MET:HE2 | 1:A:43:LEU:HD22 | 3        | 1.86          |
| (1,2253) | 1:A:79:MET:HE2 | 1:A:43:LEU:HD23 | 3        | 1.86          |
| (1,2253) | 1:A:79:MET:HE3 | 1:A:43:LEU:HD21 | 3        | 1.86          |
| (1,2253) | 1:A:79:MET:HE3 | 1:A:43:LEU:HD22 | 3        | 1.86          |
| (1,2253) | 1:A:79:MET:HE3 | 1:A:43:LEU:HD23 | 3        | 1.86          |
| (1,1168) | 1:A:6:VAL:HG21 | 1:A:11:MET:HB2  | 3        | 1.84          |
| (1,1168) | 1:A:6:VAL:HG21 | 1:A:11:MET:HB3  | 3        | 1.84          |
| (1,1168) | 1:A:6:VAL:HG22 | 1:A:11:MET:HB2  | 3        | 1.84          |
| (1,1168) | 1:A:6:VAL:HG22 | 1:A:11:MET:HB3  | 3        | 1.84          |
| (1,1168) | 1:A:6:VAL:HG23 | 1:A:11:MET:HB2  | 3        | 1.84          |
| (1,1168) | 1:A:6:VAL:HG23 | 1:A:11:MET:HB3  | 3        | 1.84          |
| (1,2623) | 1:A:56:TYR:HB3 | 1:A:44:ILE:HG12 | 1        | 1.82          |
| (1,695)  | 1:A:62:ASN:H   | 1:A:65:LYS:H    | 9        | 1.8           |
| (1,1168) | 1:A:6:VAL:HG21 | 1:A:11:MET:HB2  | 11       | 1.78          |
| (1,1168) | 1:A:6:VAL:HG21 | 1:A:11:MET:HB3  | 11       | 1.78          |
| (1,1168) | 1:A:6:VAL:HG22 | 1:A:11:MET:HB2  | 11       | 1.78          |
| (1,1168) | 1:A:6:VAL:HG22 | 1:A:11:MET:HB3  | 11       | 1.78          |
| (1,1168) | 1:A:6:VAL:HG23 | 1:A:11:MET:HB2  | 11       | 1.78          |
| (1,1168) | 1:A:6:VAL:HG23 | 1:A:11:MET:HB3  | 11       | 1.78          |
| (1,2623) | 1:A:56:TYR:HB3 | 1:A:44:ILE:HG12 | 7        | 1.77          |
| (1,1021) | 1:A:6:VAL:HG11 | 1:A:80:LYS:HG3  | 7        | 1.77          |
| (1,1021) | 1:A:6:VAL:HG12 | 1:A:80:LYS:HG3  | 7        | 1.77          |
| (1,1021) | 1:A:6:VAL:HG13 | 1:A:80:LYS:HG3  | 7        | 1.77          |
| (1,2623) | 1:A:56:TYR:HB3 | 1:A:44:ILE:HG12 | 12       | 1.76          |
| (1,2253) | 1:A:79:MET:HE1 | 1:A:43:LEU:HD21 | 10       | 1.76          |
| (1,2253) | 1:A:79:MET:HE1 | 1:A:43:LEU:HD22 | 10       | 1.76          |
| (1,2253) | 1:A:79:MET:HE1 | 1:A:43:LEU:HD23 | 10       | 1.76          |
| (1,2253) | 1:A:79:MET:HE2 | 1:A:43:LEU:HD21 | 10       | 1.76          |
| (1,2253) | 1:A:79:MET:HE2 | 1:A:43:LEU:HD22 | 10       | 1.76          |
| (1,2253) | 1:A:79:MET:HE2 | 1:A:43:LEU:HD23 | 10       | 1.76          |
| (1,2253) | 1:A:79:MET:HE3 | 1:A:43:LEU:HD21 | 10       | 1.76          |
| (1,2253) | 1:A:79:MET:HE3 | 1:A:43:LEU:HD22 | 10       | 1.76          |
| (1,2253) | 1:A:79:MET:HE3 | 1:A:43:LEU:HD23 | 10       | 1.76          |
| (1,1724) | 1:A:56:TYR:HE1 | 1:A:38:LEU:HD21 | 12       | 1.76          |
| (1,1724) | 1:A:56:TYR:HE1 | 1:A:38:LEU:HD22 | 12       | 1.76          |
| (1,1724) | 1:A:56:TYR:HE1 | 1:A:38:LEU:HD23 | 12       | 1.76          |
| (1,1724) | 1:A:56:TYR:HE2 | 1:A:38:LEU:HD21 | 12       | 1.76          |
| (1,1724) | 1:A:56:TYR:HE2 | 1:A:38:LEU:HD22 | 12       | 1.76          |
| (1,1724) | 1:A:56:TYR:HE2 | 1:A:38:LEU:HD23 | 12       | 1.76          |
| (1,2623) | 1:A:56:TYR:HB3 | 1:A:44:ILE:HG12 | 10       | 1.73          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2393) | 1:A:6:VAL:HG11   | 1:A:80:LYS:HD3  | 5        | 1.72          |
| (1,2393) | 1:A:6:VAL:HG12   | 1:A:80:LYS:HD3  | 5        | 1.72          |
| (1,2393) | 1:A:6:VAL:HG13   | 1:A:80:LYS:HD3  | 5        | 1.72          |
| (1,1168) | 1:A:6:VAL:HG21   | 1:A:11:MET:HB2  | 1        | 1.72          |
| (1,1168) | 1:A:6:VAL:HG21   | 1:A:11:MET:HB3  | 1        | 1.72          |
| (1,1168) | 1:A:6:VAL:HG22   | 1:A:11:MET:HB2  | 1        | 1.72          |
| (1,1168) | 1:A:6:VAL:HG22   | 1:A:11:MET:HB3  | 1        | 1.72          |
| (1,1168) | 1:A:6:VAL:HG23   | 1:A:11:MET:HB2  | 1        | 1.72          |
| (1,1168) | 1:A:6:VAL:HG23   | 1:A:11:MET:HB3  | 1        | 1.72          |
| (1,947)  | 1:A:6:VAL:HG11   | 1:A:80:LYS:HD3  | 5        | 1.71          |
| (1,947)  | 1:A:6:VAL:HG12   | 1:A:80:LYS:HD3  | 5        | 1.71          |
| (1,947)  | 1:A:6:VAL:HG13   | 1:A:80:LYS:HD3  | 5        | 1.71          |
| (1,695)  | 1:A:62:ASN:H     | 1:A:65:LYS:H    | 3        | 1.71          |
| (1,2623) | 1:A:56:TYR:HB3   | 1:A:44:ILE:HG12 | 11       | 1.7           |
| (2,335)  | 1:A:71:SER:HB3   | 1:A:28:ILE:HG12 | 11       | 1.68          |
| (2,268)  | 1:A:134:GLY:H    | 1:A:130:GLN:H   | 12       | 1.68          |
| (1,56)   | 1:A:52:GLU:HA    | 1:A:50:GLY:H    | 10       | 1.68          |
| (1,2118) | 1:A:89:PRO:HA    | 1:A:92:LEU:HB2  | 7        | 1.65          |
| (1,1631) | 1:A:109:THR:HB   | 1:A:108:GLU:HG3 | 2        | 1.65          |
| (1,1631) | 1:A:109:THR:HB   | 1:A:108:GLU:HG3 | 4        | 1.62          |
| (1,1631) | 1:A:109:THR:HB   | 1:A:108:GLU:HG3 | 5        | 1.62          |
| (1,2623) | 1:A:56:TYR:HB3   | 1:A:44:ILE:HG12 | 4        | 1.6           |
| (1,2118) | 1:A:89:PRO:HA    | 1:A:92:LEU:HB2  | 2        | 1.6           |
| (1,1872) | 1:A:65:LYS:HE3   | 1:A:64:THR:HG21 | 5        | 1.6           |
| (1,1872) | 1:A:65:LYS:HE3   | 1:A:64:THR:HG22 | 5        | 1.6           |
| (1,1872) | 1:A:65:LYS:HE3   | 1:A:64:THR:HG23 | 5        | 1.6           |
| (1,1631) | 1:A:109:THR:HB   | 1:A:108:GLU:HG3 | 10       | 1.6           |
| (1,1168) | 1:A:6:VAL:HG21   | 1:A:11:MET:HB2  | 7        | 1.58          |
| (1,1168) | 1:A:6:VAL:HG21   | 1:A:11:MET:HB3  | 7        | 1.58          |
| (1,1168) | 1:A:6:VAL:HG22   | 1:A:11:MET:HB2  | 7        | 1.58          |
| (1,1168) | 1:A:6:VAL:HG22   | 1:A:11:MET:HB3  | 7        | 1.58          |
| (1,1168) | 1:A:6:VAL:HG23   | 1:A:11:MET:HB2  | 7        | 1.58          |
| (1,1168) | 1:A:6:VAL:HG23   | 1:A:11:MET:HB3  | 7        | 1.58          |
| (1,695)  | 1:A:62:ASN:H     | 1:A:65:LYS:H    | 11       | 1.56          |
| (1,2573) | 1:A:109:THR:HG21 | 1:A:113:LYS:HG2 | 8        | 1.56          |
| (1,2573) | 1:A:109:THR:HG22 | 1:A:113:LYS:HG2 | 8        | 1.56          |
| (1,2573) | 1:A:109:THR:HG23 | 1:A:113:LYS:HG2 | 8        | 1.56          |
| (1,2083) | 1:A:89:PRO:HA    | 1:A:92:LEU:HD21 | 11       | 1.56          |
| (1,2083) | 1:A:89:PRO:HA    | 1:A:92:LEU:HD22 | 11       | 1.56          |
| (1,2083) | 1:A:89:PRO:HA    | 1:A:92:LEU:HD23 | 11       | 1.56          |
| (1,1274) | 1:A:6:VAL:HG21   | 1:A:11:MET:HB2  | 5        | 1.56          |
| (1,1274) | 1:A:6:VAL:HG21   | 1:A:11:MET:HB3  | 5        | 1.56          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1274) | 1:A:6:VAL:HG22   | 1:A:11:MET:HB2  | 5        | 1.56          |
| (1,1274) | 1:A:6:VAL:HG22   | 1:A:11:MET:HB3  | 5        | 1.56          |
| (1,1274) | 1:A:6:VAL:HG23   | 1:A:11:MET:HB2  | 5        | 1.56          |
| (1,1274) | 1:A:6:VAL:HG23   | 1:A:11:MET:HB3  | 5        | 1.56          |
| (2,335)  | 1:A:71:SER:HB3   | 1:A:28:ILE:HG12 | 2        | 1.54          |
| (2,313)  | 1:A:41:MET:HG3   | 1:A:43:LEU:HD21 | 3        | 1.54          |
| (2,313)  | 1:A:41:MET:HG3   | 1:A:43:LEU:HD22 | 3        | 1.54          |
| (2,313)  | 1:A:41:MET:HG3   | 1:A:43:LEU:HD23 | 3        | 1.54          |
| (1,1274) | 1:A:6:VAL:HG21   | 1:A:11:MET:HB2  | 6        | 1.54          |
| (1,1274) | 1:A:6:VAL:HG21   | 1:A:11:MET:HB3  | 6        | 1.54          |
| (1,1274) | 1:A:6:VAL:HG22   | 1:A:11:MET:HB2  | 6        | 1.54          |
| (1,1274) | 1:A:6:VAL:HG22   | 1:A:11:MET:HB3  | 6        | 1.54          |
| (1,1274) | 1:A:6:VAL:HG23   | 1:A:11:MET:HB2  | 6        | 1.54          |
| (1,1274) | 1:A:6:VAL:HG23   | 1:A:11:MET:HB3  | 6        | 1.54          |
| (2,35)   | 1:A:29:LEU:H     | 1:A:33:GLU:H    | 11       | 1.52          |
| (1,1045) | 1:A:41:MET:HB3   | 1:A:43:LEU:HD21 | 3        | 1.52          |
| (1,1045) | 1:A:41:MET:HB3   | 1:A:43:LEU:HD22 | 3        | 1.52          |
| (1,1045) | 1:A:41:MET:HB3   | 1:A:43:LEU:HD23 | 3        | 1.52          |
| (1,1631) | 1:A:109:THR:HB   | 1:A:108:GLU:HG3 | 3        | 1.51          |
| (1,1274) | 1:A:6:VAL:HG21   | 1:A:11:MET:HB2  | 8        | 1.51          |
| (1,1274) | 1:A:6:VAL:HG21   | 1:A:11:MET:HB3  | 8        | 1.51          |
| (1,1274) | 1:A:6:VAL:HG22   | 1:A:11:MET:HB2  | 8        | 1.51          |
| (1,1274) | 1:A:6:VAL:HG22   | 1:A:11:MET:HB3  | 8        | 1.51          |
| (1,1274) | 1:A:6:VAL:HG23   | 1:A:11:MET:HB2  | 8        | 1.51          |
| (1,1274) | 1:A:6:VAL:HG23   | 1:A:11:MET:HB3  | 8        | 1.51          |
| (1,1631) | 1:A:109:THR:HB   | 1:A:108:GLU:HG3 | 9        | 1.49          |
| (1,2253) | 1:A:79:MET:HE1   | 1:A:43:LEU:HD21 | 7        | 1.48          |
| (1,2253) | 1:A:79:MET:HE1   | 1:A:43:LEU:HD22 | 7        | 1.48          |
| (1,2253) | 1:A:79:MET:HE1   | 1:A:43:LEU:HD23 | 7        | 1.48          |
| (1,2253) | 1:A:79:MET:HE2   | 1:A:43:LEU:HD21 | 7        | 1.48          |
| (1,2253) | 1:A:79:MET:HE2   | 1:A:43:LEU:HD22 | 7        | 1.48          |
| (1,2253) | 1:A:79:MET:HE2   | 1:A:43:LEU:HD23 | 7        | 1.48          |
| (1,2253) | 1:A:79:MET:HE3   | 1:A:43:LEU:HD21 | 7        | 1.48          |
| (1,2253) | 1:A:79:MET:HE3   | 1:A:43:LEU:HD22 | 7        | 1.48          |
| (1,2253) | 1:A:79:MET:HE3   | 1:A:43:LEU:HD23 | 7        | 1.48          |
| (1,1812) | 1:A:41:MET:HB3   | 1:A:43:LEU:HD21 | 3        | 1.48          |
| (1,1812) | 1:A:41:MET:HB3   | 1:A:43:LEU:HD22 | 3        | 1.48          |
| (1,1812) | 1:A:41:MET:HB3   | 1:A:43:LEU:HD23 | 3        | 1.48          |
| (1,1387) | 1:A:109:THR:HG21 | 1:A:113:LYS:HE3 | 1        | 1.48          |
| (1,1387) | 1:A:109:THR:HG22 | 1:A:113:LYS:HE3 | 1        | 1.48          |
| (1,1387) | 1:A:109:THR:HG23 | 1:A:113:LYS:HE3 | 1        | 1.48          |
| (1,1274) | 1:A:6:VAL:HG21   | 1:A:11:MET:HB2  | 3        | 1.47          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1274) | 1:A:6:VAL:HG21  | 1:A:11:MET:HB3  | 3        | 1.47          |
| (1,1274) | 1:A:6:VAL:HG22  | 1:A:11:MET:HB2  | 3        | 1.47          |
| (1,1274) | 1:A:6:VAL:HG22  | 1:A:11:MET:HB3  | 3        | 1.47          |
| (1,1274) | 1:A:6:VAL:HG23  | 1:A:11:MET:HB2  | 3        | 1.47          |
| (1,1274) | 1:A:6:VAL:HG23  | 1:A:11:MET:HB3  | 3        | 1.47          |
| (1,2623) | 1:A:56:TYR:HB3  | 1:A:44:ILE:HG12 | 5        | 1.45          |
| (1,2124) | 1:A:38:LEU:HD11 | 1:A:43:LEU:HD21 | 1        | 1.45          |
| (1,2124) | 1:A:38:LEU:HD11 | 1:A:43:LEU:HD22 | 1        | 1.45          |
| (1,2124) | 1:A:38:LEU:HD11 | 1:A:43:LEU:HD23 | 1        | 1.45          |
| (1,2124) | 1:A:38:LEU:HD12 | 1:A:43:LEU:HD21 | 1        | 1.45          |
| (1,2124) | 1:A:38:LEU:HD12 | 1:A:43:LEU:HD22 | 1        | 1.45          |
| (1,2124) | 1:A:38:LEU:HD12 | 1:A:43:LEU:HD23 | 1        | 1.45          |
| (1,2124) | 1:A:38:LEU:HD13 | 1:A:43:LEU:HD21 | 1        | 1.45          |
| (1,2124) | 1:A:38:LEU:HD13 | 1:A:43:LEU:HD22 | 1        | 1.45          |
| (1,2124) | 1:A:38:LEU:HD13 | 1:A:43:LEU:HD23 | 1        | 1.45          |
| (1,2314) | 1:A:6:VAL:HG21  | 1:A:11:MET:HA   | 2        | 1.44          |
| (1,2314) | 1:A:6:VAL:HG22  | 1:A:11:MET:HA   | 2        | 1.44          |
| (1,2314) | 1:A:6:VAL:HG23  | 1:A:11:MET:HA   | 2        | 1.44          |
| (1,835)  | 1:A:78:TYR:HB2  | 1:A:75:TYR:HD1  | 3        | 1.43          |
| (1,835)  | 1:A:78:TYR:HB2  | 1:A:75:TYR:HD2  | 3        | 1.43          |
| (1,2124) | 1:A:38:LEU:HD11 | 1:A:43:LEU:HD21 | 2        | 1.43          |
| (1,2124) | 1:A:38:LEU:HD11 | 1:A:43:LEU:HD22 | 2        | 1.43          |
| (1,2124) | 1:A:38:LEU:HD11 | 1:A:43:LEU:HD23 | 2        | 1.43          |
| (1,2124) | 1:A:38:LEU:HD12 | 1:A:43:LEU:HD21 | 2        | 1.43          |
| (1,2124) | 1:A:38:LEU:HD12 | 1:A:43:LEU:HD22 | 2        | 1.43          |
| (1,2124) | 1:A:38:LEU:HD12 | 1:A:43:LEU:HD23 | 2        | 1.43          |
| (1,2124) | 1:A:38:LEU:HD13 | 1:A:43:LEU:HD21 | 2        | 1.43          |
| (1,2124) | 1:A:38:LEU:HD13 | 1:A:43:LEU:HD22 | 2        | 1.43          |
| (1,2124) | 1:A:38:LEU:HD13 | 1:A:43:LEU:HD23 | 2        | 1.43          |
| (1,1872) | 1:A:65:LYS:HE3  | 1:A:64:THR:HG21 | 8        | 1.43          |
| (1,1872) | 1:A:65:LYS:HE3  | 1:A:64:THR:HG22 | 8        | 1.43          |
| (1,1872) | 1:A:65:LYS:HE3  | 1:A:64:THR:HG23 | 8        | 1.43          |
| (1,1872) | 1:A:65:LYS:HE3  | 1:A:64:THR:HG21 | 2        | 1.42          |
| (1,1872) | 1:A:65:LYS:HE3  | 1:A:64:THR:HG22 | 2        | 1.42          |
| (1,1872) | 1:A:65:LYS:HE3  | 1:A:64:THR:HG23 | 2        | 1.42          |
| (1,1510) | 1:A:78:TYR:HB2  | 1:A:79:MET:HE1  | 3        | 1.42          |
| (1,1510) | 1:A:78:TYR:HB2  | 1:A:79:MET:HE2  | 3        | 1.42          |
| (1,1510) | 1:A:78:TYR:HB2  | 1:A:79:MET:HE3  | 3        | 1.42          |
| (1,1447) | 1:A:89:PRO:HA   | 1:A:92:LEU:HD21 | 11       | 1.42          |
| (1,1447) | 1:A:89:PRO:HA   | 1:A:92:LEU:HD22 | 11       | 1.42          |
| (1,1447) | 1:A:89:PRO:HA   | 1:A:92:LEU:HD23 | 11       | 1.42          |
| (1,835)  | 1:A:78:TYR:HB2  | 1:A:75:TYR:HD1  | 10       | 1.41          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,835)  | 1:A:78:TYR:HB2  | 1:A:75:TYR:HD2  | 10       | 1.41          |
| (1,1872) | 1:A:65:LYS:HE3  | 1:A:64:THR:HG21 | 1        | 1.41          |
| (1,1872) | 1:A:65:LYS:HE3  | 1:A:64:THR:HG22 | 1        | 1.41          |
| (1,1872) | 1:A:65:LYS:HE3  | 1:A:64:THR:HG23 | 1        | 1.41          |
| (1,1631) | 1:A:109:THR:HB  | 1:A:108:GLU:HG3 | 7        | 1.41          |
| (1,1274) | 1:A:6:VAL:HG21  | 1:A:11:MET:HB2  | 11       | 1.41          |
| (1,1274) | 1:A:6:VAL:HG21  | 1:A:11:MET:HB3  | 11       | 1.41          |
| (1,1274) | 1:A:6:VAL:HG22  | 1:A:11:MET:HB2  | 11       | 1.41          |
| (1,1274) | 1:A:6:VAL:HG22  | 1:A:11:MET:HB3  | 11       | 1.41          |
| (1,1274) | 1:A:6:VAL:HG23  | 1:A:11:MET:HB2  | 11       | 1.41          |
| (1,1274) | 1:A:6:VAL:HG23  | 1:A:11:MET:HB3  | 11       | 1.41          |
| (1,2118) | 1:A:89:PRO:HA   | 1:A:92:LEU:HB2  | 8        | 1.4           |
| (1,827)  | 1:A:6:VAL:HG21  | 1:A:10:GLN:HG3  | 3        | 1.38          |
| (1,827)  | 1:A:6:VAL:HG22  | 1:A:10:GLN:HG3  | 3        | 1.38          |
| (1,827)  | 1:A:6:VAL:HG23  | 1:A:10:GLN:HG3  | 3        | 1.38          |
| (1,2124) | 1:A:38:LEU:HD11 | 1:A:43:LEU:HD21 | 10       | 1.38          |
| (1,2124) | 1:A:38:LEU:HD11 | 1:A:43:LEU:HD22 | 10       | 1.38          |
| (1,2124) | 1:A:38:LEU:HD11 | 1:A:43:LEU:HD23 | 10       | 1.38          |
| (1,2124) | 1:A:38:LEU:HD12 | 1:A:43:LEU:HD21 | 10       | 1.38          |
| (1,2124) | 1:A:38:LEU:HD12 | 1:A:43:LEU:HD22 | 10       | 1.38          |
| (1,2124) | 1:A:38:LEU:HD12 | 1:A:43:LEU:HD23 | 10       | 1.38          |
| (1,2124) | 1:A:38:LEU:HD13 | 1:A:43:LEU:HD21 | 10       | 1.38          |
| (1,2124) | 1:A:38:LEU:HD13 | 1:A:43:LEU:HD22 | 10       | 1.38          |
| (1,2124) | 1:A:38:LEU:HD13 | 1:A:43:LEU:HD23 | 10       | 1.38          |
| (2,300)  | 1:A:109:THR:HB  | 1:A:112:GLN:HG3 | 10       | 1.37          |
| (1,2167) | 1:A:81:GLU:HA   | 1:A:84:ASP:HB3  | 8        | 1.37          |
| (1,1872) | 1:A:65:LYS:HE3  | 1:A:64:THR:HG21 | 11       | 1.37          |
| (1,1872) | 1:A:65:LYS:HE3  | 1:A:64:THR:HG22 | 11       | 1.37          |
| (1,1872) | 1:A:65:LYS:HE3  | 1:A:64:THR:HG23 | 11       | 1.37          |
| (1,1218) | 1:A:6:VAL:HG11  | 1:A:80:LYS:HG3  | 4        | 1.37          |
| (1,1218) | 1:A:6:VAL:HG12  | 1:A:80:LYS:HG3  | 4        | 1.37          |
| (1,1218) | 1:A:6:VAL:HG13  | 1:A:80:LYS:HG3  | 4        | 1.37          |
| (1,1168) | 1:A:6:VAL:HG21  | 1:A:11:MET:HB2  | 2        | 1.37          |
| (1,1168) | 1:A:6:VAL:HG21  | 1:A:11:MET:HB3  | 2        | 1.37          |
| (1,1168) | 1:A:6:VAL:HG22  | 1:A:11:MET:HB2  | 2        | 1.37          |
| (1,1168) | 1:A:6:VAL:HG22  | 1:A:11:MET:HB3  | 2        | 1.37          |
| (1,1168) | 1:A:6:VAL:HG23  | 1:A:11:MET:HB2  | 2        | 1.37          |
| (1,1168) | 1:A:6:VAL:HG23  | 1:A:11:MET:HB3  | 2        | 1.37          |
| (1,2167) | 1:A:81:GLU:HA   | 1:A:84:ASP:HB3  | 12       | 1.36          |
| (1,835)  | 1:A:78:TYR:HB2  | 1:A:75:TYR:HD1  | 2        | 1.35          |
| (1,835)  | 1:A:78:TYR:HB2  | 1:A:75:TYR:HD2  | 2        | 1.35          |
| (1,1274) | 1:A:6:VAL:HG21  | 1:A:11:MET:HB2  | 1        | 1.35          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1274) | 1:A:6:VAL:HG21   | 1:A:11:MET:HB3  | 1        | 1.35          |
| (1,1274) | 1:A:6:VAL:HG22   | 1:A:11:MET:HB2  | 1        | 1.35          |
| (1,1274) | 1:A:6:VAL:HG22   | 1:A:11:MET:HB3  | 1        | 1.35          |
| (1,1274) | 1:A:6:VAL:HG23   | 1:A:11:MET:HB2  | 1        | 1.35          |
| (1,1274) | 1:A:6:VAL:HG23   | 1:A:11:MET:HB3  | 1        | 1.35          |
| (2,18)   | 1:A:142:LYS:HB2  | 1:A:144:ASN:H   | 6        | 1.34          |
| (1,2326) | 1:A:74:ASN:HA    | 1:A:77:GLN:HG3  | 7        | 1.34          |
| (1,2326) | 1:A:74:ASN:HA    | 1:A:77:GLN:HG3  | 12       | 1.34          |
| (1,1565) | 1:A:38:LEU:HD11  | 1:A:43:LEU:HD21 | 1        | 1.34          |
| (1,1565) | 1:A:38:LEU:HD11  | 1:A:43:LEU:HD22 | 1        | 1.34          |
| (1,1565) | 1:A:38:LEU:HD11  | 1:A:43:LEU:HD23 | 1        | 1.34          |
| (1,1565) | 1:A:38:LEU:HD12  | 1:A:43:LEU:HD21 | 1        | 1.34          |
| (1,1565) | 1:A:38:LEU:HD12  | 1:A:43:LEU:HD22 | 1        | 1.34          |
| (1,1565) | 1:A:38:LEU:HD12  | 1:A:43:LEU:HD23 | 1        | 1.34          |
| (1,1565) | 1:A:38:LEU:HD13  | 1:A:43:LEU:HD21 | 1        | 1.34          |
| (1,1565) | 1:A:38:LEU:HD13  | 1:A:43:LEU:HD22 | 1        | 1.34          |
| (1,1565) | 1:A:38:LEU:HD13  | 1:A:43:LEU:HD23 | 1        | 1.34          |
| (2,268)  | 1:A:134:GLY:H    | 1:A:130:GLN:H   | 8        | 1.33          |
| (1,835)  | 1:A:78:TYR:HB2   | 1:A:75:TYR:HD1  | 6        | 1.32          |
| (1,835)  | 1:A:78:TYR:HB2   | 1:A:75:TYR:HD2  | 6        | 1.32          |
| (1,1565) | 1:A:38:LEU:HD11  | 1:A:43:LEU:HD21 | 2        | 1.32          |
| (1,1565) | 1:A:38:LEU:HD11  | 1:A:43:LEU:HD22 | 2        | 1.32          |
| (1,1565) | 1:A:38:LEU:HD11  | 1:A:43:LEU:HD23 | 2        | 1.32          |
| (1,1565) | 1:A:38:LEU:HD12  | 1:A:43:LEU:HD21 | 2        | 1.32          |
| (1,1565) | 1:A:38:LEU:HD12  | 1:A:43:LEU:HD22 | 2        | 1.32          |
| (1,1565) | 1:A:38:LEU:HD12  | 1:A:43:LEU:HD23 | 2        | 1.32          |
| (1,1565) | 1:A:38:LEU:HD13  | 1:A:43:LEU:HD21 | 2        | 1.32          |
| (1,1565) | 1:A:38:LEU:HD13  | 1:A:43:LEU:HD22 | 2        | 1.32          |
| (1,1565) | 1:A:38:LEU:HD13  | 1:A:43:LEU:HD23 | 2        | 1.32          |
| (1,1499) | 1:A:99:ILE:HG21  | 1:A:103:LYS:HE2 | 2        | 1.32          |
| (1,1499) | 1:A:99:ILE:HG22  | 1:A:103:LYS:HE2 | 2        | 1.32          |
| (1,1499) | 1:A:99:ILE:HG23  | 1:A:103:LYS:HE2 | 2        | 1.32          |
| (1,2573) | 1:A:109:THR:HG21 | 1:A:113:LYS:HG2 | 10       | 1.31          |
| (1,2573) | 1:A:109:THR:HG22 | 1:A:113:LYS:HG2 | 10       | 1.31          |
| (1,2573) | 1:A:109:THR:HG23 | 1:A:113:LYS:HG2 | 10       | 1.31          |
| (1,835)  | 1:A:78:TYR:HB2   | 1:A:75:TYR:HD1  | 1        | 1.3           |
| (1,835)  | 1:A:78:TYR:HB2   | 1:A:75:TYR:HD2  | 1        | 1.3           |
| (1,1387) | 1:A:109:THR:HG21 | 1:A:113:LYS:HE3 | 6        | 1.29          |
| (1,1387) | 1:A:109:THR:HG22 | 1:A:113:LYS:HE3 | 6        | 1.29          |
| (1,1387) | 1:A:109:THR:HG23 | 1:A:113:LYS:HE3 | 6        | 1.29          |
| (1,835)  | 1:A:78:TYR:HB2   | 1:A:75:TYR:HD1  | 4        | 1.28          |
| (1,835)  | 1:A:78:TYR:HB2   | 1:A:75:TYR:HD2  | 4        | 1.28          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,835)  | 1:A:78:TYR:HB2  | 1:A:75:TYR:HD1  | 7        | 1.28          |
| (1,835)  | 1:A:78:TYR:HB2  | 1:A:75:TYR:HD2  | 7        | 1.28          |
| (1,2253) | 1:A:79:MET:HE1  | 1:A:43:LEU:HD21 | 4        | 1.28          |
| (1,2253) | 1:A:79:MET:HE1  | 1:A:43:LEU:HD22 | 4        | 1.28          |
| (1,2253) | 1:A:79:MET:HE1  | 1:A:43:LEU:HD23 | 4        | 1.28          |
| (1,2253) | 1:A:79:MET:HE2  | 1:A:43:LEU:HD21 | 4        | 1.28          |
| (1,2253) | 1:A:79:MET:HE2  | 1:A:43:LEU:HD22 | 4        | 1.28          |
| (1,2253) | 1:A:79:MET:HE2  | 1:A:43:LEU:HD23 | 4        | 1.28          |
| (1,2253) | 1:A:79:MET:HE3  | 1:A:43:LEU:HD21 | 4        | 1.28          |
| (1,2253) | 1:A:79:MET:HE3  | 1:A:43:LEU:HD22 | 4        | 1.28          |
| (1,2253) | 1:A:79:MET:HE3  | 1:A:43:LEU:HD23 | 4        | 1.28          |
| (2,359)  | 1:A:109:THR:HA  | 1:A:113:LYS:HD3 | 10       | 1.27          |
| (2,358)  | 1:A:41:MET:HG2  | 1:A:43:LEU:HD21 | 3        | 1.27          |
| (2,358)  | 1:A:41:MET:HG2  | 1:A:43:LEU:HD22 | 3        | 1.27          |
| (2,358)  | 1:A:41:MET:HG2  | 1:A:43:LEU:HD23 | 3        | 1.27          |
| (1,1565) | 1:A:38:LEU:HD11 | 1:A:43:LEU:HD21 | 10       | 1.27          |
| (1,1565) | 1:A:38:LEU:HD11 | 1:A:43:LEU:HD22 | 10       | 1.27          |
| (1,1565) | 1:A:38:LEU:HD11 | 1:A:43:LEU:HD23 | 10       | 1.27          |
| (1,1565) | 1:A:38:LEU:HD12 | 1:A:43:LEU:HD21 | 10       | 1.27          |
| (1,1565) | 1:A:38:LEU:HD12 | 1:A:43:LEU:HD22 | 10       | 1.27          |
| (1,1565) | 1:A:38:LEU:HD12 | 1:A:43:LEU:HD23 | 10       | 1.27          |
| (1,1565) | 1:A:38:LEU:HD13 | 1:A:43:LEU:HD21 | 10       | 1.27          |
| (1,1565) | 1:A:38:LEU:HD13 | 1:A:43:LEU:HD22 | 10       | 1.27          |
| (1,1565) | 1:A:38:LEU:HD13 | 1:A:43:LEU:HD23 | 10       | 1.27          |
| (2,268)  | 1:A:134:GLY:H   | 1:A:130:GLN:H   | 11       | 1.26          |
| (1,1900) | 1:A:41:MET:HE1  | 1:A:43:LEU:HD21 | 4        | 1.26          |
| (1,1900) | 1:A:41:MET:HE1  | 1:A:43:LEU:HD22 | 4        | 1.26          |
| (1,1900) | 1:A:41:MET:HE1  | 1:A:43:LEU:HD23 | 4        | 1.26          |
| (1,1900) | 1:A:41:MET:HE2  | 1:A:43:LEU:HD21 | 4        | 1.26          |
| (1,1900) | 1:A:41:MET:HE2  | 1:A:43:LEU:HD22 | 4        | 1.26          |
| (1,1900) | 1:A:41:MET:HE2  | 1:A:43:LEU:HD23 | 4        | 1.26          |
| (1,1900) | 1:A:41:MET:HE3  | 1:A:43:LEU:HD21 | 4        | 1.26          |
| (1,1900) | 1:A:41:MET:HE3  | 1:A:43:LEU:HD22 | 4        | 1.26          |
| (1,1900) | 1:A:41:MET:HE3  | 1:A:43:LEU:HD23 | 4        | 1.26          |
| (1,1081) | 1:A:6:VAL:HG21  | 1:A:11:MET:HG2  | 1        | 1.26          |
| (1,1081) | 1:A:6:VAL:HG22  | 1:A:11:MET:HG2  | 1        | 1.26          |
| (1,1081) | 1:A:6:VAL:HG23  | 1:A:11:MET:HG2  | 1        | 1.26          |
| (1,835)  | 1:A:78:TYR:HB2  | 1:A:75:TYR:HD1  | 5        | 1.24          |
| (1,835)  | 1:A:78:TYR:HB2  | 1:A:75:TYR:HD2  | 5        | 1.24          |
| (1,827)  | 1:A:6:VAL:HG21  | 1:A:10:GLN:HG3  | 7        | 1.24          |
| (1,827)  | 1:A:6:VAL:HG22  | 1:A:10:GLN:HG3  | 7        | 1.24          |
| (1,827)  | 1:A:6:VAL:HG23  | 1:A:10:GLN:HG3  | 7        | 1.24          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2642) | 1:A:81:GLU:HA    | 1:A:84:ASP:HB3  | 8        | 1.24          |
| (1,2564) | 1:A:89:PRO:HA    | 1:A:92:LEU:HB2  | 7        | 1.24          |
| (1,1021) | 1:A:6:VAL:HG11   | 1:A:80:LYS:HG3  | 4        | 1.24          |
| (1,1021) | 1:A:6:VAL:HG12   | 1:A:80:LYS:HG3  | 4        | 1.24          |
| (1,1021) | 1:A:6:VAL:HG13   | 1:A:80:LYS:HG3  | 4        | 1.24          |
| (1,2642) | 1:A:81:GLU:HA    | 1:A:84:ASP:HB3  | 12       | 1.23          |
| (1,2273) | 1:A:109:THR:HG21 | 1:A:108:GLU:HG3 | 3        | 1.23          |
| (1,2273) | 1:A:109:THR:HG22 | 1:A:108:GLU:HG3 | 3        | 1.23          |
| (1,2273) | 1:A:109:THR:HG23 | 1:A:108:GLU:HG3 | 3        | 1.23          |
| (1,2273) | 1:A:109:THR:HG21 | 1:A:108:GLU:HG3 | 7        | 1.23          |
| (1,2273) | 1:A:109:THR:HG22 | 1:A:108:GLU:HG3 | 7        | 1.23          |
| (1,2273) | 1:A:109:THR:HG23 | 1:A:108:GLU:HG3 | 7        | 1.23          |
| (1,835)  | 1:A:78:TYR:HB2   | 1:A:75:TYR:HD1  | 8        | 1.22          |
| (1,835)  | 1:A:78:TYR:HB2   | 1:A:75:TYR:HD2  | 8        | 1.22          |
| (1,835)  | 1:A:78:TYR:HB2   | 1:A:75:TYR:HD1  | 12       | 1.22          |
| (1,835)  | 1:A:78:TYR:HB2   | 1:A:75:TYR:HD2  | 12       | 1.22          |
| (1,56)   | 1:A:52:GLU:HA    | 1:A:50:GLY:H    | 12       | 1.21          |
| (1,2273) | 1:A:109:THR:HG21 | 1:A:108:GLU:HG3 | 9        | 1.21          |
| (1,2273) | 1:A:109:THR:HG22 | 1:A:108:GLU:HG3 | 9        | 1.21          |
| (1,2273) | 1:A:109:THR:HG23 | 1:A:108:GLU:HG3 | 9        | 1.21          |
| (1,1499) | 1:A:99:ILE:HG21  | 1:A:103:LYS:HE2 | 4        | 1.21          |
| (1,1499) | 1:A:99:ILE:HG22  | 1:A:103:LYS:HE2 | 4        | 1.21          |
| (1,1499) | 1:A:99:ILE:HG23  | 1:A:103:LYS:HE2 | 4        | 1.21          |
| (1,1274) | 1:A:6:VAL:HG21   | 1:A:11:MET:HB2  | 7        | 1.21          |
| (1,1274) | 1:A:6:VAL:HG21   | 1:A:11:MET:HB3  | 7        | 1.21          |
| (1,1274) | 1:A:6:VAL:HG22   | 1:A:11:MET:HB2  | 7        | 1.21          |
| (1,1274) | 1:A:6:VAL:HG22   | 1:A:11:MET:HB3  | 7        | 1.21          |
| (1,1274) | 1:A:6:VAL:HG23   | 1:A:11:MET:HB2  | 7        | 1.21          |
| (1,1274) | 1:A:6:VAL:HG23   | 1:A:11:MET:HB3  | 7        | 1.21          |
| (1,2273) | 1:A:109:THR:HG21 | 1:A:108:GLU:HG3 | 5        | 1.2           |
| (1,2273) | 1:A:109:THR:HG22 | 1:A:108:GLU:HG3 | 5        | 1.2           |
| (1,2273) | 1:A:109:THR:HG23 | 1:A:108:GLU:HG3 | 5        | 1.2           |
| (1,2124) | 1:A:38:LEU:HD11  | 1:A:43:LEU:HD21 | 4        | 1.2           |
| (1,2124) | 1:A:38:LEU:HD11  | 1:A:43:LEU:HD22 | 4        | 1.2           |
| (1,2124) | 1:A:38:LEU:HD11  | 1:A:43:LEU:HD23 | 4        | 1.2           |
| (1,2124) | 1:A:38:LEU:HD12  | 1:A:43:LEU:HD21 | 4        | 1.2           |
| (1,2124) | 1:A:38:LEU:HD12  | 1:A:43:LEU:HD22 | 4        | 1.2           |
| (1,2124) | 1:A:38:LEU:HD12  | 1:A:43:LEU:HD23 | 4        | 1.2           |
| (1,2124) | 1:A:38:LEU:HD13  | 1:A:43:LEU:HD21 | 4        | 1.2           |
| (1,2124) | 1:A:38:LEU:HD13  | 1:A:43:LEU:HD22 | 4        | 1.2           |
| (1,2124) | 1:A:38:LEU:HD13  | 1:A:43:LEU:HD23 | 4        | 1.2           |
| (1,2641) | 1:A:122:GLU:HB2  | 1:A:126:ALA:HB1 | 2        | 1.19          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2641) | 1:A:122:GLU:HB2  | 1:A:126:ALA:HB2 | 2        | 1.19          |
| (1,2641) | 1:A:122:GLU:HB2  | 1:A:126:ALA:HB3 | 2        | 1.19          |
| (1,2564) | 1:A:89:PRO:HA    | 1:A:92:LEU:HB2  | 2        | 1.19          |
| (1,2273) | 1:A:109:THR:HG21 | 1:A:108:GLU:HG3 | 2        | 1.19          |
| (1,2273) | 1:A:109:THR:HG22 | 1:A:108:GLU:HG3 | 2        | 1.19          |
| (1,2273) | 1:A:109:THR:HG23 | 1:A:108:GLU:HG3 | 2        | 1.19          |
| (1,1890) | 1:A:79:MET:HE1   | 1:A:38:LEU:HD11 | 6        | 1.18          |
| (1,1890) | 1:A:79:MET:HE1   | 1:A:38:LEU:HD12 | 6        | 1.18          |
| (1,1890) | 1:A:79:MET:HE1   | 1:A:38:LEU:HD13 | 6        | 1.18          |
| (1,1890) | 1:A:79:MET:HE2   | 1:A:38:LEU:HD11 | 6        | 1.18          |
| (1,1890) | 1:A:79:MET:HE2   | 1:A:38:LEU:HD12 | 6        | 1.18          |
| (1,1890) | 1:A:79:MET:HE2   | 1:A:38:LEU:HD13 | 6        | 1.18          |
| (1,1890) | 1:A:79:MET:HE3   | 1:A:38:LEU:HD11 | 6        | 1.18          |
| (1,1890) | 1:A:79:MET:HE3   | 1:A:38:LEU:HD12 | 6        | 1.18          |
| (1,1890) | 1:A:79:MET:HE3   | 1:A:38:LEU:HD13 | 6        | 1.18          |
| (1,2167) | 1:A:81:GLU:HA    | 1:A:84:ASP:HB3  | 2        | 1.17          |
| (1,1829) | 1:A:103:LYS:HE2  | 1:A:101:ALA:HB1 | 7        | 1.17          |
| (1,1829) | 1:A:103:LYS:HE2  | 1:A:101:ALA:HB2 | 7        | 1.17          |
| (1,1829) | 1:A:103:LYS:HE2  | 1:A:101:ALA:HB3 | 7        | 1.17          |
| (1,827)  | 1:A:6:VAL:HG21   | 1:A:10:GLN:HG3  | 1        | 1.16          |
| (1,827)  | 1:A:6:VAL:HG22   | 1:A:10:GLN:HG3  | 1        | 1.16          |
| (1,827)  | 1:A:6:VAL:HG23   | 1:A:10:GLN:HG3  | 1        | 1.16          |
| (1,827)  | 1:A:6:VAL:HG21   | 1:A:10:GLN:HG3  | 6        | 1.16          |
| (1,827)  | 1:A:6:VAL:HG22   | 1:A:10:GLN:HG3  | 6        | 1.16          |
| (1,827)  | 1:A:6:VAL:HG23   | 1:A:10:GLN:HG3  | 6        | 1.16          |
| (1,2573) | 1:A:109:THR:HG21 | 1:A:113:LYS:HG2 | 6        | 1.16          |
| (1,2573) | 1:A:109:THR:HG22 | 1:A:113:LYS:HG2 | 6        | 1.16          |
| (1,2573) | 1:A:109:THR:HG23 | 1:A:113:LYS:HG2 | 6        | 1.16          |
| (1,835)  | 1:A:78:TYR:HB2   | 1:A:75:TYR:HD1  | 11       | 1.15          |
| (1,835)  | 1:A:78:TYR:HB2   | 1:A:75:TYR:HD2  | 11       | 1.15          |
| (1,1890) | 1:A:79:MET:HE1   | 1:A:38:LEU:HD11 | 9        | 1.15          |
| (1,1890) | 1:A:79:MET:HE1   | 1:A:38:LEU:HD12 | 9        | 1.15          |
| (1,1890) | 1:A:79:MET:HE1   | 1:A:38:LEU:HD13 | 9        | 1.15          |
| (1,1890) | 1:A:79:MET:HE2   | 1:A:38:LEU:HD11 | 9        | 1.15          |
| (1,1890) | 1:A:79:MET:HE2   | 1:A:38:LEU:HD12 | 9        | 1.15          |
| (1,1890) | 1:A:79:MET:HE2   | 1:A:38:LEU:HD13 | 9        | 1.15          |
| (1,1890) | 1:A:79:MET:HE3   | 1:A:38:LEU:HD11 | 9        | 1.15          |
| (1,1890) | 1:A:79:MET:HE3   | 1:A:38:LEU:HD12 | 9        | 1.15          |
| (1,1890) | 1:A:79:MET:HE3   | 1:A:38:LEU:HD13 | 9        | 1.15          |
| (1,1890) | 1:A:79:MET:HE1   | 1:A:38:LEU:HD11 | 7        | 1.14          |
| (1,1890) | 1:A:79:MET:HE1   | 1:A:38:LEU:HD12 | 7        | 1.14          |
| (1,1890) | 1:A:79:MET:HE1   | 1:A:38:LEU:HD13 | 7        | 1.14          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1890) | 1:A:79:MET:HE2   | 1:A:38:LEU:HD11 | 7        | 1.14          |
| (1,1890) | 1:A:79:MET:HE2   | 1:A:38:LEU:HD12 | 7        | 1.14          |
| (1,1890) | 1:A:79:MET:HE2   | 1:A:38:LEU:HD13 | 7        | 1.14          |
| (1,1890) | 1:A:79:MET:HE3   | 1:A:38:LEU:HD11 | 7        | 1.14          |
| (1,1890) | 1:A:79:MET:HE3   | 1:A:38:LEU:HD12 | 7        | 1.14          |
| (1,1890) | 1:A:79:MET:HE3   | 1:A:38:LEU:HD13 | 7        | 1.14          |
| (1,1890) | 1:A:79:MET:HE1   | 1:A:38:LEU:HD11 | 12       | 1.13          |
| (1,1890) | 1:A:79:MET:HE1   | 1:A:38:LEU:HD12 | 12       | 1.13          |
| (1,1890) | 1:A:79:MET:HE1   | 1:A:38:LEU:HD13 | 12       | 1.13          |
| (1,1890) | 1:A:79:MET:HE2   | 1:A:38:LEU:HD11 | 12       | 1.13          |
| (1,1890) | 1:A:79:MET:HE2   | 1:A:38:LEU:HD12 | 12       | 1.13          |
| (1,1890) | 1:A:79:MET:HE2   | 1:A:38:LEU:HD13 | 12       | 1.13          |
| (1,1890) | 1:A:79:MET:HE3   | 1:A:38:LEU:HD11 | 12       | 1.13          |
| (1,1890) | 1:A:79:MET:HE3   | 1:A:38:LEU:HD12 | 12       | 1.13          |
| (1,1890) | 1:A:79:MET:HE3   | 1:A:38:LEU:HD13 | 12       | 1.13          |
| (1,1002) | 1:A:41:MET:HE1   | 1:A:17:SER:HB3  | 9        | 1.13          |
| (1,1002) | 1:A:41:MET:HE2   | 1:A:17:SER:HB3  | 9        | 1.13          |
| (1,1002) | 1:A:41:MET:HE3   | 1:A:17:SER:HB3  | 9        | 1.13          |
| (1,2573) | 1:A:109:THR:HG21 | 1:A:113:LYS:HG2 | 2        | 1.12          |
| (1,2573) | 1:A:109:THR:HG22 | 1:A:113:LYS:HG2 | 2        | 1.12          |
| (1,2573) | 1:A:109:THR:HG23 | 1:A:113:LYS:HG2 | 2        | 1.12          |
| (1,1890) | 1:A:79:MET:HE1   | 1:A:38:LEU:HD11 | 4        | 1.12          |
| (1,1890) | 1:A:79:MET:HE1   | 1:A:38:LEU:HD12 | 4        | 1.12          |
| (1,1890) | 1:A:79:MET:HE1   | 1:A:38:LEU:HD13 | 4        | 1.12          |
| (1,1890) | 1:A:79:MET:HE2   | 1:A:38:LEU:HD11 | 4        | 1.12          |
| (1,1890) | 1:A:79:MET:HE2   | 1:A:38:LEU:HD12 | 4        | 1.12          |
| (1,1890) | 1:A:79:MET:HE2   | 1:A:38:LEU:HD13 | 4        | 1.12          |
| (1,1890) | 1:A:79:MET:HE3   | 1:A:38:LEU:HD11 | 4        | 1.12          |
| (1,1890) | 1:A:79:MET:HE3   | 1:A:38:LEU:HD12 | 4        | 1.12          |
| (1,1890) | 1:A:79:MET:HE3   | 1:A:38:LEU:HD13 | 4        | 1.12          |
| (1,1510) | 1:A:78:TYR:HB2   | 1:A:79:MET:HE1  | 12       | 1.12          |
| (1,1510) | 1:A:78:TYR:HB2   | 1:A:79:MET:HE2  | 12       | 1.12          |
| (1,1510) | 1:A:78:TYR:HB2   | 1:A:79:MET:HE3  | 12       | 1.12          |
| (2,300)  | 1:A:109:THR:HB   | 1:A:112:GLN:HG3 | 8        | 1.11          |
| (1,1872) | 1:A:65:LYS:HE3   | 1:A:64:THR:HG21 | 9        | 1.11          |
| (1,1872) | 1:A:65:LYS:HE3   | 1:A:64:THR:HG22 | 9        | 1.11          |
| (1,1872) | 1:A:65:LYS:HE3   | 1:A:64:THR:HG23 | 9        | 1.11          |
| (1,2623) | 1:A:56:TYR:HB3   | 1:A:44:ILE:HG12 | 8        | 1.1           |
| (1,1149) | 1:A:82:LYS:HA    | 1:A:85:GLU:HG3  | 12       | 1.1           |
| (2,18)   | 1:A:142:LYS:HB2  | 1:A:144:ASN:H   | 3        | 1.09          |
| (1,827)  | 1:A:6:VAL:HG21   | 1:A:10:GLN:HG3  | 11       | 1.09          |
| (1,827)  | 1:A:6:VAL:HG22   | 1:A:10:GLN:HG3  | 11       | 1.09          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,827)  | 1:A:6:VAL:HG23   | 1:A:10:GLN:HG3  | 11       | 1.09          |
| (1,1890) | 1:A:79:MET:HE1   | 1:A:38:LEU:HD11 | 5        | 1.09          |
| (1,1890) | 1:A:79:MET:HE1   | 1:A:38:LEU:HD12 | 5        | 1.09          |
| (1,1890) | 1:A:79:MET:HE1   | 1:A:38:LEU:HD13 | 5        | 1.09          |
| (1,1890) | 1:A:79:MET:HE2   | 1:A:38:LEU:HD11 | 5        | 1.09          |
| (1,1890) | 1:A:79:MET:HE2   | 1:A:38:LEU:HD12 | 5        | 1.09          |
| (1,1890) | 1:A:79:MET:HE2   | 1:A:38:LEU:HD13 | 5        | 1.09          |
| (1,1890) | 1:A:79:MET:HE3   | 1:A:38:LEU:HD11 | 5        | 1.09          |
| (1,1890) | 1:A:79:MET:HE3   | 1:A:38:LEU:HD12 | 5        | 1.09          |
| (1,1890) | 1:A:79:MET:HE3   | 1:A:38:LEU:HD13 | 5        | 1.09          |
| (1,1565) | 1:A:38:LEU:HD11  | 1:A:43:LEU:HD21 | 4        | 1.09          |
| (1,1565) | 1:A:38:LEU:HD11  | 1:A:43:LEU:HD22 | 4        | 1.09          |
| (1,1565) | 1:A:38:LEU:HD11  | 1:A:43:LEU:HD23 | 4        | 1.09          |
| (1,1565) | 1:A:38:LEU:HD12  | 1:A:43:LEU:HD21 | 4        | 1.09          |
| (1,1565) | 1:A:38:LEU:HD12  | 1:A:43:LEU:HD22 | 4        | 1.09          |
| (1,1565) | 1:A:38:LEU:HD12  | 1:A:43:LEU:HD23 | 4        | 1.09          |
| (1,1565) | 1:A:38:LEU:HD13  | 1:A:43:LEU:HD21 | 4        | 1.09          |
| (1,1565) | 1:A:38:LEU:HD13  | 1:A:43:LEU:HD22 | 4        | 1.09          |
| (1,1565) | 1:A:38:LEU:HD13  | 1:A:43:LEU:HD23 | 4        | 1.09          |
| (2,335)  | 1:A:71:SER:HB3   | 1:A:28:ILE:HG12 | 12       | 1.08          |
| (2,268)  | 1:A:134:GLY:H    | 1:A:130:GLN:H   | 3        | 1.08          |
| (1,835)  | 1:A:78:TYR:HB2   | 1:A:75:TYR:HD1  | 9        | 1.08          |
| (1,835)  | 1:A:78:TYR:HB2   | 1:A:75:TYR:HD2  | 9        | 1.08          |
| (1,2273) | 1:A:109:THR:HG21 | 1:A:108:GLU:HG3 | 4        | 1.08          |
| (1,2273) | 1:A:109:THR:HG22 | 1:A:108:GLU:HG3 | 4        | 1.08          |
| (1,2273) | 1:A:109:THR:HG23 | 1:A:108:GLU:HG3 | 4        | 1.08          |
| (1,1145) | 1:A:6:VAL:HG21   | 1:A:11:MET:HA   | 5        | 1.08          |
| (1,1145) | 1:A:6:VAL:HG22   | 1:A:11:MET:HA   | 5        | 1.08          |
| (1,1145) | 1:A:6:VAL:HG23   | 1:A:11:MET:HA   | 5        | 1.08          |
| (1,2573) | 1:A:109:THR:HG21 | 1:A:113:LYS:HG2 | 11       | 1.07          |
| (1,2573) | 1:A:109:THR:HG22 | 1:A:113:LYS:HG2 | 11       | 1.07          |
| (1,2573) | 1:A:109:THR:HG23 | 1:A:113:LYS:HG2 | 11       | 1.07          |
| (1,2267) | 1:A:92:LEU:HD21  | 1:A:123:TYR:HE1 | 8        | 1.06          |
| (1,2267) | 1:A:92:LEU:HD21  | 1:A:123:TYR:HE2 | 8        | 1.06          |
| (1,2267) | 1:A:92:LEU:HD22  | 1:A:123:TYR:HE1 | 8        | 1.06          |
| (1,2267) | 1:A:92:LEU:HD22  | 1:A:123:TYR:HE2 | 8        | 1.06          |
| (1,2267) | 1:A:92:LEU:HD23  | 1:A:123:TYR:HE1 | 8        | 1.06          |
| (1,2267) | 1:A:92:LEU:HD23  | 1:A:123:TYR:HE2 | 8        | 1.06          |
| (1,1122) | 1:A:29:LEU:HD11  | 1:A:38:LEU:HD11 | 7        | 1.06          |
| (1,1122) | 1:A:29:LEU:HD11  | 1:A:38:LEU:HD12 | 7        | 1.06          |
| (1,1122) | 1:A:29:LEU:HD11  | 1:A:38:LEU:HD13 | 7        | 1.06          |
| (1,1122) | 1:A:29:LEU:HD12  | 1:A:38:LEU:HD11 | 7        | 1.06          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1122) | 1:A:29:LEU:HD12 | 1:A:38:LEU:HD12 | 7        | 1.06          |
| (1,1122) | 1:A:29:LEU:HD12 | 1:A:38:LEU:HD13 | 7        | 1.06          |
| (1,1122) | 1:A:29:LEU:HD13 | 1:A:38:LEU:HD11 | 7        | 1.06          |
| (1,1122) | 1:A:29:LEU:HD13 | 1:A:38:LEU:HD12 | 7        | 1.06          |
| (1,1122) | 1:A:29:LEU:HD13 | 1:A:38:LEU:HD13 | 7        | 1.06          |
| (1,1119) | 1:A:70:VAL:HG21 | 1:A:71:SER:HB3  | 12       | 1.06          |
| (1,1119) | 1:A:70:VAL:HG22 | 1:A:71:SER:HB3  | 12       | 1.06          |
| (1,1119) | 1:A:70:VAL:HG23 | 1:A:71:SER:HB3  | 12       | 1.06          |
| (1,813)  | 1:A:10:GLN:HB2  | 1:A:6:VAL:HG21  | 7        | 1.04          |
| (1,813)  | 1:A:10:GLN:HB2  | 1:A:6:VAL:HG22  | 7        | 1.04          |
| (1,813)  | 1:A:10:GLN:HB2  | 1:A:6:VAL:HG23  | 7        | 1.04          |
| (1,2642) | 1:A:81:GLU:HA   | 1:A:84:ASP:HB3  | 2        | 1.04          |
| (1,2001) | 1:A:52:GLU:HG2  | 1:A:51:GLY:HA3  | 1        | 1.04          |
| (1,1499) | 1:A:99:ILE:HG21 | 1:A:103:LYS:HE2 | 9        | 1.04          |
| (1,1499) | 1:A:99:ILE:HG22 | 1:A:103:LYS:HE2 | 9        | 1.04          |
| (1,1499) | 1:A:99:ILE:HG23 | 1:A:103:LYS:HE2 | 9        | 1.04          |
| (1,1122) | 1:A:29:LEU:HD11 | 1:A:38:LEU:HD11 | 12       | 1.04          |
| (1,1122) | 1:A:29:LEU:HD11 | 1:A:38:LEU:HD12 | 12       | 1.04          |
| (1,1122) | 1:A:29:LEU:HD11 | 1:A:38:LEU:HD13 | 12       | 1.04          |
| (1,1122) | 1:A:29:LEU:HD12 | 1:A:38:LEU:HD11 | 12       | 1.04          |
| (1,1122) | 1:A:29:LEU:HD12 | 1:A:38:LEU:HD12 | 12       | 1.04          |
| (1,1122) | 1:A:29:LEU:HD12 | 1:A:38:LEU:HD13 | 12       | 1.04          |
| (1,1122) | 1:A:29:LEU:HD13 | 1:A:38:LEU:HD11 | 12       | 1.04          |
| (1,1122) | 1:A:29:LEU:HD13 | 1:A:38:LEU:HD12 | 12       | 1.04          |
| (1,1122) | 1:A:29:LEU:HD13 | 1:A:38:LEU:HD13 | 12       | 1.04          |
| (1,695)  | 1:A:62:ASN:H    | 1:A:65:LYS:H    | 12       | 1.03          |
| (1,1122) | 1:A:29:LEU:HD11 | 1:A:38:LEU:HD11 | 8        | 1.03          |
| (1,1122) | 1:A:29:LEU:HD11 | 1:A:38:LEU:HD12 | 8        | 1.03          |
| (1,1122) | 1:A:29:LEU:HD11 | 1:A:38:LEU:HD13 | 8        | 1.03          |
| (1,1122) | 1:A:29:LEU:HD12 | 1:A:38:LEU:HD11 | 8        | 1.03          |
| (1,1122) | 1:A:29:LEU:HD12 | 1:A:38:LEU:HD12 | 8        | 1.03          |
| (1,1122) | 1:A:29:LEU:HD12 | 1:A:38:LEU:HD13 | 8        | 1.03          |
| (1,1122) | 1:A:29:LEU:HD13 | 1:A:38:LEU:HD11 | 8        | 1.03          |
| (1,1122) | 1:A:29:LEU:HD13 | 1:A:38:LEU:HD12 | 8        | 1.03          |
| (1,1122) | 1:A:29:LEU:HD13 | 1:A:38:LEU:HD13 | 8        | 1.03          |
| (1,1119) | 1:A:70:VAL:HG21 | 1:A:71:SER:HB3  | 6        | 1.03          |
| (1,1119) | 1:A:70:VAL:HG22 | 1:A:71:SER:HB3  | 6        | 1.03          |
| (1,1119) | 1:A:70:VAL:HG23 | 1:A:71:SER:HB3  | 6        | 1.03          |
| (1,813)  | 1:A:10:GLN:HB2  | 1:A:6:VAL:HG21  | 1        | 1.02          |
| (1,813)  | 1:A:10:GLN:HB2  | 1:A:6:VAL:HG22  | 1        | 1.02          |
| (1,813)  | 1:A:10:GLN:HB2  | 1:A:6:VAL:HG23  | 1        | 1.02          |
| (1,2641) | 1:A:122:GLU:HB2 | 1:A:126:ALA:HB1 | 7        | 1.02          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2641) | 1:A:122:GLU:HB2 | 1:A:126:ALA:HB2 | 7        | 1.02          |
| (1,2641) | 1:A:122:GLU:HB2 | 1:A:126:ALA:HB3 | 7        | 1.02          |
| (1,1016) | 1:A:6:VAL:HG21  | 1:A:11:MET:HG3  | 6        | 1.02          |
| (1,1016) | 1:A:6:VAL:HG22  | 1:A:11:MET:HG3  | 6        | 1.02          |
| (1,1016) | 1:A:6:VAL:HG23  | 1:A:11:MET:HG3  | 6        | 1.02          |
| (1,882)  | 1:A:80:LYS:HE3  | 1:A:6:VAL:HG11  | 8        | 1.01          |
| (1,882)  | 1:A:80:LYS:HE3  | 1:A:6:VAL:HG12  | 8        | 1.01          |
| (1,882)  | 1:A:80:LYS:HE3  | 1:A:6:VAL:HG13  | 8        | 1.01          |
| (1,2124) | 1:A:38:LEU:HD11 | 1:A:43:LEU:HD21 | 7        | 1.01          |
| (1,2124) | 1:A:38:LEU:HD11 | 1:A:43:LEU:HD22 | 7        | 1.01          |
| (1,2124) | 1:A:38:LEU:HD11 | 1:A:43:LEU:HD23 | 7        | 1.01          |
| (1,2124) | 1:A:38:LEU:HD12 | 1:A:43:LEU:HD21 | 7        | 1.01          |
| (1,2124) | 1:A:38:LEU:HD12 | 1:A:43:LEU:HD22 | 7        | 1.01          |
| (1,2124) | 1:A:38:LEU:HD12 | 1:A:43:LEU:HD23 | 7        | 1.01          |
| (1,2124) | 1:A:38:LEU:HD13 | 1:A:43:LEU:HD21 | 7        | 1.01          |
| (1,2124) | 1:A:38:LEU:HD13 | 1:A:43:LEU:HD22 | 7        | 1.01          |
| (1,2124) | 1:A:38:LEU:HD13 | 1:A:43:LEU:HD23 | 7        | 1.01          |
| (1,1900) | 1:A:41:MET:HE1  | 1:A:43:LEU:HD21 | 7        | 1.01          |
| (1,1900) | 1:A:41:MET:HE1  | 1:A:43:LEU:HD22 | 7        | 1.01          |
| (1,1900) | 1:A:41:MET:HE1  | 1:A:43:LEU:HD23 | 7        | 1.01          |
| (1,1900) | 1:A:41:MET:HE2  | 1:A:43:LEU:HD21 | 7        | 1.01          |
| (1,1900) | 1:A:41:MET:HE2  | 1:A:43:LEU:HD22 | 7        | 1.01          |
| (1,1900) | 1:A:41:MET:HE2  | 1:A:43:LEU:HD23 | 7        | 1.01          |
| (1,1900) | 1:A:41:MET:HE3  | 1:A:43:LEU:HD21 | 7        | 1.01          |
| (1,1900) | 1:A:41:MET:HE3  | 1:A:43:LEU:HD22 | 7        | 1.01          |
| (1,1900) | 1:A:41:MET:HE3  | 1:A:43:LEU:HD23 | 7        | 1.01          |
| (1,1829) | 1:A:103:LYS:HE2 | 1:A:101:ALA:HB1 | 1        | 1.01          |
| (1,1829) | 1:A:103:LYS:HE2 | 1:A:101:ALA:HB2 | 1        | 1.01          |
| (1,1829) | 1:A:103:LYS:HE2 | 1:A:101:ALA:HB3 | 1        | 1.01          |
| (1,1712) | 1:A:106:ILE:HA  | 1:A:103:LYS:HE3 | 8        | 1.01          |
| (1,882)  | 1:A:80:LYS:HE3  | 1:A:6:VAL:HG11  | 3        | 1.0           |
| (1,882)  | 1:A:80:LYS:HE3  | 1:A:6:VAL:HG12  | 3        | 1.0           |
| (1,882)  | 1:A:80:LYS:HE3  | 1:A:6:VAL:HG13  | 3        | 1.0           |
| (1,2393) | 1:A:6:VAL:HG11  | 1:A:80:LYS:HD3  | 2        | 1.0           |
| (1,2393) | 1:A:6:VAL:HG12  | 1:A:80:LYS:HD3  | 2        | 1.0           |
| (1,2393) | 1:A:6:VAL:HG13  | 1:A:80:LYS:HD3  | 2        | 1.0           |
| (1,1900) | 1:A:41:MET:HE1  | 1:A:43:LEU:HD21 | 2        | 1.0           |
| (1,1900) | 1:A:41:MET:HE1  | 1:A:43:LEU:HD22 | 2        | 1.0           |
| (1,1900) | 1:A:41:MET:HE1  | 1:A:43:LEU:HD23 | 2        | 1.0           |
| (1,1900) | 1:A:41:MET:HE2  | 1:A:43:LEU:HD21 | 2        | 1.0           |
| (1,1900) | 1:A:41:MET:HE2  | 1:A:43:LEU:HD22 | 2        | 1.0           |
| (1,1900) | 1:A:41:MET:HE2  | 1:A:43:LEU:HD23 | 2        | 1.0           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1900) | 1:A:41:MET:HE3  | 1:A:43:LEU:HD21 | 2        | 1.0           |
| (1,1900) | 1:A:41:MET:HE3  | 1:A:43:LEU:HD22 | 2        | 1.0           |
| (1,1900) | 1:A:41:MET:HE3  | 1:A:43:LEU:HD23 | 2        | 1.0           |
| (1,1274) | 1:A:6:VAL:HG21  | 1:A:11:MET:HB2  | 2        | 1.0           |
| (1,1274) | 1:A:6:VAL:HG21  | 1:A:11:MET:HB3  | 2        | 1.0           |
| (1,1274) | 1:A:6:VAL:HG22  | 1:A:11:MET:HB2  | 2        | 1.0           |
| (1,1274) | 1:A:6:VAL:HG22  | 1:A:11:MET:HB3  | 2        | 1.0           |
| (1,1274) | 1:A:6:VAL:HG23  | 1:A:11:MET:HB2  | 2        | 1.0           |
| (1,1274) | 1:A:6:VAL:HG23  | 1:A:11:MET:HB3  | 2        | 1.0           |
| (1,947)  | 1:A:6:VAL:HG11  | 1:A:80:LYS:HD3  | 2        | 0.99          |
| (1,947)  | 1:A:6:VAL:HG12  | 1:A:80:LYS:HD3  | 2        | 0.99          |
| (1,947)  | 1:A:6:VAL:HG13  | 1:A:80:LYS:HD3  | 2        | 0.99          |
| (1,882)  | 1:A:80:LYS:HE3  | 1:A:6:VAL:HG11  | 10       | 0.99          |
| (1,882)  | 1:A:80:LYS:HE3  | 1:A:6:VAL:HG12  | 10       | 0.99          |
| (1,882)  | 1:A:80:LYS:HE3  | 1:A:6:VAL:HG13  | 10       | 0.99          |
| (1,827)  | 1:A:6:VAL:HG21  | 1:A:10:GLN:HG3  | 5        | 0.99          |
| (1,827)  | 1:A:6:VAL:HG22  | 1:A:10:GLN:HG3  | 5        | 0.99          |
| (1,827)  | 1:A:6:VAL:HG23  | 1:A:10:GLN:HG3  | 5        | 0.99          |
| (1,827)  | 1:A:6:VAL:HG21  | 1:A:10:GLN:HG3  | 8        | 0.99          |
| (1,827)  | 1:A:6:VAL:HG22  | 1:A:10:GLN:HG3  | 8        | 0.99          |
| (1,827)  | 1:A:6:VAL:HG23  | 1:A:10:GLN:HG3  | 8        | 0.99          |
| (1,2564) | 1:A:89:PRO:HA   | 1:A:92:LEU:HB2  | 8        | 0.99          |
| (1,2001) | 1:A:52:GLU:HG2  | 1:A:51:GLY:HA3  | 8        | 0.99          |
| (1,1122) | 1:A:29:LEU:HD11 | 1:A:38:LEU:HD11 | 5        | 0.99          |
| (1,1122) | 1:A:29:LEU:HD11 | 1:A:38:LEU:HD12 | 5        | 0.99          |
| (1,1122) | 1:A:29:LEU:HD11 | 1:A:38:LEU:HD13 | 5        | 0.99          |
| (1,1122) | 1:A:29:LEU:HD12 | 1:A:38:LEU:HD11 | 5        | 0.99          |
| (1,1122) | 1:A:29:LEU:HD12 | 1:A:38:LEU:HD12 | 5        | 0.99          |
| (1,1122) | 1:A:29:LEU:HD12 | 1:A:38:LEU:HD13 | 5        | 0.99          |
| (1,1122) | 1:A:29:LEU:HD13 | 1:A:38:LEU:HD11 | 5        | 0.99          |
| (1,1122) | 1:A:29:LEU:HD13 | 1:A:38:LEU:HD12 | 5        | 0.99          |
| (1,1122) | 1:A:29:LEU:HD13 | 1:A:38:LEU:HD13 | 5        | 0.99          |
| (2,335)  | 1:A:71:SER:HB3  | 1:A:28:ILE:HG12 | 6        | 0.98          |
| (1,882)  | 1:A:80:LYS:HE3  | 1:A:6:VAL:HG11  | 12       | 0.98          |
| (1,882)  | 1:A:80:LYS:HE3  | 1:A:6:VAL:HG12  | 12       | 0.98          |
| (1,882)  | 1:A:80:LYS:HE3  | 1:A:6:VAL:HG13  | 12       | 0.98          |
| (1,813)  | 1:A:10:GLN:HB2  | 1:A:6:VAL:HG21  | 8        | 0.98          |
| (1,813)  | 1:A:10:GLN:HB2  | 1:A:6:VAL:HG22  | 8        | 0.98          |
| (1,813)  | 1:A:10:GLN:HB2  | 1:A:6:VAL:HG23  | 8        | 0.98          |
| (2,268)  | 1:A:134:GLY:H   | 1:A:130:GLN:H   | 9        | 0.97          |
| (1,813)  | 1:A:10:GLN:HB2  | 1:A:6:VAL:HG21  | 11       | 0.97          |
| (1,813)  | 1:A:10:GLN:HB2  | 1:A:6:VAL:HG22  | 11       | 0.97          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,813)  | 1:A:10:GLN:HB2   | 1:A:6:VAL:HG23  | 11       | 0.97          |
| (1,850)  | 1:A:109:THR:HA   | 1:A:108:GLU:HG3 | 1        | 0.96          |
| (1,813)  | 1:A:10:GLN:HB2   | 1:A:6:VAL:HG21  | 6        | 0.96          |
| (1,813)  | 1:A:10:GLN:HB2   | 1:A:6:VAL:HG22  | 6        | 0.96          |
| (1,813)  | 1:A:10:GLN:HB2   | 1:A:6:VAL:HG23  | 6        | 0.96          |
| (1,1145) | 1:A:6:VAL:HG21   | 1:A:11:MET:HA   | 6        | 0.96          |
| (1,1145) | 1:A:6:VAL:HG22   | 1:A:11:MET:HA   | 6        | 0.96          |
| (1,1145) | 1:A:6:VAL:HG23   | 1:A:11:MET:HA   | 6        | 0.96          |
| (1,882)  | 1:A:80:LYS:HE3   | 1:A:6:VAL:HG11  | 6        | 0.95          |
| (1,882)  | 1:A:80:LYS:HE3   | 1:A:6:VAL:HG12  | 6        | 0.95          |
| (1,882)  | 1:A:80:LYS:HE3   | 1:A:6:VAL:HG13  | 6        | 0.95          |
| (1,882)  | 1:A:80:LYS:HE3   | 1:A:6:VAL:HG11  | 7        | 0.95          |
| (1,882)  | 1:A:80:LYS:HE3   | 1:A:6:VAL:HG12  | 7        | 0.95          |
| (1,882)  | 1:A:80:LYS:HE3   | 1:A:6:VAL:HG13  | 7        | 0.95          |
| (1,418)  | 1:A:117:SER:H    | 1:A:120:GLN:HB3 | 7        | 0.95          |
| (1,2393) | 1:A:6:VAL:HG11   | 1:A:80:LYS:HD3  | 3        | 0.95          |
| (1,2393) | 1:A:6:VAL:HG12   | 1:A:80:LYS:HD3  | 3        | 0.95          |
| (1,2393) | 1:A:6:VAL:HG13   | 1:A:80:LYS:HD3  | 3        | 0.95          |
| (1,1387) | 1:A:109:THR:HG21 | 1:A:113:LYS:HE3 | 2        | 0.95          |
| (1,1387) | 1:A:109:THR:HG22 | 1:A:113:LYS:HE3 | 2        | 0.95          |
| (1,1387) | 1:A:109:THR:HG23 | 1:A:113:LYS:HE3 | 2        | 0.95          |
| (1,1016) | 1:A:6:VAL:HG21   | 1:A:11:MET:HG3  | 5        | 0.95          |
| (1,1016) | 1:A:6:VAL:HG22   | 1:A:11:MET:HG3  | 5        | 0.95          |
| (1,1016) | 1:A:6:VAL:HG23   | 1:A:11:MET:HG3  | 5        | 0.95          |
| (1,947)  | 1:A:6:VAL:HG11   | 1:A:80:LYS:HD3  | 3        | 0.94          |
| (1,947)  | 1:A:6:VAL:HG12   | 1:A:80:LYS:HD3  | 3        | 0.94          |
| (1,947)  | 1:A:6:VAL:HG13   | 1:A:80:LYS:HD3  | 3        | 0.94          |
| (1,882)  | 1:A:80:LYS:HE3   | 1:A:6:VAL:HG11  | 1        | 0.94          |
| (1,882)  | 1:A:80:LYS:HE3   | 1:A:6:VAL:HG12  | 1        | 0.94          |
| (1,882)  | 1:A:80:LYS:HE3   | 1:A:6:VAL:HG13  | 1        | 0.94          |
| (2,268)  | 1:A:134:GLY:H    | 1:A:130:GLN:H   | 10       | 0.93          |
| (1,1872) | 1:A:65:LYS:HE3   | 1:A:64:THR:HG21 | 3        | 0.93          |
| (1,1872) | 1:A:65:LYS:HE3   | 1:A:64:THR:HG22 | 3        | 0.93          |
| (1,1872) | 1:A:65:LYS:HE3   | 1:A:64:THR:HG23 | 3        | 0.93          |
| (1,1145) | 1:A:6:VAL:HG21   | 1:A:11:MET:HA   | 8        | 0.93          |
| (1,1145) | 1:A:6:VAL:HG22   | 1:A:11:MET:HA   | 8        | 0.93          |
| (1,1145) | 1:A:6:VAL:HG23   | 1:A:11:MET:HA   | 8        | 0.93          |
| (2,300)  | 1:A:109:THR:HB   | 1:A:112:GLN:HG3 | 9        | 0.92          |
| (1,2083) | 1:A:89:PRO:HA    | 1:A:92:LEU:HD21 | 9        | 0.92          |
| (1,2083) | 1:A:89:PRO:HA    | 1:A:92:LEU:HD22 | 9        | 0.92          |
| (1,2083) | 1:A:89:PRO:HA    | 1:A:92:LEU:HD23 | 9        | 0.92          |
| (1,1510) | 1:A:78:TYR:HB2   | 1:A:79:MET:HE1  | 6        | 0.92          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1510) | 1:A:78:TYR:HB2   | 1:A:79:MET:HE2  | 6        | 0.92          |
| (1,1510) | 1:A:78:TYR:HB2   | 1:A:79:MET:HE3  | 6        | 0.92          |
| (1,1407) | 1:A:41:MET:HB3   | 1:A:43:LEU:HG   | 9        | 0.92          |
| (1,1016) | 1:A:6:VAL:HG21   | 1:A:11:MET:HG3  | 8        | 0.92          |
| (1,1016) | 1:A:6:VAL:HG22   | 1:A:11:MET:HG3  | 8        | 0.92          |
| (1,1016) | 1:A:6:VAL:HG23   | 1:A:11:MET:HG3  | 8        | 0.92          |
| (1,813)  | 1:A:10:GLN:HB2   | 1:A:6:VAL:HG21  | 5        | 0.91          |
| (1,813)  | 1:A:10:GLN:HB2   | 1:A:6:VAL:HG22  | 5        | 0.91          |
| (1,813)  | 1:A:10:GLN:HB2   | 1:A:6:VAL:HG23  | 5        | 0.91          |
| (1,1016) | 1:A:6:VAL:HG21   | 1:A:11:MET:HG3  | 1        | 0.91          |
| (1,1016) | 1:A:6:VAL:HG22   | 1:A:11:MET:HG3  | 1        | 0.91          |
| (1,1016) | 1:A:6:VAL:HG23   | 1:A:11:MET:HG3  | 1        | 0.91          |
| (1,2273) | 1:A:109:THR:HG21 | 1:A:108:GLU:HG3 | 10       | 0.9           |
| (1,2273) | 1:A:109:THR:HG22 | 1:A:108:GLU:HG3 | 10       | 0.9           |
| (1,2273) | 1:A:109:THR:HG23 | 1:A:108:GLU:HG3 | 10       | 0.9           |
| (1,1565) | 1:A:38:LEU:HD11  | 1:A:43:LEU:HD21 | 7        | 0.9           |
| (1,1565) | 1:A:38:LEU:HD11  | 1:A:43:LEU:HD22 | 7        | 0.9           |
| (1,1565) | 1:A:38:LEU:HD11  | 1:A:43:LEU:HD23 | 7        | 0.9           |
| (1,1565) | 1:A:38:LEU:HD12  | 1:A:43:LEU:HD21 | 7        | 0.9           |
| (1,1565) | 1:A:38:LEU:HD12  | 1:A:43:LEU:HD22 | 7        | 0.9           |
| (1,1565) | 1:A:38:LEU:HD12  | 1:A:43:LEU:HD23 | 7        | 0.9           |
| (1,1565) | 1:A:38:LEU:HD13  | 1:A:43:LEU:HD21 | 7        | 0.9           |
| (1,1565) | 1:A:38:LEU:HD13  | 1:A:43:LEU:HD22 | 7        | 0.9           |
| (1,1565) | 1:A:38:LEU:HD13  | 1:A:43:LEU:HD23 | 7        | 0.9           |
| (1,1119) | 1:A:70:VAL:HG21  | 1:A:71:SER:HB3  | 11       | 0.9           |
| (1,1119) | 1:A:70:VAL:HG22  | 1:A:71:SER:HB3  | 11       | 0.9           |
| (1,1119) | 1:A:70:VAL:HG23  | 1:A:71:SER:HB3  | 11       | 0.9           |
| (1,882)  | 1:A:80:LYS:HE3   | 1:A:6:VAL:HG11  | 5        | 0.89          |
| (1,882)  | 1:A:80:LYS:HE3   | 1:A:6:VAL:HG12  | 5        | 0.89          |
| (1,882)  | 1:A:80:LYS:HE3   | 1:A:6:VAL:HG13  | 5        | 0.89          |
| (1,1016) | 1:A:6:VAL:HG21   | 1:A:11:MET:HG3  | 3        | 0.89          |
| (1,1016) | 1:A:6:VAL:HG22   | 1:A:11:MET:HG3  | 3        | 0.89          |
| (1,1016) | 1:A:6:VAL:HG23   | 1:A:11:MET:HG3  | 3        | 0.89          |
| (1,2124) | 1:A:38:LEU:HD11  | 1:A:43:LEU:HD21 | 3        | 0.87          |
| (1,2124) | 1:A:38:LEU:HD11  | 1:A:43:LEU:HD22 | 3        | 0.87          |
| (1,2124) | 1:A:38:LEU:HD11  | 1:A:43:LEU:HD23 | 3        | 0.87          |
| (1,2124) | 1:A:38:LEU:HD12  | 1:A:43:LEU:HD21 | 3        | 0.87          |
| (1,2124) | 1:A:38:LEU:HD12  | 1:A:43:LEU:HD22 | 3        | 0.87          |
| (1,2124) | 1:A:38:LEU:HD12  | 1:A:43:LEU:HD23 | 3        | 0.87          |
| (1,2124) | 1:A:38:LEU:HD13  | 1:A:43:LEU:HD21 | 3        | 0.87          |
| (1,2124) | 1:A:38:LEU:HD13  | 1:A:43:LEU:HD22 | 3        | 0.87          |
| (1,2124) | 1:A:38:LEU:HD13  | 1:A:43:LEU:HD23 | 3        | 0.87          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1145) | 1:A:6:VAL:HG21  | 1:A:11:MET:HA   | 11       | 0.87          |
| (1,1145) | 1:A:6:VAL:HG22  | 1:A:11:MET:HA   | 11       | 0.87          |
| (1,1145) | 1:A:6:VAL:HG23  | 1:A:11:MET:HA   | 11       | 0.87          |
| (1,1122) | 1:A:29:LEU:HD11 | 1:A:38:LEU:HD11 | 6        | 0.87          |
| (1,1122) | 1:A:29:LEU:HD11 | 1:A:38:LEU:HD12 | 6        | 0.87          |
| (1,1122) | 1:A:29:LEU:HD11 | 1:A:38:LEU:HD13 | 6        | 0.87          |
| (1,1122) | 1:A:29:LEU:HD12 | 1:A:38:LEU:HD11 | 6        | 0.87          |
| (1,1122) | 1:A:29:LEU:HD12 | 1:A:38:LEU:HD12 | 6        | 0.87          |
| (1,1122) | 1:A:29:LEU:HD12 | 1:A:38:LEU:HD13 | 6        | 0.87          |
| (1,1122) | 1:A:29:LEU:HD13 | 1:A:38:LEU:HD11 | 6        | 0.87          |
| (1,1122) | 1:A:29:LEU:HD13 | 1:A:38:LEU:HD12 | 6        | 0.87          |
| (1,1122) | 1:A:29:LEU:HD13 | 1:A:38:LEU:HD13 | 6        | 0.87          |
| (1,2393) | 1:A:6:VAL:HG11  | 1:A:80:LYS:HD3  | 12       | 0.86          |
| (1,2393) | 1:A:6:VAL:HG12  | 1:A:80:LYS:HD3  | 12       | 0.86          |
| (1,2393) | 1:A:6:VAL:HG13  | 1:A:80:LYS:HD3  | 12       | 0.86          |
| (1,1779) | 1:A:43:LEU:HD11 | 1:A:82:LYS:HE2  | 4        | 0.86          |
| (1,1779) | 1:A:43:LEU:HD12 | 1:A:82:LYS:HE2  | 4        | 0.86          |
| (1,1779) | 1:A:43:LEU:HD13 | 1:A:82:LYS:HE2  | 4        | 0.86          |
| (1,1145) | 1:A:6:VAL:HG21  | 1:A:11:MET:HA   | 1        | 0.86          |
| (1,1145) | 1:A:6:VAL:HG22  | 1:A:11:MET:HA   | 1        | 0.86          |
| (1,1145) | 1:A:6:VAL:HG23  | 1:A:11:MET:HA   | 1        | 0.86          |
| (1,947)  | 1:A:6:VAL:HG11  | 1:A:80:LYS:HD3  | 12       | 0.85          |
| (1,947)  | 1:A:6:VAL:HG12  | 1:A:80:LYS:HD3  | 12       | 0.85          |
| (1,947)  | 1:A:6:VAL:HG13  | 1:A:80:LYS:HD3  | 12       | 0.85          |
| (1,850)  | 1:A:109:THR:HA  | 1:A:108:GLU:HG3 | 7        | 0.85          |
| (1,1145) | 1:A:6:VAL:HG21  | 1:A:11:MET:HA   | 3        | 0.85          |
| (1,1145) | 1:A:6:VAL:HG22  | 1:A:11:MET:HA   | 3        | 0.85          |
| (1,1145) | 1:A:6:VAL:HG23  | 1:A:11:MET:HA   | 3        | 0.85          |
| (1,1122) | 1:A:29:LEU:HD11 | 1:A:38:LEU:HD11 | 4        | 0.85          |
| (1,1122) | 1:A:29:LEU:HD11 | 1:A:38:LEU:HD12 | 4        | 0.85          |
| (1,1122) | 1:A:29:LEU:HD11 | 1:A:38:LEU:HD13 | 4        | 0.85          |
| (1,1122) | 1:A:29:LEU:HD12 | 1:A:38:LEU:HD11 | 4        | 0.85          |
| (1,1122) | 1:A:29:LEU:HD12 | 1:A:38:LEU:HD12 | 4        | 0.85          |
| (1,1122) | 1:A:29:LEU:HD12 | 1:A:38:LEU:HD13 | 4        | 0.85          |
| (1,1122) | 1:A:29:LEU:HD13 | 1:A:38:LEU:HD11 | 4        | 0.85          |
| (1,1122) | 1:A:29:LEU:HD13 | 1:A:38:LEU:HD12 | 4        | 0.85          |
| (1,1122) | 1:A:29:LEU:HD13 | 1:A:38:LEU:HD13 | 4        | 0.85          |
| (1,882)  | 1:A:80:LYS:HE3  | 1:A:6:VAL:HG11  | 11       | 0.84          |
| (1,882)  | 1:A:80:LYS:HE3  | 1:A:6:VAL:HG12  | 11       | 0.84          |
| (1,882)  | 1:A:80:LYS:HE3  | 1:A:6:VAL:HG13  | 11       | 0.84          |
| (1,1168) | 1:A:6:VAL:HG21  | 1:A:11:MET:HB2  | 12       | 0.83          |
| (1,1168) | 1:A:6:VAL:HG21  | 1:A:11:MET:HB3  | 12       | 0.83          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1168) | 1:A:6:VAL:HG22   | 1:A:11:MET:HB2  | 12       | 0.83          |
| (1,1168) | 1:A:6:VAL:HG22   | 1:A:11:MET:HB3  | 12       | 0.83          |
| (1,1168) | 1:A:6:VAL:HG23   | 1:A:11:MET:HB2  | 12       | 0.83          |
| (1,1168) | 1:A:6:VAL:HG23   | 1:A:11:MET:HB3  | 12       | 0.83          |
| (1,1847) | 1:A:6:VAL:HG11   | 1:A:80:LYS:HB3  | 2        | 0.82          |
| (1,1847) | 1:A:6:VAL:HG12   | 1:A:80:LYS:HB3  | 2        | 0.82          |
| (1,1847) | 1:A:6:VAL:HG13   | 1:A:80:LYS:HB3  | 2        | 0.82          |
| (1,1379) | 1:A:141:VAL:HG11 | 1:A:140:TRP:HA  | 6        | 0.82          |
| (1,1379) | 1:A:141:VAL:HG12 | 1:A:140:TRP:HA  | 6        | 0.82          |
| (1,1379) | 1:A:141:VAL:HG13 | 1:A:140:TRP:HA  | 6        | 0.82          |
| (1,1168) | 1:A:6:VAL:HG21   | 1:A:11:MET:HB2  | 10       | 0.82          |
| (1,1168) | 1:A:6:VAL:HG21   | 1:A:11:MET:HB3  | 10       | 0.82          |
| (1,1168) | 1:A:6:VAL:HG22   | 1:A:11:MET:HB2  | 10       | 0.82          |
| (1,1168) | 1:A:6:VAL:HG22   | 1:A:11:MET:HB3  | 10       | 0.82          |
| (1,1168) | 1:A:6:VAL:HG23   | 1:A:11:MET:HB2  | 10       | 0.82          |
| (1,1168) | 1:A:6:VAL:HG23   | 1:A:11:MET:HB3  | 10       | 0.82          |
| (1,1000) | 1:A:20:ALA:HB1   | 1:A:17:SER:HB3  | 12       | 0.82          |
| (1,1000) | 1:A:20:ALA:HB2   | 1:A:17:SER:HB3  | 12       | 0.82          |
| (1,1000) | 1:A:20:ALA:HB3   | 1:A:17:SER:HB3  | 12       | 0.82          |
| (2,300)  | 1:A:109:THR:HB   | 1:A:112:GLN:HG3 | 7        | 0.81          |
| (1,2641) | 1:A:122:GLU:HB2  | 1:A:126:ALA:HB1 | 5        | 0.81          |
| (1,2641) | 1:A:122:GLU:HB2  | 1:A:126:ALA:HB2 | 5        | 0.81          |
| (1,2641) | 1:A:122:GLU:HB2  | 1:A:126:ALA:HB3 | 5        | 0.81          |
| (1,2001) | 1:A:52:GLU:HG2   | 1:A:51:GLY:HA3  | 2        | 0.81          |
| (1,1900) | 1:A:41:MET:HE1   | 1:A:43:LEU:HD21 | 1        | 0.81          |
| (1,1900) | 1:A:41:MET:HE1   | 1:A:43:LEU:HD22 | 1        | 0.81          |
| (1,1900) | 1:A:41:MET:HE1   | 1:A:43:LEU:HD23 | 1        | 0.81          |
| (1,1900) | 1:A:41:MET:HE2   | 1:A:43:LEU:HD21 | 1        | 0.81          |
| (1,1900) | 1:A:41:MET:HE2   | 1:A:43:LEU:HD22 | 1        | 0.81          |
| (1,1900) | 1:A:41:MET:HE2   | 1:A:43:LEU:HD23 | 1        | 0.81          |
| (1,1900) | 1:A:41:MET:HE3   | 1:A:43:LEU:HD21 | 1        | 0.81          |
| (1,1900) | 1:A:41:MET:HE3   | 1:A:43:LEU:HD22 | 1        | 0.81          |
| (1,1900) | 1:A:41:MET:HE3   | 1:A:43:LEU:HD23 | 1        | 0.81          |
| (1,1900) | 1:A:41:MET:HE1   | 1:A:43:LEU:HD21 | 3        | 0.81          |
| (1,1900) | 1:A:41:MET:HE1   | 1:A:43:LEU:HD22 | 3        | 0.81          |
| (1,1900) | 1:A:41:MET:HE1   | 1:A:43:LEU:HD23 | 3        | 0.81          |
| (1,1900) | 1:A:41:MET:HE2   | 1:A:43:LEU:HD21 | 3        | 0.81          |
| (1,1900) | 1:A:41:MET:HE2   | 1:A:43:LEU:HD22 | 3        | 0.81          |
| (1,1900) | 1:A:41:MET:HE2   | 1:A:43:LEU:HD23 | 3        | 0.81          |
| (1,1900) | 1:A:41:MET:HE3   | 1:A:43:LEU:HD21 | 3        | 0.81          |
| (1,1900) | 1:A:41:MET:HE3   | 1:A:43:LEU:HD22 | 3        | 0.81          |
| (1,1900) | 1:A:41:MET:HE3   | 1:A:43:LEU:HD23 | 3        | 0.81          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (2,268)  | 1:A:134:GLY:H    | 1:A:130:GLN:H   | 2        | 0.8           |
| (1,2327) | 1:A:113:LYS:HB3  | 1:A:113:LYS:HE3 | 5        | 0.8           |
| (1,1872) | 1:A:65:LYS:HE3   | 1:A:64:THR:HG21 | 10       | 0.8           |
| (1,1872) | 1:A:65:LYS:HE3   | 1:A:64:THR:HG22 | 10       | 0.8           |
| (1,1872) | 1:A:65:LYS:HE3   | 1:A:64:THR:HG23 | 10       | 0.8           |
| (1,2047) | 1:A:43:LEU:HD11  | 1:A:82:LYS:HE3  | 3        | 0.79          |
| (1,2047) | 1:A:43:LEU:HD12  | 1:A:82:LYS:HE3  | 3        | 0.79          |
| (1,2047) | 1:A:43:LEU:HD13  | 1:A:82:LYS:HE3  | 3        | 0.79          |
| (1,1510) | 1:A:78:TYR:HB2   | 1:A:79:MET:HE1  | 2        | 0.79          |
| (1,1510) | 1:A:78:TYR:HB2   | 1:A:79:MET:HE2  | 2        | 0.79          |
| (1,1510) | 1:A:78:TYR:HB2   | 1:A:79:MET:HE3  | 2        | 0.79          |
| (1,1499) | 1:A:99:ILE:HG21  | 1:A:103:LYS:HE2 | 12       | 0.79          |
| (1,1499) | 1:A:99:ILE:HG22  | 1:A:103:LYS:HE2 | 12       | 0.79          |
| (1,1499) | 1:A:99:ILE:HG23  | 1:A:103:LYS:HE2 | 12       | 0.79          |
| (1,1379) | 1:A:141:VAL:HG11 | 1:A:140:TRP:HA  | 11       | 0.79          |
| (1,1379) | 1:A:141:VAL:HG12 | 1:A:140:TRP:HA  | 11       | 0.79          |
| (1,1379) | 1:A:141:VAL:HG13 | 1:A:140:TRP:HA  | 11       | 0.79          |
| (1,1119) | 1:A:70:VAL:HG21  | 1:A:71:SER:HB3  | 10       | 0.79          |
| (1,1119) | 1:A:70:VAL:HG22  | 1:A:71:SER:HB3  | 10       | 0.79          |
| (1,1119) | 1:A:70:VAL:HG23  | 1:A:71:SER:HB3  | 10       | 0.79          |
| (1,2393) | 1:A:6:VAL:HG11   | 1:A:80:LYS:HD3  | 1        | 0.78          |
| (1,2393) | 1:A:6:VAL:HG12   | 1:A:80:LYS:HD3  | 1        | 0.78          |
| (1,2393) | 1:A:6:VAL:HG13   | 1:A:80:LYS:HD3  | 1        | 0.78          |
| (1,2327) | 1:A:113:LYS:HB3  | 1:A:113:LYS:HE3 | 9        | 0.78          |
| (1,1941) | 1:A:44:ILE:HG21  | 1:A:38:LEU:HD21 | 9        | 0.78          |
| (1,1941) | 1:A:44:ILE:HG21  | 1:A:38:LEU:HD22 | 9        | 0.78          |
| (1,1941) | 1:A:44:ILE:HG21  | 1:A:38:LEU:HD23 | 9        | 0.78          |
| (1,1941) | 1:A:44:ILE:HG22  | 1:A:38:LEU:HD21 | 9        | 0.78          |
| (1,1941) | 1:A:44:ILE:HG22  | 1:A:38:LEU:HD22 | 9        | 0.78          |
| (1,1941) | 1:A:44:ILE:HG22  | 1:A:38:LEU:HD23 | 9        | 0.78          |
| (1,1941) | 1:A:44:ILE:HG23  | 1:A:38:LEU:HD21 | 9        | 0.78          |
| (1,1941) | 1:A:44:ILE:HG23  | 1:A:38:LEU:HD22 | 9        | 0.78          |
| (1,1941) | 1:A:44:ILE:HG23  | 1:A:38:LEU:HD23 | 9        | 0.78          |
| (1,1847) | 1:A:6:VAL:HG11   | 1:A:80:LYS:HB3  | 10       | 0.78          |
| (1,1847) | 1:A:6:VAL:HG12   | 1:A:80:LYS:HB3  | 10       | 0.78          |
| (1,1847) | 1:A:6:VAL:HG13   | 1:A:80:LYS:HB3  | 10       | 0.78          |
| (1,1447) | 1:A:89:PRO:HA    | 1:A:92:LEU:HD21 | 9        | 0.78          |
| (1,1447) | 1:A:89:PRO:HA    | 1:A:92:LEU:HD22 | 9        | 0.78          |
| (1,1447) | 1:A:89:PRO:HA    | 1:A:92:LEU:HD23 | 9        | 0.78          |
| (1,1016) | 1:A:6:VAL:HG21   | 1:A:11:MET:HG3  | 11       | 0.78          |
| (1,1016) | 1:A:6:VAL:HG22   | 1:A:11:MET:HG3  | 11       | 0.78          |
| (1,1016) | 1:A:6:VAL:HG23   | 1:A:11:MET:HG3  | 11       | 0.78          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,947)  | 1:A:6:VAL:HG11   | 1:A:80:LYS:HD3  | 1        | 0.77          |
| (1,947)  | 1:A:6:VAL:HG12   | 1:A:80:LYS:HD3  | 1        | 0.77          |
| (1,947)  | 1:A:6:VAL:HG13   | 1:A:80:LYS:HD3  | 1        | 0.77          |
| (1,2331) | 1:A:6:VAL:HB     | 1:A:11:MET:HG2  | 10       | 0.77          |
| (1,1277) | 1:A:41:MET:HE1   | 1:A:17:SER:HB3  | 9        | 0.77          |
| (1,1277) | 1:A:41:MET:HE2   | 1:A:17:SER:HB3  | 9        | 0.77          |
| (1,1277) | 1:A:41:MET:HE3   | 1:A:17:SER:HB3  | 9        | 0.77          |
| (1,2314) | 1:A:6:VAL:HG21   | 1:A:11:MET:HA   | 10       | 0.76          |
| (1,2314) | 1:A:6:VAL:HG22   | 1:A:11:MET:HA   | 10       | 0.76          |
| (1,2314) | 1:A:6:VAL:HG23   | 1:A:11:MET:HA   | 10       | 0.76          |
| (1,2138) | 1:A:6:VAL:HG11   | 1:A:5:GLY:HA3   | 1        | 0.76          |
| (1,2138) | 1:A:6:VAL:HG12   | 1:A:5:GLY:HA3   | 1        | 0.76          |
| (1,2138) | 1:A:6:VAL:HG13   | 1:A:5:GLY:HA3   | 1        | 0.76          |
| (1,1565) | 1:A:38:LEU:HD11  | 1:A:43:LEU:HD21 | 3        | 0.76          |
| (1,1565) | 1:A:38:LEU:HD11  | 1:A:43:LEU:HD22 | 3        | 0.76          |
| (1,1565) | 1:A:38:LEU:HD11  | 1:A:43:LEU:HD23 | 3        | 0.76          |
| (1,1565) | 1:A:38:LEU:HD12  | 1:A:43:LEU:HD21 | 3        | 0.76          |
| (1,1565) | 1:A:38:LEU:HD12  | 1:A:43:LEU:HD22 | 3        | 0.76          |
| (1,1565) | 1:A:38:LEU:HD12  | 1:A:43:LEU:HD23 | 3        | 0.76          |
| (1,1565) | 1:A:38:LEU:HD13  | 1:A:43:LEU:HD21 | 3        | 0.76          |
| (1,1565) | 1:A:38:LEU:HD13  | 1:A:43:LEU:HD22 | 3        | 0.76          |
| (1,1565) | 1:A:38:LEU:HD13  | 1:A:43:LEU:HD23 | 3        | 0.76          |
| (1,1379) | 1:A:141:VAL:HG11 | 1:A:140:TRP:HA  | 7        | 0.76          |
| (1,1379) | 1:A:141:VAL:HG12 | 1:A:140:TRP:HA  | 7        | 0.76          |
| (1,1379) | 1:A:141:VAL:HG13 | 1:A:140:TRP:HA  | 7        | 0.76          |
| (1,1218) | 1:A:6:VAL:HG11   | 1:A:80:LYS:HG3  | 10       | 0.76          |
| (1,1218) | 1:A:6:VAL:HG12   | 1:A:80:LYS:HG3  | 10       | 0.76          |
| (1,1218) | 1:A:6:VAL:HG13   | 1:A:80:LYS:HG3  | 10       | 0.76          |
| (1,1379) | 1:A:141:VAL:HG11 | 1:A:140:TRP:HA  | 1        | 0.75          |
| (1,1379) | 1:A:141:VAL:HG12 | 1:A:140:TRP:HA  | 1        | 0.75          |
| (1,1379) | 1:A:141:VAL:HG13 | 1:A:140:TRP:HA  | 1        | 0.75          |
| (1,1379) | 1:A:141:VAL:HG11 | 1:A:140:TRP:HA  | 2        | 0.75          |
| (1,1379) | 1:A:141:VAL:HG12 | 1:A:140:TRP:HA  | 2        | 0.75          |
| (1,1379) | 1:A:141:VAL:HG13 | 1:A:140:TRP:HA  | 2        | 0.75          |
| (1,2543) | 1:A:59:ILE:HD11  | 1:A:55:GLN:HG3  | 8        | 0.74          |
| (1,2543) | 1:A:59:ILE:HD12  | 1:A:55:GLN:HG3  | 8        | 0.74          |
| (1,2543) | 1:A:59:ILE:HD13  | 1:A:55:GLN:HG3  | 8        | 0.74          |
| (1,2142) | 1:A:79:MET:HA    | 1:A:82:LYS:HB3  | 8        | 0.74          |
| (1,1847) | 1:A:6:VAL:HG11   | 1:A:80:LYS:HB3  | 8        | 0.74          |
| (1,1847) | 1:A:6:VAL:HG12   | 1:A:80:LYS:HB3  | 8        | 0.74          |
| (1,1847) | 1:A:6:VAL:HG13   | 1:A:80:LYS:HB3  | 8        | 0.74          |
| (1,1379) | 1:A:141:VAL:HG11 | 1:A:140:TRP:HA  | 9        | 0.74          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1379) | 1:A:141:VAL:HG12 | 1:A:140:TRP:HA  | 9        | 0.74          |
| (1,1379) | 1:A:141:VAL:HG13 | 1:A:140:TRP:HA  | 9        | 0.74          |
| (1,1379) | 1:A:141:VAL:HG11 | 1:A:140:TRP:HA  | 3        | 0.73          |
| (1,1379) | 1:A:141:VAL:HG12 | 1:A:140:TRP:HA  | 3        | 0.73          |
| (1,1379) | 1:A:141:VAL:HG13 | 1:A:140:TRP:HA  | 3        | 0.73          |
| (1,1336) | 1:A:38:LEU:HA    | 1:A:43:LEU:HD21 | 4        | 0.73          |
| (1,1336) | 1:A:38:LEU:HA    | 1:A:43:LEU:HD22 | 4        | 0.73          |
| (1,1336) | 1:A:38:LEU:HA    | 1:A:43:LEU:HD23 | 4        | 0.73          |
| (2,335)  | 1:A:71:SER:HB3   | 1:A:28:ILE:HG12 | 10       | 0.72          |
| (1,2399) | 1:A:103:LYS:HE2  | 1:A:100:ALA:HB1 | 2        | 0.72          |
| (1,2399) | 1:A:103:LYS:HE2  | 1:A:100:ALA:HB2 | 2        | 0.72          |
| (1,2399) | 1:A:103:LYS:HE2  | 1:A:100:ALA:HB3 | 2        | 0.72          |
| (1,2167) | 1:A:81:GLU:HA    | 1:A:84:ASP:HB3  | 9        | 0.72          |
| (1,2001) | 1:A:52:GLU:HG2   | 1:A:51:GLY:HA3  | 6        | 0.72          |
| (1,1900) | 1:A:41:MET:HE1   | 1:A:43:LEU:HD21 | 10       | 0.72          |
| (1,1900) | 1:A:41:MET:HE1   | 1:A:43:LEU:HD22 | 10       | 0.72          |
| (1,1900) | 1:A:41:MET:HE1   | 1:A:43:LEU:HD23 | 10       | 0.72          |
| (1,1900) | 1:A:41:MET:HE2   | 1:A:43:LEU:HD21 | 10       | 0.72          |
| (1,1900) | 1:A:41:MET:HE2   | 1:A:43:LEU:HD22 | 10       | 0.72          |
| (1,1900) | 1:A:41:MET:HE2   | 1:A:43:LEU:HD23 | 10       | 0.72          |
| (1,1900) | 1:A:41:MET:HE3   | 1:A:43:LEU:HD21 | 10       | 0.72          |
| (1,1900) | 1:A:41:MET:HE3   | 1:A:43:LEU:HD22 | 10       | 0.72          |
| (1,1900) | 1:A:41:MET:HE3   | 1:A:43:LEU:HD23 | 10       | 0.72          |
| (1,56)   | 1:A:52:GLU:HA    | 1:A:50:GLY:H    | 6        | 0.71          |
| (1,1638) | 1:A:21:PHE:HE1   | 1:A:17:SER:HB3  | 12       | 0.71          |
| (1,1638) | 1:A:21:PHE:HE2   | 1:A:17:SER:HB3  | 12       | 0.71          |
| (1,1890) | 1:A:79:MET:HE1   | 1:A:38:LEU:HD11 | 8        | 0.7           |
| (1,1890) | 1:A:79:MET:HE1   | 1:A:38:LEU:HD12 | 8        | 0.7           |
| (1,1890) | 1:A:79:MET:HE1   | 1:A:38:LEU:HD13 | 8        | 0.7           |
| (1,1890) | 1:A:79:MET:HE2   | 1:A:38:LEU:HD11 | 8        | 0.7           |
| (1,1890) | 1:A:79:MET:HE2   | 1:A:38:LEU:HD12 | 8        | 0.7           |
| (1,1890) | 1:A:79:MET:HE2   | 1:A:38:LEU:HD13 | 8        | 0.7           |
| (1,1890) | 1:A:79:MET:HE3   | 1:A:38:LEU:HD11 | 8        | 0.7           |
| (1,1890) | 1:A:79:MET:HE3   | 1:A:38:LEU:HD12 | 8        | 0.7           |
| (1,1890) | 1:A:79:MET:HE3   | 1:A:38:LEU:HD13 | 8        | 0.7           |
| (1,1000) | 1:A:20:ALA:HB1   | 1:A:17:SER:HB3  | 9        | 0.7           |
| (1,1000) | 1:A:20:ALA:HB2   | 1:A:17:SER:HB3  | 9        | 0.7           |
| (1,1000) | 1:A:20:ALA:HB3   | 1:A:17:SER:HB3  | 9        | 0.7           |
| (1,1259) | 1:A:38:LEU:HD21  | 1:A:59:ILE:HG21 | 4        | 0.69          |
| (1,1259) | 1:A:38:LEU:HD21  | 1:A:59:ILE:HG22 | 4        | 0.69          |
| (1,1259) | 1:A:38:LEU:HD21  | 1:A:59:ILE:HG23 | 4        | 0.69          |
| (1,1259) | 1:A:38:LEU:HD22  | 1:A:59:ILE:HG21 | 4        | 0.69          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1259) | 1:A:38:LEU:HD22 | 1:A:59:ILE:HG22 | 4        | 0.69          |
| (1,1259) | 1:A:38:LEU:HD22 | 1:A:59:ILE:HG23 | 4        | 0.69          |
| (1,1259) | 1:A:38:LEU:HD23 | 1:A:59:ILE:HG21 | 4        | 0.69          |
| (1,1259) | 1:A:38:LEU:HD23 | 1:A:59:ILE:HG22 | 4        | 0.69          |
| (1,1259) | 1:A:38:LEU:HD23 | 1:A:59:ILE:HG23 | 4        | 0.69          |
| (1,1259) | 1:A:38:LEU:HD21 | 1:A:59:ILE:HG21 | 5        | 0.69          |
| (1,1259) | 1:A:38:LEU:HD21 | 1:A:59:ILE:HG22 | 5        | 0.69          |
| (1,1259) | 1:A:38:LEU:HD21 | 1:A:59:ILE:HG23 | 5        | 0.69          |
| (1,1259) | 1:A:38:LEU:HD22 | 1:A:59:ILE:HG21 | 5        | 0.69          |
| (1,1259) | 1:A:38:LEU:HD22 | 1:A:59:ILE:HG22 | 5        | 0.69          |
| (1,1259) | 1:A:38:LEU:HD22 | 1:A:59:ILE:HG23 | 5        | 0.69          |
| (1,1259) | 1:A:38:LEU:HD23 | 1:A:59:ILE:HG21 | 5        | 0.69          |
| (1,1259) | 1:A:38:LEU:HD23 | 1:A:59:ILE:HG22 | 5        | 0.69          |
| (1,1259) | 1:A:38:LEU:HD23 | 1:A:59:ILE:HG23 | 5        | 0.69          |
| (1,1145) | 1:A:6:VAL:HG21  | 1:A:11:MET:HA   | 7        | 0.69          |
| (1,1145) | 1:A:6:VAL:HG22  | 1:A:11:MET:HA   | 7        | 0.69          |
| (1,1145) | 1:A:6:VAL:HG23  | 1:A:11:MET:HA   | 7        | 0.69          |
| (1,1122) | 1:A:29:LEU:HD11 | 1:A:38:LEU:HD11 | 9        | 0.69          |
| (1,1122) | 1:A:29:LEU:HD11 | 1:A:38:LEU:HD12 | 9        | 0.69          |
| (1,1122) | 1:A:29:LEU:HD11 | 1:A:38:LEU:HD13 | 9        | 0.69          |
| (1,1122) | 1:A:29:LEU:HD12 | 1:A:38:LEU:HD11 | 9        | 0.69          |
| (1,1122) | 1:A:29:LEU:HD12 | 1:A:38:LEU:HD12 | 9        | 0.69          |
| (1,1122) | 1:A:29:LEU:HD12 | 1:A:38:LEU:HD13 | 9        | 0.69          |
| (1,1122) | 1:A:29:LEU:HD13 | 1:A:38:LEU:HD11 | 9        | 0.69          |
| (1,1122) | 1:A:29:LEU:HD13 | 1:A:38:LEU:HD12 | 9        | 0.69          |
| (1,1122) | 1:A:29:LEU:HD13 | 1:A:38:LEU:HD13 | 9        | 0.69          |
| (1,1119) | 1:A:70:VAL:HG21 | 1:A:71:SER:HB3  | 2        | 0.68          |
| (1,1119) | 1:A:70:VAL:HG22 | 1:A:71:SER:HB3  | 2        | 0.68          |
| (1,1119) | 1:A:70:VAL:HG23 | 1:A:71:SER:HB3  | 2        | 0.68          |
| (1,2331) | 1:A:6:VAL:HB    | 1:A:11:MET:HG2  | 9        | 0.67          |
| (1,813)  | 1:A:10:GLN:HB2  | 1:A:6:VAL:HG21  | 3        | 0.66          |
| (1,813)  | 1:A:10:GLN:HB2  | 1:A:6:VAL:HG22  | 3        | 0.66          |
| (1,813)  | 1:A:10:GLN:HB2  | 1:A:6:VAL:HG23  | 3        | 0.66          |
| (1,2462) | 1:A:65:LYS:HE3  | 1:A:65:LYS:HA   | 9        | 0.66          |
| (1,2431) | 1:A:6:VAL:HG21  | 1:A:10:GLN:HG2  | 3        | 0.66          |
| (1,2431) | 1:A:6:VAL:HG22  | 1:A:10:GLN:HG2  | 3        | 0.66          |
| (1,2431) | 1:A:6:VAL:HG23  | 1:A:10:GLN:HG2  | 3        | 0.66          |
| (1,2304) | 1:A:43:LEU:HD21 | 1:A:82:LYS:HE2  | 4        | 0.66          |
| (1,2304) | 1:A:43:LEU:HD22 | 1:A:82:LYS:HE2  | 4        | 0.66          |
| (1,2304) | 1:A:43:LEU:HD23 | 1:A:82:LYS:HE2  | 4        | 0.66          |
| (1,2304) | 1:A:43:LEU:HD21 | 1:A:82:LYS:HE2  | 6        | 0.66          |
| (1,2304) | 1:A:43:LEU:HD22 | 1:A:82:LYS:HE2  | 6        | 0.66          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2304) | 1:A:43:LEU:HD23  | 1:A:82:LYS:HE2  | 6        | 0.66          |
| (2,298)  | 1:A:92:LEU:HD11  | 1:A:123:TYR:HE1 | 5        | 0.65          |
| (2,298)  | 1:A:92:LEU:HD11  | 1:A:123:TYR:HE2 | 5        | 0.65          |
| (2,298)  | 1:A:92:LEU:HD12  | 1:A:123:TYR:HE1 | 5        | 0.65          |
| (2,298)  | 1:A:92:LEU:HD12  | 1:A:123:TYR:HE2 | 5        | 0.65          |
| (2,298)  | 1:A:92:LEU:HD13  | 1:A:123:TYR:HE1 | 5        | 0.65          |
| (2,298)  | 1:A:92:LEU:HD13  | 1:A:123:TYR:HE2 | 5        | 0.65          |
| (1,2292) | 1:A:113:LYS:HB3  | 1:A:113:LYS:HE3 | 5        | 0.65          |
| (1,2273) | 1:A:109:THR:HG21 | 1:A:108:GLU:HG3 | 1        | 0.65          |
| (1,2273) | 1:A:109:THR:HG22 | 1:A:108:GLU:HG3 | 1        | 0.65          |
| (1,2273) | 1:A:109:THR:HG23 | 1:A:108:GLU:HG3 | 1        | 0.65          |
| (1,2138) | 1:A:6:VAL:HG11   | 1:A:5:GLY:HA3   | 8        | 0.65          |
| (1,2138) | 1:A:6:VAL:HG12   | 1:A:5:GLY:HA3   | 8        | 0.65          |
| (1,2138) | 1:A:6:VAL:HG13   | 1:A:5:GLY:HA3   | 8        | 0.65          |
| (1,2653) | 1:A:61:ASN:HB3   | 1:A:58:ALA:HB1  | 4        | 0.64          |
| (1,2653) | 1:A:61:ASN:HB3   | 1:A:58:ALA:HB2  | 4        | 0.64          |
| (1,2653) | 1:A:61:ASN:HB3   | 1:A:58:ALA:HB3  | 4        | 0.64          |
| (1,1489) | 1:A:20:ALA:HB1   | 1:A:17:SER:HB3  | 12       | 0.64          |
| (1,1489) | 1:A:20:ALA:HB2   | 1:A:17:SER:HB3  | 12       | 0.64          |
| (1,1489) | 1:A:20:ALA:HB3   | 1:A:17:SER:HB3  | 12       | 0.64          |
| (1,1067) | 1:A:10:GLN:HB3   | 1:A:6:VAL:HG21  | 8        | 0.64          |
| (1,1067) | 1:A:10:GLN:HB3   | 1:A:6:VAL:HG22  | 8        | 0.64          |
| (1,1067) | 1:A:10:GLN:HB3   | 1:A:6:VAL:HG23  | 8        | 0.64          |
| (1,2314) | 1:A:6:VAL:HG21   | 1:A:11:MET:HA   | 12       | 0.63          |
| (1,2314) | 1:A:6:VAL:HG22   | 1:A:11:MET:HA   | 12       | 0.63          |
| (1,2314) | 1:A:6:VAL:HG23   | 1:A:11:MET:HA   | 12       | 0.63          |
| (1,2292) | 1:A:113:LYS:HB3  | 1:A:113:LYS:HE3 | 9        | 0.63          |
| (1,1021) | 1:A:6:VAL:HG11   | 1:A:80:LYS:HG3  | 10       | 0.63          |
| (1,1021) | 1:A:6:VAL:HG12   | 1:A:80:LYS:HG3  | 10       | 0.63          |
| (1,1021) | 1:A:6:VAL:HG13   | 1:A:80:LYS:HG3  | 10       | 0.63          |
| (2,300)  | 1:A:109:THR:HB   | 1:A:112:GLN:HG3 | 5        | 0.62          |
| (1,2331) | 1:A:6:VAL:HB     | 1:A:11:MET:HG2  | 4        | 0.62          |
| (1,1724) | 1:A:56:TYR:HE1   | 1:A:38:LEU:HD21 | 8        | 0.62          |
| (1,1724) | 1:A:56:TYR:HE1   | 1:A:38:LEU:HD22 | 8        | 0.62          |
| (1,1724) | 1:A:56:TYR:HE1   | 1:A:38:LEU:HD23 | 8        | 0.62          |
| (1,1724) | 1:A:56:TYR:HE2   | 1:A:38:LEU:HD21 | 8        | 0.62          |
| (1,1724) | 1:A:56:TYR:HE2   | 1:A:38:LEU:HD22 | 8        | 0.62          |
| (1,1724) | 1:A:56:TYR:HE2   | 1:A:38:LEU:HD23 | 8        | 0.62          |
| (1,1081) | 1:A:6:VAL:HG21   | 1:A:11:MET:HG2  | 2        | 0.62          |
| (1,1081) | 1:A:6:VAL:HG22   | 1:A:11:MET:HG2  | 2        | 0.62          |
| (1,1081) | 1:A:6:VAL:HG23   | 1:A:11:MET:HG2  | 2        | 0.62          |
| (1,1067) | 1:A:10:GLN:HB3   | 1:A:6:VAL:HG21  | 3        | 0.62          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1067) | 1:A:10:GLN:HB3   | 1:A:6:VAL:HG22  | 3        | 0.62          |
| (1,1067) | 1:A:10:GLN:HB3   | 1:A:6:VAL:HG23  | 3        | 0.62          |
| (2,300)  | 1:A:109:THR:HB   | 1:A:112:GLN:HG3 | 6        | 0.61          |
| (1,2331) | 1:A:6:VAL:HB     | 1:A:11:MET:HG2  | 12       | 0.61          |
| (1,2167) | 1:A:81:GLU:HA    | 1:A:84:ASP:HB3  | 4        | 0.61          |
| (1,1191) | 1:A:38:LEU:HD11  | 1:A:43:LEU:HB2  | 9        | 0.61          |
| (1,1191) | 1:A:38:LEU:HD12  | 1:A:43:LEU:HB2  | 9        | 0.61          |
| (1,1191) | 1:A:38:LEU:HD13  | 1:A:43:LEU:HB2  | 9        | 0.61          |
| (1,1067) | 1:A:10:GLN:HB3   | 1:A:6:VAL:HG21  | 1        | 0.61          |
| (1,1067) | 1:A:10:GLN:HB3   | 1:A:6:VAL:HG22  | 1        | 0.61          |
| (1,1067) | 1:A:10:GLN:HB3   | 1:A:6:VAL:HG23  | 1        | 0.61          |
| (1,1024) | 1:A:15:LYS:HE3   | 1:A:15:LYS:HA   | 4        | 0.61          |
| (1,2653) | 1:A:61:ASN:HB3   | 1:A:58:ALA:HB1  | 5        | 0.6           |
| (1,2653) | 1:A:61:ASN:HB3   | 1:A:58:ALA:HB2  | 5        | 0.6           |
| (1,2653) | 1:A:61:ASN:HB3   | 1:A:58:ALA:HB3  | 5        | 0.6           |
| (1,2602) | 1:A:141:VAL:HG11 | 1:A:137:TYR:HD1 | 1        | 0.6           |
| (1,2602) | 1:A:141:VAL:HG11 | 1:A:137:TYR:HD2 | 1        | 0.6           |
| (1,2602) | 1:A:141:VAL:HG12 | 1:A:137:TYR:HD1 | 1        | 0.6           |
| (1,2602) | 1:A:141:VAL:HG12 | 1:A:137:TYR:HD2 | 1        | 0.6           |
| (1,2602) | 1:A:141:VAL:HG13 | 1:A:137:TYR:HD1 | 1        | 0.6           |
| (1,2602) | 1:A:141:VAL:HG13 | 1:A:137:TYR:HD2 | 1        | 0.6           |
| (1,2462) | 1:A:65:LYS:HE3   | 1:A:65:LYS:HA   | 11       | 0.6           |
| (1,1741) | 1:A:69:GLY:HA3   | 1:A:60:TYR:HE1  | 3        | 0.6           |
| (1,1741) | 1:A:69:GLY:HA3   | 1:A:60:TYR:HE2  | 3        | 0.6           |
| (1,1510) | 1:A:78:TYR:HB2   | 1:A:79:MET:HE1  | 10       | 0.6           |
| (1,1510) | 1:A:78:TYR:HB2   | 1:A:79:MET:HE2  | 10       | 0.6           |
| (1,1510) | 1:A:78:TYR:HB2   | 1:A:79:MET:HE3  | 10       | 0.6           |
| (1,1067) | 1:A:10:GLN:HB3   | 1:A:6:VAL:HG21  | 5        | 0.6           |
| (1,1067) | 1:A:10:GLN:HB3   | 1:A:6:VAL:HG22  | 5        | 0.6           |
| (1,1067) | 1:A:10:GLN:HB3   | 1:A:6:VAL:HG23  | 5        | 0.6           |
| (1,1067) | 1:A:10:GLN:HB3   | 1:A:6:VAL:HG21  | 6        | 0.6           |
| (1,1067) | 1:A:10:GLN:HB3   | 1:A:6:VAL:HG22  | 6        | 0.6           |
| (1,1067) | 1:A:10:GLN:HB3   | 1:A:6:VAL:HG23  | 6        | 0.6           |
| (1,1067) | 1:A:10:GLN:HB3   | 1:A:6:VAL:HG21  | 7        | 0.6           |
| (1,1067) | 1:A:10:GLN:HB3   | 1:A:6:VAL:HG22  | 7        | 0.6           |
| (1,1067) | 1:A:10:GLN:HB3   | 1:A:6:VAL:HG23  | 7        | 0.6           |
| (1,2642) | 1:A:81:GLU:HA    | 1:A:84:ASP:HB3  | 9        | 0.59          |
| (1,2001) | 1:A:52:GLU:HG2   | 1:A:51:GLY:HA3  | 10       | 0.59          |
| (1,1067) | 1:A:10:GLN:HB3   | 1:A:6:VAL:HG21  | 11       | 0.59          |
| (1,1067) | 1:A:10:GLN:HB3   | 1:A:6:VAL:HG22  | 11       | 0.59          |
| (1,1067) | 1:A:10:GLN:HB3   | 1:A:6:VAL:HG23  | 11       | 0.59          |
| (1,2653) | 1:A:61:ASN:HB3   | 1:A:58:ALA:HB1  | 9        | 0.58          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2653) | 1:A:61:ASN:HB3   | 1:A:58:ALA:HB2  | 9        | 0.58          |
| (1,2653) | 1:A:61:ASN:HB3   | 1:A:58:ALA:HB3  | 9        | 0.58          |
| (1,2331) | 1:A:6:VAL:HB     | 1:A:11:MET:HG2  | 2        | 0.58          |
| (1,2138) | 1:A:6:VAL:HG11   | 1:A:5:GLY:HA3   | 5        | 0.58          |
| (1,2138) | 1:A:6:VAL:HG12   | 1:A:5:GLY:HA3   | 5        | 0.58          |
| (1,2138) | 1:A:6:VAL:HG13   | 1:A:5:GLY:HA3   | 5        | 0.58          |
| (1,542)  | 1:A:108:GLU:HG2  | 1:A:113:LYS:H   | 12       | 0.57          |
| (1,2326) | 1:A:74:ASN:HA    | 1:A:77:GLN:HG3  | 5        | 0.57          |
| (1,2312) | 1:A:14:PHE:HB2   | 1:A:11:MET:HA   | 10       | 0.57          |
| (1,1829) | 1:A:103:LYS:HE2  | 1:A:101:ALA:HB1 | 8        | 0.57          |
| (1,1829) | 1:A:103:LYS:HE2  | 1:A:101:ALA:HB2 | 8        | 0.57          |
| (1,1829) | 1:A:103:LYS:HE2  | 1:A:101:ALA:HB3 | 8        | 0.57          |
| (1,1149) | 1:A:82:LYS:HA    | 1:A:85:GLU:HG3  | 5        | 0.57          |
| (1,2393) | 1:A:6:VAL:HG11   | 1:A:80:LYS:HD3  | 9        | 0.56          |
| (1,2393) | 1:A:6:VAL:HG12   | 1:A:80:LYS:HD3  | 9        | 0.56          |
| (1,2393) | 1:A:6:VAL:HG13   | 1:A:80:LYS:HD3  | 9        | 0.56          |
| (1,2253) | 1:A:79:MET:HE1   | 1:A:43:LEU:HD21 | 12       | 0.56          |
| (1,2253) | 1:A:79:MET:HE1   | 1:A:43:LEU:HD22 | 12       | 0.56          |
| (1,2253) | 1:A:79:MET:HE1   | 1:A:43:LEU:HD23 | 12       | 0.56          |
| (1,2253) | 1:A:79:MET:HE2   | 1:A:43:LEU:HD21 | 12       | 0.56          |
| (1,2253) | 1:A:79:MET:HE2   | 1:A:43:LEU:HD22 | 12       | 0.56          |
| (1,2253) | 1:A:79:MET:HE2   | 1:A:43:LEU:HD23 | 12       | 0.56          |
| (1,2253) | 1:A:79:MET:HE3   | 1:A:43:LEU:HD21 | 12       | 0.56          |
| (1,2253) | 1:A:79:MET:HE3   | 1:A:43:LEU:HD22 | 12       | 0.56          |
| (1,2253) | 1:A:79:MET:HE3   | 1:A:43:LEU:HD23 | 12       | 0.56          |
| (1,1712) | 1:A:106:ILE:HA   | 1:A:103:LYS:HE3 | 9        | 0.56          |
| (1,1259) | 1:A:38:LEU:HD21  | 1:A:59:ILE:HG21 | 6        | 0.56          |
| (1,1259) | 1:A:38:LEU:HD21  | 1:A:59:ILE:HG22 | 6        | 0.56          |
| (1,1259) | 1:A:38:LEU:HD21  | 1:A:59:ILE:HG23 | 6        | 0.56          |
| (1,1259) | 1:A:38:LEU:HD22  | 1:A:59:ILE:HG21 | 6        | 0.56          |
| (1,1259) | 1:A:38:LEU:HD22  | 1:A:59:ILE:HG22 | 6        | 0.56          |
| (1,1259) | 1:A:38:LEU:HD22  | 1:A:59:ILE:HG23 | 6        | 0.56          |
| (1,1259) | 1:A:38:LEU:HD23  | 1:A:59:ILE:HG21 | 6        | 0.56          |
| (1,1259) | 1:A:38:LEU:HD23  | 1:A:59:ILE:HG22 | 6        | 0.56          |
| (1,1259) | 1:A:38:LEU:HD23  | 1:A:59:ILE:HG23 | 6        | 0.56          |
| (1,947)  | 1:A:6:VAL:HG11   | 1:A:80:LYS:HD3  | 9        | 0.55          |
| (1,947)  | 1:A:6:VAL:HG12   | 1:A:80:LYS:HD3  | 9        | 0.55          |
| (1,947)  | 1:A:6:VAL:HG13   | 1:A:80:LYS:HD3  | 9        | 0.55          |
| (1,2573) | 1:A:109:THR:HG21 | 1:A:113:LYS:HG2 | 4        | 0.55          |
| (1,2573) | 1:A:109:THR:HG22 | 1:A:113:LYS:HG2 | 4        | 0.55          |
| (1,2573) | 1:A:109:THR:HG23 | 1:A:113:LYS:HG2 | 4        | 0.55          |
| (1,2312) | 1:A:14:PHE:HB2   | 1:A:11:MET:HA   | 9        | 0.55          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2304) | 1:A:43:LEU:HD21 | 1:A:82:LYS:HE2  | 2        | 0.55          |
| (1,2304) | 1:A:43:LEU:HD22 | 1:A:82:LYS:HE2  | 2        | 0.55          |
| (1,2304) | 1:A:43:LEU:HD23 | 1:A:82:LYS:HE2  | 2        | 0.55          |
| (1,2138) | 1:A:6:VAL:HG11  | 1:A:5:GLY:HA3   | 6        | 0.55          |
| (1,2138) | 1:A:6:VAL:HG12  | 1:A:5:GLY:HA3   | 6        | 0.55          |
| (1,2138) | 1:A:6:VAL:HG13  | 1:A:5:GLY:HA3   | 6        | 0.55          |
| (1,2047) | 1:A:43:LEU:HD11 | 1:A:82:LYS:HE3  | 7        | 0.55          |
| (1,2047) | 1:A:43:LEU:HD12 | 1:A:82:LYS:HE3  | 7        | 0.55          |
| (1,2047) | 1:A:43:LEU:HD13 | 1:A:82:LYS:HE3  | 7        | 0.55          |
| (1,1631) | 1:A:109:THR:HB  | 1:A:108:GLU:HG3 | 1        | 0.55          |
| (1,1458) | 1:A:77:GLN:HB3  | 1:A:74:ASN:HA   | 7        | 0.55          |
| (1,2138) | 1:A:6:VAL:HG11  | 1:A:5:GLY:HA3   | 3        | 0.54          |
| (1,2138) | 1:A:6:VAL:HG12  | 1:A:5:GLY:HA3   | 3        | 0.54          |
| (1,2138) | 1:A:6:VAL:HG13  | 1:A:5:GLY:HA3   | 3        | 0.54          |
| (1,1407) | 1:A:41:MET:HB3  | 1:A:43:LEU:HG   | 3        | 0.54          |
| (1,1336) | 1:A:38:LEU:HA   | 1:A:43:LEU:HD21 | 7        | 0.54          |
| (1,1336) | 1:A:38:LEU:HA   | 1:A:43:LEU:HD22 | 7        | 0.54          |
| (1,1336) | 1:A:38:LEU:HA   | 1:A:43:LEU:HD23 | 7        | 0.54          |
| (1,850)  | 1:A:109:THR:HA  | 1:A:108:GLU:HG3 | 4        | 0.53          |
| (1,2462) | 1:A:65:LYS:HE3  | 1:A:65:LYS:HA   | 8        | 0.53          |
| (1,2312) | 1:A:14:PHE:HB2  | 1:A:11:MET:HA   | 6        | 0.53          |
| (1,2312) | 1:A:14:PHE:HB2  | 1:A:11:MET:HA   | 8        | 0.53          |
| (1,1978) | 1:A:38:LEU:HA   | 1:A:43:LEU:HD21 | 4        | 0.53          |
| (1,1978) | 1:A:38:LEU:HA   | 1:A:43:LEU:HD22 | 4        | 0.53          |
| (1,1978) | 1:A:38:LEU:HA   | 1:A:43:LEU:HD23 | 4        | 0.53          |
| (1,1762) | 1:A:6:VAL:HG21  | 1:A:14:PHE:HE1  | 8        | 0.53          |
| (1,1762) | 1:A:6:VAL:HG21  | 1:A:14:PHE:HE2  | 8        | 0.53          |
| (1,1762) | 1:A:6:VAL:HG22  | 1:A:14:PHE:HE1  | 8        | 0.53          |
| (1,1762) | 1:A:6:VAL:HG22  | 1:A:14:PHE:HE2  | 8        | 0.53          |
| (1,1762) | 1:A:6:VAL:HG23  | 1:A:14:PHE:HE1  | 8        | 0.53          |
| (1,1762) | 1:A:6:VAL:HG23  | 1:A:14:PHE:HE2  | 8        | 0.53          |
| (1,1351) | 1:A:80:LYS:HD3  | 1:A:80:LYS:HA   | 1        | 0.53          |
| (1,1351) | 1:A:80:LYS:HD3  | 1:A:80:LYS:HA   | 12       | 0.53          |
| (1,1119) | 1:A:70:VAL:HG21 | 1:A:71:SER:HB3  | 4        | 0.53          |
| (1,1119) | 1:A:70:VAL:HG22 | 1:A:71:SER:HB3  | 4        | 0.53          |
| (1,1119) | 1:A:70:VAL:HG23 | 1:A:71:SER:HB3  | 4        | 0.53          |
| (1,56)   | 1:A:52:GLU:HA   | 1:A:50:GLY:H    | 11       | 0.52          |
| (1,2408) | 1:A:6:VAL:HG21  | 1:A:14:PHE:HD1  | 5        | 0.52          |
| (1,2408) | 1:A:6:VAL:HG21  | 1:A:14:PHE:HD2  | 5        | 0.52          |
| (1,2408) | 1:A:6:VAL:HG22  | 1:A:14:PHE:HD1  | 5        | 0.52          |
| (1,2408) | 1:A:6:VAL:HG22  | 1:A:14:PHE:HD2  | 5        | 0.52          |
| (1,2408) | 1:A:6:VAL:HG23  | 1:A:14:PHE:HD1  | 5        | 0.52          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2408) | 1:A:6:VAL:HG23  | 1:A:14:PHE:HD2  | 5        | 0.52          |
| (1,2312) | 1:A:14:PHE:HB2  | 1:A:11:MET:HA   | 1        | 0.52          |
| (1,2312) | 1:A:14:PHE:HB2  | 1:A:11:MET:HA   | 7        | 0.52          |
| (1,1489) | 1:A:20:ALA:HB1  | 1:A:17:SER:HB3  | 9        | 0.52          |
| (1,1489) | 1:A:20:ALA:HB2  | 1:A:17:SER:HB3  | 9        | 0.52          |
| (1,1489) | 1:A:20:ALA:HB3  | 1:A:17:SER:HB3  | 9        | 0.52          |
| (1,542)  | 1:A:108:GLU:HG2 | 1:A:113:LYS:H   | 11       | 0.51          |
| (1,2459) | 1:A:41:MET:HB3  | 1:A:43:LEU:HG   | 9        | 0.51          |
| (1,2408) | 1:A:6:VAL:HG21  | 1:A:14:PHE:HD1  | 6        | 0.51          |
| (1,2408) | 1:A:6:VAL:HG21  | 1:A:14:PHE:HD2  | 6        | 0.51          |
| (1,2408) | 1:A:6:VAL:HG22  | 1:A:14:PHE:HD1  | 6        | 0.51          |
| (1,2408) | 1:A:6:VAL:HG22  | 1:A:14:PHE:HD2  | 6        | 0.51          |
| (1,2408) | 1:A:6:VAL:HG23  | 1:A:14:PHE:HD1  | 6        | 0.51          |
| (1,2408) | 1:A:6:VAL:HG23  | 1:A:14:PHE:HD2  | 6        | 0.51          |
| (1,1762) | 1:A:6:VAL:HG21  | 1:A:14:PHE:HE1  | 6        | 0.51          |
| (1,1762) | 1:A:6:VAL:HG21  | 1:A:14:PHE:HE2  | 6        | 0.51          |
| (1,1762) | 1:A:6:VAL:HG22  | 1:A:14:PHE:HE1  | 6        | 0.51          |
| (1,1762) | 1:A:6:VAL:HG22  | 1:A:14:PHE:HE2  | 6        | 0.51          |
| (1,1762) | 1:A:6:VAL:HG23  | 1:A:14:PHE:HE1  | 6        | 0.51          |
| (1,1762) | 1:A:6:VAL:HG23  | 1:A:14:PHE:HE2  | 6        | 0.51          |
| (1,1351) | 1:A:80:LYS:HD3  | 1:A:80:LYS:HA   | 7        | 0.51          |
| (1,1218) | 1:A:6:VAL:HG11  | 1:A:80:LYS:HG3  | 8        | 0.51          |
| (1,1218) | 1:A:6:VAL:HG12  | 1:A:80:LYS:HG3  | 8        | 0.51          |
| (1,1218) | 1:A:6:VAL:HG13  | 1:A:80:LYS:HG3  | 8        | 0.51          |
| (1,1000) | 1:A:20:ALA:HB1  | 1:A:17:SER:HB3  | 5        | 0.51          |
| (1,1000) | 1:A:20:ALA:HB2  | 1:A:17:SER:HB3  | 5        | 0.51          |
| (1,1000) | 1:A:20:ALA:HB3  | 1:A:17:SER:HB3  | 5        | 0.51          |
| (2,223)  | 1:A:52:GLU:HB3  | 1:A:50:GLY:H    | 12       | 0.5           |
| (1,2462) | 1:A:65:LYS:HE3  | 1:A:65:LYS:HA   | 2        | 0.5           |
| (1,2431) | 1:A:6:VAL:HG21  | 1:A:10:GLN:HG2  | 5        | 0.5           |
| (1,2431) | 1:A:6:VAL:HG22  | 1:A:10:GLN:HG2  | 5        | 0.5           |
| (1,2431) | 1:A:6:VAL:HG23  | 1:A:10:GLN:HG2  | 5        | 0.5           |
| (1,2312) | 1:A:14:PHE:HB2  | 1:A:11:MET:HA   | 3        | 0.5           |
| (1,1872) | 1:A:65:LYS:HE3  | 1:A:64:THR:HG21 | 4        | 0.5           |
| (1,1872) | 1:A:65:LYS:HE3  | 1:A:64:THR:HG22 | 4        | 0.5           |
| (1,1872) | 1:A:65:LYS:HE3  | 1:A:64:THR:HG23 | 4        | 0.5           |
| (1,1847) | 1:A:6:VAL:HG11  | 1:A:80:LYS:HB3  | 3        | 0.5           |
| (1,1847) | 1:A:6:VAL:HG12  | 1:A:80:LYS:HB3  | 3        | 0.5           |
| (1,1847) | 1:A:6:VAL:HG13  | 1:A:80:LYS:HB3  | 3        | 0.5           |
| (1,1455) | 1:A:10:GLN:HA   | 1:A:13:GLU:HB2  | 1        | 0.5           |
| (1,1081) | 1:A:6:VAL:HG21  | 1:A:11:MET:HG2  | 6        | 0.5           |
| (1,1081) | 1:A:6:VAL:HG22  | 1:A:11:MET:HG2  | 6        | 0.5           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1081) | 1:A:6:VAL:HG23  | 1:A:11:MET:HG2  | 6        | 0.5           |
| (2,359)  | 1:A:109:THR:HA  | 1:A:113:LYS:HD3 | 3        | 0.49          |
| (2,223)  | 1:A:52:GLU:HB3  | 1:A:50:GLY:H    | 1        | 0.49          |
| (1,850)  | 1:A:109:THR:HA  | 1:A:108:GLU:HG3 | 2        | 0.49          |
| (1,56)   | 1:A:52:GLU:HA   | 1:A:50:GLY:H    | 5        | 0.49          |
| (1,2312) | 1:A:14:PHE:HB2  | 1:A:11:MET:HA   | 4        | 0.49          |
| (1,2312) | 1:A:14:PHE:HB2  | 1:A:11:MET:HA   | 5        | 0.49          |
| (1,2312) | 1:A:14:PHE:HB2  | 1:A:11:MET:HA   | 11       | 0.49          |
| (1,1983) | 1:A:126:ALA:HB1 | 1:A:122:GLU:HG3 | 8        | 0.49          |
| (1,1983) | 1:A:126:ALA:HB2 | 1:A:122:GLU:HG3 | 8        | 0.49          |
| (1,1983) | 1:A:126:ALA:HB3 | 1:A:122:GLU:HG3 | 8        | 0.49          |
| (1,1762) | 1:A:6:VAL:HG21  | 1:A:14:PHE:HE1  | 1        | 0.49          |
| (1,1762) | 1:A:6:VAL:HG21  | 1:A:14:PHE:HE2  | 1        | 0.49          |
| (1,1762) | 1:A:6:VAL:HG22  | 1:A:14:PHE:HE1  | 1        | 0.49          |
| (1,1762) | 1:A:6:VAL:HG22  | 1:A:14:PHE:HE2  | 1        | 0.49          |
| (1,1762) | 1:A:6:VAL:HG23  | 1:A:14:PHE:HE1  | 1        | 0.49          |
| (1,1762) | 1:A:6:VAL:HG23  | 1:A:14:PHE:HE2  | 1        | 0.49          |
| (1,1745) | 1:A:80:LYS:HE3  | 1:A:6:VAL:HG11  | 8        | 0.49          |
| (1,1745) | 1:A:80:LYS:HE3  | 1:A:6:VAL:HG12  | 8        | 0.49          |
| (1,1745) | 1:A:80:LYS:HE3  | 1:A:6:VAL:HG13  | 8        | 0.49          |
| (1,1016) | 1:A:6:VAL:HG21  | 1:A:11:MET:HG3  | 7        | 0.49          |
| (1,1016) | 1:A:6:VAL:HG22  | 1:A:11:MET:HG3  | 7        | 0.49          |
| (1,1016) | 1:A:6:VAL:HG23  | 1:A:11:MET:HG3  | 7        | 0.49          |
| (1,850)  | 1:A:109:THR:HA  | 1:A:108:GLU:HG3 | 5        | 0.48          |
| (1,2642) | 1:A:81:GLU:HA   | 1:A:84:ASP:HB3  | 4        | 0.48          |
| (1,2312) | 1:A:14:PHE:HB2  | 1:A:11:MET:HA   | 12       | 0.48          |
| (1,1983) | 1:A:126:ALA:HB1 | 1:A:122:GLU:HG3 | 6        | 0.48          |
| (1,1983) | 1:A:126:ALA:HB2 | 1:A:122:GLU:HG3 | 6        | 0.48          |
| (1,1983) | 1:A:126:ALA:HB3 | 1:A:122:GLU:HG3 | 6        | 0.48          |
| (1,1983) | 1:A:126:ALA:HB1 | 1:A:122:GLU:HG3 | 12       | 0.48          |
| (1,1983) | 1:A:126:ALA:HB2 | 1:A:122:GLU:HG3 | 12       | 0.48          |
| (1,1983) | 1:A:126:ALA:HB3 | 1:A:122:GLU:HG3 | 12       | 0.48          |
| (1,1745) | 1:A:80:LYS:HE3  | 1:A:6:VAL:HG11  | 3        | 0.48          |
| (1,1745) | 1:A:80:LYS:HE3  | 1:A:6:VAL:HG12  | 3        | 0.48          |
| (1,1745) | 1:A:80:LYS:HE3  | 1:A:6:VAL:HG13  | 3        | 0.48          |
| (2,300)  | 1:A:109:THR:HB  | 1:A:112:GLN:HG3 | 11       | 0.47          |
| (1,542)  | 1:A:108:GLU:HG2 | 1:A:113:LYS:H   | 6        | 0.47          |
| (1,542)  | 1:A:108:GLU:HG2 | 1:A:113:LYS:H   | 8        | 0.47          |
| (1,2431) | 1:A:6:VAL:HG21  | 1:A:10:GLN:HG2  | 6        | 0.47          |
| (1,2431) | 1:A:6:VAL:HG22  | 1:A:10:GLN:HG2  | 6        | 0.47          |
| (1,2431) | 1:A:6:VAL:HG23  | 1:A:10:GLN:HG2  | 6        | 0.47          |
| (1,2399) | 1:A:103:LYS:HE2 | 1:A:100:ALA:HB1 | 9        | 0.47          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2399) | 1:A:103:LYS:HE2 | 1:A:100:ALA:HB2 | 9        | 0.47          |
| (1,2399) | 1:A:103:LYS:HE2 | 1:A:100:ALA:HB3 | 9        | 0.47          |
| (1,1762) | 1:A:6:VAL:HG21  | 1:A:14:PHE:HE1  | 11       | 0.47          |
| (1,1762) | 1:A:6:VAL:HG21  | 1:A:14:PHE:HE2  | 11       | 0.47          |
| (1,1762) | 1:A:6:VAL:HG22  | 1:A:14:PHE:HE1  | 11       | 0.47          |
| (1,1762) | 1:A:6:VAL:HG22  | 1:A:14:PHE:HE2  | 11       | 0.47          |
| (1,1762) | 1:A:6:VAL:HG23  | 1:A:14:PHE:HE1  | 11       | 0.47          |
| (1,1762) | 1:A:6:VAL:HG23  | 1:A:14:PHE:HE2  | 11       | 0.47          |
| (1,1745) | 1:A:80:LYS:HE3  | 1:A:6:VAL:HG11  | 10       | 0.47          |
| (1,1745) | 1:A:80:LYS:HE3  | 1:A:6:VAL:HG12  | 10       | 0.47          |
| (1,1745) | 1:A:80:LYS:HE3  | 1:A:6:VAL:HG13  | 10       | 0.47          |
| (1,2543) | 1:A:59:ILE:HD11 | 1:A:55:GLN:HG3  | 9        | 0.46          |
| (1,2543) | 1:A:59:ILE:HD12 | 1:A:55:GLN:HG3  | 9        | 0.46          |
| (1,2543) | 1:A:59:ILE:HD13 | 1:A:55:GLN:HG3  | 9        | 0.46          |
| (1,2436) | 1:A:6:VAL:HG11  | 1:A:80:LYS:HB3  | 2        | 0.46          |
| (1,2436) | 1:A:6:VAL:HG12  | 1:A:80:LYS:HB3  | 2        | 0.46          |
| (1,2436) | 1:A:6:VAL:HG13  | 1:A:80:LYS:HB3  | 2        | 0.46          |
| (1,2267) | 1:A:92:LEU:HD21 | 1:A:123:TYR:HE1 | 6        | 0.46          |
| (1,2267) | 1:A:92:LEU:HD21 | 1:A:123:TYR:HE2 | 6        | 0.46          |
| (1,2267) | 1:A:92:LEU:HD22 | 1:A:123:TYR:HE1 | 6        | 0.46          |
| (1,2267) | 1:A:92:LEU:HD22 | 1:A:123:TYR:HE2 | 6        | 0.46          |
| (1,2267) | 1:A:92:LEU:HD23 | 1:A:123:TYR:HE1 | 6        | 0.46          |
| (1,2267) | 1:A:92:LEU:HD23 | 1:A:123:TYR:HE2 | 6        | 0.46          |
| (1,2024) | 1:A:10:GLN:HB3  | 1:A:6:VAL:HG21  | 8        | 0.46          |
| (1,2024) | 1:A:10:GLN:HB3  | 1:A:6:VAL:HG22  | 8        | 0.46          |
| (1,2024) | 1:A:10:GLN:HB3  | 1:A:6:VAL:HG23  | 8        | 0.46          |
| (1,2001) | 1:A:52:GLU:HG2  | 1:A:51:GLY:HA3  | 7        | 0.46          |
| (1,2001) | 1:A:52:GLU:HG2  | 1:A:51:GLY:HA3  | 11       | 0.46          |
| (1,1745) | 1:A:80:LYS:HE3  | 1:A:6:VAL:HG11  | 12       | 0.46          |
| (1,1745) | 1:A:80:LYS:HE3  | 1:A:6:VAL:HG12  | 12       | 0.46          |
| (1,1745) | 1:A:80:LYS:HE3  | 1:A:6:VAL:HG13  | 12       | 0.46          |
| (1,1510) | 1:A:78:TYR:HB2  | 1:A:79:MET:HE1  | 5        | 0.46          |
| (1,1510) | 1:A:78:TYR:HB2  | 1:A:79:MET:HE2  | 5        | 0.46          |
| (1,1510) | 1:A:78:TYR:HB2  | 1:A:79:MET:HE3  | 5        | 0.46          |
| (1,1274) | 1:A:6:VAL:HG21  | 1:A:11:MET:HB2  | 12       | 0.46          |
| (1,1274) | 1:A:6:VAL:HG21  | 1:A:11:MET:HB3  | 12       | 0.46          |
| (1,1274) | 1:A:6:VAL:HG22  | 1:A:11:MET:HB2  | 12       | 0.46          |
| (1,1274) | 1:A:6:VAL:HG22  | 1:A:11:MET:HB3  | 12       | 0.46          |
| (1,1274) | 1:A:6:VAL:HG23  | 1:A:11:MET:HB2  | 12       | 0.46          |
| (1,1274) | 1:A:6:VAL:HG23  | 1:A:11:MET:HB3  | 12       | 0.46          |
| (1,2312) | 1:A:14:PHE:HB2  | 1:A:11:MET:HA   | 2        | 0.45          |
| (1,1847) | 1:A:6:VAL:HG11  | 1:A:80:LYS:HB3  | 6        | 0.45          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1847) | 1:A:6:VAL:HG12  | 1:A:80:LYS:HB3  | 6        | 0.45          |
| (1,1847) | 1:A:6:VAL:HG13  | 1:A:80:LYS:HB3  | 6        | 0.45          |
| (1,1762) | 1:A:6:VAL:HG21  | 1:A:14:PHE:HE1  | 3        | 0.45          |
| (1,1762) | 1:A:6:VAL:HG21  | 1:A:14:PHE:HE2  | 3        | 0.45          |
| (1,1762) | 1:A:6:VAL:HG22  | 1:A:14:PHE:HE1  | 3        | 0.45          |
| (1,1762) | 1:A:6:VAL:HG22  | 1:A:14:PHE:HE2  | 3        | 0.45          |
| (1,1762) | 1:A:6:VAL:HG23  | 1:A:14:PHE:HE1  | 3        | 0.45          |
| (1,1762) | 1:A:6:VAL:HG23  | 1:A:14:PHE:HE2  | 3        | 0.45          |
| (1,1455) | 1:A:10:GLN:HA   | 1:A:13:GLU:HB2  | 8        | 0.45          |
| (1,1336) | 1:A:38:LEU:HA   | 1:A:43:LEU:HD21 | 2        | 0.45          |
| (1,1336) | 1:A:38:LEU:HA   | 1:A:43:LEU:HD22 | 2        | 0.45          |
| (1,1336) | 1:A:38:LEU:HA   | 1:A:43:LEU:HD23 | 2        | 0.45          |
| (1,1274) | 1:A:6:VAL:HG21  | 1:A:11:MET:HB2  | 10       | 0.45          |
| (1,1274) | 1:A:6:VAL:HG21  | 1:A:11:MET:HB3  | 10       | 0.45          |
| (1,1274) | 1:A:6:VAL:HG22  | 1:A:11:MET:HB2  | 10       | 0.45          |
| (1,1274) | 1:A:6:VAL:HG22  | 1:A:11:MET:HB3  | 10       | 0.45          |
| (1,1274) | 1:A:6:VAL:HG23  | 1:A:11:MET:HB2  | 10       | 0.45          |
| (1,1274) | 1:A:6:VAL:HG23  | 1:A:11:MET:HB3  | 10       | 0.45          |
| (1,865)  | 1:A:139:ALA:HA  | 1:A:142:LYS:HB3 | 5        | 0.44          |
| (1,2408) | 1:A:6:VAL:HG21  | 1:A:14:PHE:HD1  | 11       | 0.44          |
| (1,2408) | 1:A:6:VAL:HG21  | 1:A:14:PHE:HD2  | 11       | 0.44          |
| (1,2408) | 1:A:6:VAL:HG22  | 1:A:14:PHE:HD1  | 11       | 0.44          |
| (1,2408) | 1:A:6:VAL:HG22  | 1:A:14:PHE:HD2  | 11       | 0.44          |
| (1,2408) | 1:A:6:VAL:HG23  | 1:A:14:PHE:HD1  | 11       | 0.44          |
| (1,2408) | 1:A:6:VAL:HG23  | 1:A:14:PHE:HD2  | 11       | 0.44          |
| (1,2024) | 1:A:10:GLN:HB3  | 1:A:6:VAL:HG21  | 3        | 0.44          |
| (1,2024) | 1:A:10:GLN:HB3  | 1:A:6:VAL:HG22  | 3        | 0.44          |
| (1,2024) | 1:A:10:GLN:HB3  | 1:A:6:VAL:HG23  | 3        | 0.44          |
| (1,1983) | 1:A:126:ALA:HB1 | 1:A:122:GLU:HG3 | 3        | 0.44          |
| (1,1983) | 1:A:126:ALA:HB2 | 1:A:122:GLU:HG3 | 3        | 0.44          |
| (1,1983) | 1:A:126:ALA:HB3 | 1:A:122:GLU:HG3 | 3        | 0.44          |
| (1,1983) | 1:A:126:ALA:HB1 | 1:A:122:GLU:HG3 | 11       | 0.44          |
| (1,1983) | 1:A:126:ALA:HB2 | 1:A:122:GLU:HG3 | 11       | 0.44          |
| (1,1983) | 1:A:126:ALA:HB3 | 1:A:122:GLU:HG3 | 11       | 0.44          |
| (1,1933) | 1:A:78:TYR:HB3  | 1:A:63:VAL:HA   | 4        | 0.44          |
| (1,1510) | 1:A:78:TYR:HB2  | 1:A:79:MET:HE1  | 1        | 0.44          |
| (1,1510) | 1:A:78:TYR:HB2  | 1:A:79:MET:HE2  | 1        | 0.44          |
| (1,1510) | 1:A:78:TYR:HB2  | 1:A:79:MET:HE3  | 1        | 0.44          |
| (1,1483) | 1:A:15:LYS:HD2  | 1:A:15:LYS:HA   | 12       | 0.44          |
| (1,1334) | 1:A:38:LEU:HD11 | 1:A:43:LEU:HB3  | 1        | 0.44          |
| (1,1334) | 1:A:38:LEU:HD12 | 1:A:43:LEU:HB3  | 1        | 0.44          |
| (1,1334) | 1:A:38:LEU:HD13 | 1:A:43:LEU:HB3  | 1        | 0.44          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1259) | 1:A:38:LEU:HD21  | 1:A:59:ILE:HG21 | 12       | 0.44          |
| (1,1259) | 1:A:38:LEU:HD21  | 1:A:59:ILE:HG22 | 12       | 0.44          |
| (1,1259) | 1:A:38:LEU:HD21  | 1:A:59:ILE:HG23 | 12       | 0.44          |
| (1,1259) | 1:A:38:LEU:HD22  | 1:A:59:ILE:HG21 | 12       | 0.44          |
| (1,1259) | 1:A:38:LEU:HD22  | 1:A:59:ILE:HG22 | 12       | 0.44          |
| (1,1259) | 1:A:38:LEU:HD22  | 1:A:59:ILE:HG23 | 12       | 0.44          |
| (1,1259) | 1:A:38:LEU:HD23  | 1:A:59:ILE:HG21 | 12       | 0.44          |
| (1,1259) | 1:A:38:LEU:HD23  | 1:A:59:ILE:HG22 | 12       | 0.44          |
| (1,1259) | 1:A:38:LEU:HD23  | 1:A:59:ILE:HG23 | 12       | 0.44          |
| (1,2024) | 1:A:10:GLN:HB3   | 1:A:6:VAL:HG21  | 1        | 0.43          |
| (1,2024) | 1:A:10:GLN:HB3   | 1:A:6:VAL:HG22  | 1        | 0.43          |
| (1,2024) | 1:A:10:GLN:HB3   | 1:A:6:VAL:HG23  | 1        | 0.43          |
| (1,1983) | 1:A:126:ALA:HB1  | 1:A:122:GLU:HG3 | 10       | 0.43          |
| (1,1983) | 1:A:126:ALA:HB2  | 1:A:122:GLU:HG3 | 10       | 0.43          |
| (1,1983) | 1:A:126:ALA:HB3  | 1:A:122:GLU:HG3 | 10       | 0.43          |
| (1,1762) | 1:A:6:VAL:HG21   | 1:A:14:PHE:HE1  | 5        | 0.43          |
| (1,1762) | 1:A:6:VAL:HG21   | 1:A:14:PHE:HE2  | 5        | 0.43          |
| (1,1762) | 1:A:6:VAL:HG22   | 1:A:14:PHE:HE1  | 5        | 0.43          |
| (1,1762) | 1:A:6:VAL:HG22   | 1:A:14:PHE:HE2  | 5        | 0.43          |
| (1,1762) | 1:A:6:VAL:HG23   | 1:A:14:PHE:HE1  | 5        | 0.43          |
| (1,1762) | 1:A:6:VAL:HG23   | 1:A:14:PHE:HE2  | 5        | 0.43          |
| (1,1745) | 1:A:80:LYS:HE3   | 1:A:6:VAL:HG11  | 6        | 0.43          |
| (1,1745) | 1:A:80:LYS:HE3   | 1:A:6:VAL:HG12  | 6        | 0.43          |
| (1,1745) | 1:A:80:LYS:HE3   | 1:A:6:VAL:HG13  | 6        | 0.43          |
| (1,1745) | 1:A:80:LYS:HE3   | 1:A:6:VAL:HG11  | 7        | 0.43          |
| (1,1745) | 1:A:80:LYS:HE3   | 1:A:6:VAL:HG12  | 7        | 0.43          |
| (1,1745) | 1:A:80:LYS:HE3   | 1:A:6:VAL:HG13  | 7        | 0.43          |
| (1,1510) | 1:A:78:TYR:HB2   | 1:A:79:MET:HE1  | 4        | 0.43          |
| (1,1510) | 1:A:78:TYR:HB2   | 1:A:79:MET:HE2  | 4        | 0.43          |
| (1,1510) | 1:A:78:TYR:HB2   | 1:A:79:MET:HE3  | 4        | 0.43          |
| (1,1387) | 1:A:109:THR:HG21 | 1:A:113:LYS:HE3 | 5        | 0.43          |
| (1,1387) | 1:A:109:THR:HG22 | 1:A:113:LYS:HE3 | 5        | 0.43          |
| (1,1387) | 1:A:109:THR:HG23 | 1:A:113:LYS:HE3 | 5        | 0.43          |
| (1,1334) | 1:A:38:LEU:HD11  | 1:A:43:LEU:HB3  | 10       | 0.43          |
| (1,1334) | 1:A:38:LEU:HD12  | 1:A:43:LEU:HB3  | 10       | 0.43          |
| (1,1334) | 1:A:38:LEU:HD13  | 1:A:43:LEU:HB3  | 10       | 0.43          |
| (2,300)  | 1:A:109:THR:HB   | 1:A:112:GLN:HG3 | 1        | 0.42          |
| (1,850)  | 1:A:109:THR:HA   | 1:A:108:GLU:HG3 | 9        | 0.42          |
| (1,2436) | 1:A:6:VAL:HG11   | 1:A:80:LYS:HB3  | 10       | 0.42          |
| (1,2436) | 1:A:6:VAL:HG12   | 1:A:80:LYS:HB3  | 10       | 0.42          |
| (1,2436) | 1:A:6:VAL:HG13   | 1:A:80:LYS:HB3  | 10       | 0.42          |
| (1,2290) | 1:A:40:SER:HB3   | 1:A:37:CYS:HA   | 11       | 0.42          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2054) | 1:A:69:GLY:HA3   | 1:A:28:ILE:HB   | 4        | 0.42          |
| (1,2024) | 1:A:10:GLN:HB3   | 1:A:6:VAL:HG21  | 5        | 0.42          |
| (1,2024) | 1:A:10:GLN:HB3   | 1:A:6:VAL:HG22  | 5        | 0.42          |
| (1,2024) | 1:A:10:GLN:HB3   | 1:A:6:VAL:HG23  | 5        | 0.42          |
| (1,2024) | 1:A:10:GLN:HB3   | 1:A:6:VAL:HG21  | 6        | 0.42          |
| (1,2024) | 1:A:10:GLN:HB3   | 1:A:6:VAL:HG22  | 6        | 0.42          |
| (1,2024) | 1:A:10:GLN:HB3   | 1:A:6:VAL:HG23  | 6        | 0.42          |
| (1,2024) | 1:A:10:GLN:HB3   | 1:A:6:VAL:HG21  | 7        | 0.42          |
| (1,2024) | 1:A:10:GLN:HB3   | 1:A:6:VAL:HG22  | 7        | 0.42          |
| (1,2024) | 1:A:10:GLN:HB3   | 1:A:6:VAL:HG23  | 7        | 0.42          |
| (1,1745) | 1:A:80:LYS:HE3   | 1:A:6:VAL:HG11  | 1        | 0.42          |
| (1,1745) | 1:A:80:LYS:HE3   | 1:A:6:VAL:HG12  | 1        | 0.42          |
| (1,1745) | 1:A:80:LYS:HE3   | 1:A:6:VAL:HG13  | 1        | 0.42          |
| (1,850)  | 1:A:109:THR:HA   | 1:A:108:GLU:HG3 | 3        | 0.41          |
| (1,2408) | 1:A:6:VAL:HG21   | 1:A:14:PHE:HD1  | 1        | 0.41          |
| (1,2408) | 1:A:6:VAL:HG21   | 1:A:14:PHE:HD2  | 1        | 0.41          |
| (1,2408) | 1:A:6:VAL:HG22   | 1:A:14:PHE:HD1  | 1        | 0.41          |
| (1,2408) | 1:A:6:VAL:HG22   | 1:A:14:PHE:HD2  | 1        | 0.41          |
| (1,2408) | 1:A:6:VAL:HG23   | 1:A:14:PHE:HD1  | 1        | 0.41          |
| (1,2408) | 1:A:6:VAL:HG23   | 1:A:14:PHE:HD2  | 1        | 0.41          |
| (1,2408) | 1:A:6:VAL:HG21   | 1:A:14:PHE:HD1  | 8        | 0.41          |
| (1,2408) | 1:A:6:VAL:HG21   | 1:A:14:PHE:HD2  | 8        | 0.41          |
| (1,2408) | 1:A:6:VAL:HG22   | 1:A:14:PHE:HD1  | 8        | 0.41          |
| (1,2408) | 1:A:6:VAL:HG22   | 1:A:14:PHE:HD2  | 8        | 0.41          |
| (1,2408) | 1:A:6:VAL:HG23   | 1:A:14:PHE:HD1  | 8        | 0.41          |
| (1,2408) | 1:A:6:VAL:HG23   | 1:A:14:PHE:HD2  | 8        | 0.41          |
| (1,2370) | 1:A:141:VAL:HG11 | 1:A:138:ALA:HA  | 9        | 0.41          |
| (1,2370) | 1:A:141:VAL:HG12 | 1:A:138:ALA:HA  | 9        | 0.41          |
| (1,2370) | 1:A:141:VAL:HG13 | 1:A:138:ALA:HA  | 9        | 0.41          |
| (1,2121) | 1:A:78:TYR:HE1   | 1:A:43:LEU:HD21 | 7        | 0.41          |
| (1,2121) | 1:A:78:TYR:HE1   | 1:A:43:LEU:HD22 | 7        | 0.41          |
| (1,2121) | 1:A:78:TYR:HE1   | 1:A:43:LEU:HD23 | 7        | 0.41          |
| (1,2121) | 1:A:78:TYR:HE2   | 1:A:43:LEU:HD21 | 7        | 0.41          |
| (1,2121) | 1:A:78:TYR:HE2   | 1:A:43:LEU:HD22 | 7        | 0.41          |
| (1,2121) | 1:A:78:TYR:HE2   | 1:A:43:LEU:HD23 | 7        | 0.41          |
| (1,2024) | 1:A:10:GLN:HB3   | 1:A:6:VAL:HG21  | 11       | 0.41          |
| (1,2024) | 1:A:10:GLN:HB3   | 1:A:6:VAL:HG22  | 11       | 0.41          |
| (1,2024) | 1:A:10:GLN:HB3   | 1:A:6:VAL:HG23  | 11       | 0.41          |
| (1,1539) | 1:A:6:VAL:HG21   | 1:A:11:MET:HE1  | 2        | 0.41          |
| (1,1539) | 1:A:6:VAL:HG21   | 1:A:11:MET:HE2  | 2        | 0.41          |
| (1,1539) | 1:A:6:VAL:HG21   | 1:A:11:MET:HE3  | 2        | 0.41          |
| (1,1539) | 1:A:6:VAL:HG22   | 1:A:11:MET:HE1  | 2        | 0.41          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1539) | 1:A:6:VAL:HG22  | 1:A:11:MET:HE2  | 2        | 0.41          |
| (1,1539) | 1:A:6:VAL:HG22  | 1:A:11:MET:HE3  | 2        | 0.41          |
| (1,1539) | 1:A:6:VAL:HG23  | 1:A:11:MET:HE1  | 2        | 0.41          |
| (1,1539) | 1:A:6:VAL:HG23  | 1:A:11:MET:HE2  | 2        | 0.41          |
| (1,1539) | 1:A:6:VAL:HG23  | 1:A:11:MET:HE3  | 2        | 0.41          |
| (1,1119) | 1:A:70:VAL:HG21 | 1:A:71:SER:HB3  | 3        | 0.41          |
| (1,1119) | 1:A:70:VAL:HG22 | 1:A:71:SER:HB3  | 3        | 0.41          |
| (1,1119) | 1:A:70:VAL:HG23 | 1:A:71:SER:HB3  | 3        | 0.41          |
| (2,332)  | 1:A:32:LEU:HD21 | 1:A:35:ARG:HD3  | 1        | 0.4           |
| (2,332)  | 1:A:32:LEU:HD22 | 1:A:35:ARG:HD3  | 1        | 0.4           |
| (2,332)  | 1:A:32:LEU:HD23 | 1:A:35:ARG:HD3  | 1        | 0.4           |
| (1,2641) | 1:A:122:GLU:HB2 | 1:A:126:ALA:HB1 | 4        | 0.4           |
| (1,2641) | 1:A:122:GLU:HB2 | 1:A:126:ALA:HB2 | 4        | 0.4           |
| (1,2641) | 1:A:122:GLU:HB2 | 1:A:126:ALA:HB3 | 4        | 0.4           |
| (1,2267) | 1:A:92:LEU:HD21 | 1:A:123:TYR:HE1 | 2        | 0.4           |
| (1,2267) | 1:A:92:LEU:HD21 | 1:A:123:TYR:HE2 | 2        | 0.4           |
| (1,2267) | 1:A:92:LEU:HD22 | 1:A:123:TYR:HE1 | 2        | 0.4           |
| (1,2267) | 1:A:92:LEU:HD22 | 1:A:123:TYR:HE2 | 2        | 0.4           |
| (1,2267) | 1:A:92:LEU:HD23 | 1:A:123:TYR:HE1 | 2        | 0.4           |
| (1,2267) | 1:A:92:LEU:HD23 | 1:A:123:TYR:HE2 | 2        | 0.4           |
| (1,2132) | 1:A:65:LYS:HG2  | 1:A:65:LYS:HA   | 12       | 0.4           |
| (1,1847) | 1:A:6:VAL:HG11  | 1:A:80:LYS:HB3  | 11       | 0.4           |
| (1,1847) | 1:A:6:VAL:HG12  | 1:A:80:LYS:HB3  | 11       | 0.4           |
| (1,1847) | 1:A:6:VAL:HG13  | 1:A:80:LYS:HB3  | 11       | 0.4           |
| (1,1779) | 1:A:43:LEU:HD11 | 1:A:82:LYS:HE2  | 2        | 0.4           |
| (1,1779) | 1:A:43:LEU:HD12 | 1:A:82:LYS:HE2  | 2        | 0.4           |
| (1,1779) | 1:A:43:LEU:HD13 | 1:A:82:LYS:HE2  | 2        | 0.4           |
| (1,1638) | 1:A:21:PHE:HE1  | 1:A:17:SER:HB3  | 9        | 0.4           |
| (1,1638) | 1:A:21:PHE:HE2  | 1:A:17:SER:HB3  | 9        | 0.4           |
| (1,1119) | 1:A:70:VAL:HG21 | 1:A:71:SER:HB3  | 8        | 0.4           |
| (1,1119) | 1:A:70:VAL:HG22 | 1:A:71:SER:HB3  | 8        | 0.4           |
| (1,1119) | 1:A:70:VAL:HG23 | 1:A:71:SER:HB3  | 8        | 0.4           |
| (1,1024) | 1:A:15:LYS:HE3  | 1:A:15:LYS:HA   | 1        | 0.4           |
| (1,824)  | 1:A:77:GLN:HB3  | 1:A:74:ASN:HA   | 7        | 0.39          |
| (1,56)   | 1:A:52:GLU:HA   | 1:A:50:GLY:H    | 7        | 0.39          |
| (1,2431) | 1:A:6:VAL:HG21  | 1:A:10:GLN:HG2  | 11       | 0.39          |
| (1,2431) | 1:A:6:VAL:HG22  | 1:A:10:GLN:HG2  | 11       | 0.39          |
| (1,2431) | 1:A:6:VAL:HG23  | 1:A:10:GLN:HG2  | 11       | 0.39          |
| (1,2001) | 1:A:52:GLU:HG2  | 1:A:51:GLY:HA3  | 3        | 0.39          |
| (1,1483) | 1:A:15:LYS:HD2  | 1:A:15:LYS:HA   | 9        | 0.39          |
| (1,1081) | 1:A:6:VAL:HG21  | 1:A:11:MET:HG2  | 5        | 0.39          |
| (1,1081) | 1:A:6:VAL:HG22  | 1:A:11:MET:HG2  | 5        | 0.39          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1081) | 1:A:6:VAL:HG23  | 1:A:11:MET:HG2  | 5        | 0.39          |
| (1,850)  | 1:A:109:THR:HA  | 1:A:108:GLU:HG3 | 10       | 0.38          |
| (1,2653) | 1:A:61:ASN:HB3  | 1:A:58:ALA:HB1  | 2        | 0.38          |
| (1,2653) | 1:A:61:ASN:HB3  | 1:A:58:ALA:HB2  | 2        | 0.38          |
| (1,2653) | 1:A:61:ASN:HB3  | 1:A:58:ALA:HB3  | 2        | 0.38          |
| (1,2462) | 1:A:65:LYS:HE3  | 1:A:65:LYS:HA   | 3        | 0.38          |
| (1,2436) | 1:A:6:VAL:HG11  | 1:A:80:LYS:HB3  | 8        | 0.38          |
| (1,2436) | 1:A:6:VAL:HG12  | 1:A:80:LYS:HB3  | 8        | 0.38          |
| (1,2436) | 1:A:6:VAL:HG13  | 1:A:80:LYS:HB3  | 8        | 0.38          |
| (1,2431) | 1:A:6:VAL:HG21  | 1:A:10:GLN:HG2  | 7        | 0.38          |
| (1,2431) | 1:A:6:VAL:HG22  | 1:A:10:GLN:HG2  | 7        | 0.38          |
| (1,2431) | 1:A:6:VAL:HG23  | 1:A:10:GLN:HG2  | 7        | 0.38          |
| (1,2368) | 1:A:32:LEU:HA   | 1:A:35:ARG:HD2  | 6        | 0.38          |
| (1,2167) | 1:A:81:GLU:HA   | 1:A:84:ASP:HB3  | 3        | 0.38          |
| (1,1716) | 1:A:40:SER:HB3  | 1:A:37:CYS:HA   | 11       | 0.38          |
| (1,1656) | 1:A:8:ALA:HB1   | 1:A:11:MET:HG2  | 9        | 0.38          |
| (1,1656) | 1:A:8:ALA:HB2   | 1:A:11:MET:HG2  | 9        | 0.38          |
| (1,1656) | 1:A:8:ALA:HB3   | 1:A:11:MET:HG2  | 9        | 0.38          |
| (1,1631) | 1:A:109:THR:HB  | 1:A:108:GLU:HG3 | 12       | 0.38          |
| (1,1336) | 1:A:38:LEU:HA   | 1:A:43:LEU:HD21 | 3        | 0.38          |
| (1,1336) | 1:A:38:LEU:HA   | 1:A:43:LEU:HD22 | 3        | 0.38          |
| (1,1336) | 1:A:38:LEU:HA   | 1:A:43:LEU:HD23 | 3        | 0.38          |
| (1,1334) | 1:A:38:LEU:HD11 | 1:A:43:LEU:HB3  | 11       | 0.38          |
| (1,1334) | 1:A:38:LEU:HD12 | 1:A:43:LEU:HB3  | 11       | 0.38          |
| (1,1334) | 1:A:38:LEU:HD13 | 1:A:43:LEU:HB3  | 11       | 0.38          |
| (1,1119) | 1:A:70:VAL:HG21 | 1:A:71:SER:HB3  | 7        | 0.38          |
| (1,1119) | 1:A:70:VAL:HG22 | 1:A:71:SER:HB3  | 7        | 0.38          |
| (1,1119) | 1:A:70:VAL:HG23 | 1:A:71:SER:HB3  | 7        | 0.38          |
| (1,1021) | 1:A:6:VAL:HG11  | 1:A:80:LYS:HG3  | 8        | 0.38          |
| (1,1021) | 1:A:6:VAL:HG12  | 1:A:80:LYS:HG3  | 8        | 0.38          |
| (1,1021) | 1:A:6:VAL:HG13  | 1:A:80:LYS:HG3  | 8        | 0.38          |
| (3,133)  | 1:A:91:GLN:O    | 1:A:94:GLU:N    | 5        | 0.37          |
| (3,123)  | 1:A:59:ILE:O    | 1:A:63:VAL:N    | 3        | 0.37          |
| (2,223)  | 1:A:52:GLU:HB3  | 1:A:50:GLY:H    | 5        | 0.37          |
| (1,1745) | 1:A:80:LYS:HE3  | 1:A:6:VAL:HG11  | 5        | 0.37          |
| (1,1745) | 1:A:80:LYS:HE3  | 1:A:6:VAL:HG12  | 5        | 0.37          |
| (1,1745) | 1:A:80:LYS:HE3  | 1:A:6:VAL:HG13  | 5        | 0.37          |
| (1,1721) | 1:A:15:LYS:HD2  | 1:A:15:LYS:HA   | 12       | 0.37          |
| (1,1259) | 1:A:38:LEU:HD21 | 1:A:59:ILE:HG21 | 7        | 0.37          |
| (1,1259) | 1:A:38:LEU:HD21 | 1:A:59:ILE:HG22 | 7        | 0.37          |
| (1,1259) | 1:A:38:LEU:HD21 | 1:A:59:ILE:HG23 | 7        | 0.37          |
| (1,1259) | 1:A:38:LEU:HD22 | 1:A:59:ILE:HG21 | 7        | 0.37          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1259) | 1:A:38:LEU:HD22  | 1:A:59:ILE:HG22 | 7        | 0.37          |
| (1,1259) | 1:A:38:LEU:HD22  | 1:A:59:ILE:HG23 | 7        | 0.37          |
| (1,1259) | 1:A:38:LEU:HD23  | 1:A:59:ILE:HG21 | 7        | 0.37          |
| (1,1259) | 1:A:38:LEU:HD23  | 1:A:59:ILE:HG22 | 7        | 0.37          |
| (1,1259) | 1:A:38:LEU:HD23  | 1:A:59:ILE:HG23 | 7        | 0.37          |
| (1,1149) | 1:A:82:LYS:HA    | 1:A:85:GLU:HG3  | 4        | 0.37          |
| (3,149)  | 1:A:136:ASP:O    | 1:A:139:ALA:N   | 5        | 0.36          |
| (3,119)  | 1:A:45:ASP:O     | 1:A:47:ASP:N    | 3        | 0.36          |
| (3,119)  | 1:A:45:ASP:O     | 1:A:47:ASP:N    | 12       | 0.36          |
| (3,101)  | 1:A:7:THR:O      | 1:A:11:MET:N    | 3        | 0.36          |
| (3,101)  | 1:A:7:THR:O      | 1:A:11:MET:N    | 7        | 0.36          |
| (1,2641) | 1:A:122:GLU:HB2  | 1:A:126:ALA:HB1 | 9        | 0.36          |
| (1,2641) | 1:A:122:GLU:HB2  | 1:A:126:ALA:HB2 | 9        | 0.36          |
| (1,2641) | 1:A:122:GLU:HB2  | 1:A:126:ALA:HB3 | 9        | 0.36          |
| (1,2138) | 1:A:6:VAL:HG11   | 1:A:5:GLY:HA3   | 11       | 0.36          |
| (1,2138) | 1:A:6:VAL:HG12   | 1:A:5:GLY:HA3   | 11       | 0.36          |
| (1,2138) | 1:A:6:VAL:HG13   | 1:A:5:GLY:HA3   | 11       | 0.36          |
| (1,1847) | 1:A:6:VAL:HG11   | 1:A:80:LYS:HB3  | 4        | 0.36          |
| (1,1847) | 1:A:6:VAL:HG12   | 1:A:80:LYS:HB3  | 4        | 0.36          |
| (1,1847) | 1:A:6:VAL:HG13   | 1:A:80:LYS:HB3  | 4        | 0.36          |
| (1,1712) | 1:A:106:ILE:HA   | 1:A:103:LYS:HE3 | 2        | 0.36          |
| (3,139)  | 1:A:107:THR:O    | 1:A:111:MET:N   | 5        | 0.35          |
| (3,139)  | 1:A:107:THR:O    | 1:A:111:MET:N   | 7        | 0.35          |
| (3,120)  | 1:A:54:ALA:O     | 1:A:58:ALA:N    | 9        | 0.35          |
| (3,108)  | 1:A:16:GLN:O     | 1:A:20:ALA:N    | 4        | 0.35          |
| (3,101)  | 1:A:7:THR:O      | 1:A:11:MET:N    | 10       | 0.35          |
| (2,300)  | 1:A:109:THR:HB   | 1:A:112:GLN:HG3 | 2        | 0.35          |
| (1,802)  | 1:A:54:ALA:HB1   | 1:A:57:ASP:HB3  | 11       | 0.35          |
| (1,802)  | 1:A:54:ALA:HB2   | 1:A:57:ASP:HB3  | 11       | 0.35          |
| (1,802)  | 1:A:54:ALA:HB3   | 1:A:57:ASP:HB3  | 11       | 0.35          |
| (1,2543) | 1:A:59:ILE:HD11  | 1:A:55:GLN:HG3  | 10       | 0.35          |
| (1,2543) | 1:A:59:ILE:HD12  | 1:A:55:GLN:HG3  | 10       | 0.35          |
| (1,2543) | 1:A:59:ILE:HD13  | 1:A:55:GLN:HG3  | 10       | 0.35          |
| (1,2326) | 1:A:74:ASN:HA    | 1:A:77:GLN:HG3  | 11       | 0.35          |
| (1,1455) | 1:A:10:GLN:HA    | 1:A:13:GLU:HB2  | 2        | 0.35          |
| (1,1439) | 1:A:141:VAL:HG11 | 1:A:137:TYR:HE1 | 2        | 0.35          |
| (1,1439) | 1:A:141:VAL:HG11 | 1:A:137:TYR:HE2 | 2        | 0.35          |
| (1,1439) | 1:A:141:VAL:HG12 | 1:A:137:TYR:HE1 | 2        | 0.35          |
| (1,1439) | 1:A:141:VAL:HG12 | 1:A:137:TYR:HE2 | 2        | 0.35          |
| (1,1439) | 1:A:141:VAL:HG13 | 1:A:137:TYR:HE1 | 2        | 0.35          |
| (1,1439) | 1:A:141:VAL:HG13 | 1:A:137:TYR:HE2 | 2        | 0.35          |
| (1,1334) | 1:A:38:LEU:HD11  | 1:A:43:LEU:HB3  | 2        | 0.35          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1334) | 1:A:38:LEU:HD12 | 1:A:43:LEU:HB3  | 2        | 0.35          |
| (1,1334) | 1:A:38:LEU:HD13 | 1:A:43:LEU:HB3  | 2        | 0.35          |
| (3,149)  | 1:A:136:ASP:O   | 1:A:139:ALA:N   | 6        | 0.34          |
| (3,120)  | 1:A:54:ALA:O    | 1:A:58:ALA:N    | 4        | 0.34          |
| (3,120)  | 1:A:54:ALA:O    | 1:A:58:ALA:N    | 5        | 0.34          |
| (3,120)  | 1:A:54:ALA:O    | 1:A:58:ALA:N    | 6        | 0.34          |
| (3,120)  | 1:A:54:ALA:O    | 1:A:58:ALA:N    | 8        | 0.34          |
| (3,108)  | 1:A:16:GLN:O    | 1:A:20:ALA:N    | 9        | 0.34          |
| (3,107)  | 1:A:14:PHE:O    | 1:A:18:PHE:N    | 5        | 0.34          |
| (3,101)  | 1:A:7:THR:O     | 1:A:11:MET:N    | 6        | 0.34          |
| (1,2408) | 1:A:6:VAL:HG21  | 1:A:14:PHE:HD1  | 7        | 0.34          |
| (1,2408) | 1:A:6:VAL:HG21  | 1:A:14:PHE:HD2  | 7        | 0.34          |
| (1,2408) | 1:A:6:VAL:HG22  | 1:A:14:PHE:HD1  | 7        | 0.34          |
| (1,2408) | 1:A:6:VAL:HG22  | 1:A:14:PHE:HD2  | 7        | 0.34          |
| (1,2408) | 1:A:6:VAL:HG23  | 1:A:14:PHE:HD1  | 7        | 0.34          |
| (1,2408) | 1:A:6:VAL:HG23  | 1:A:14:PHE:HD2  | 7        | 0.34          |
| (1,2211) | 1:A:136:ASP:HB3 | 1:A:129:PRO:HG3 | 10       | 0.34          |
| (1,2083) | 1:A:89:PRO:HA   | 1:A:92:LEU:HD21 | 10       | 0.34          |
| (1,2083) | 1:A:89:PRO:HA   | 1:A:92:LEU:HD22 | 10       | 0.34          |
| (1,2083) | 1:A:89:PRO:HA   | 1:A:92:LEU:HD23 | 10       | 0.34          |
| (1,2080) | 1:A:38:LEU:HD21 | 1:A:59:ILE:HG21 | 4        | 0.34          |
| (1,2080) | 1:A:38:LEU:HD21 | 1:A:59:ILE:HG22 | 4        | 0.34          |
| (1,2080) | 1:A:38:LEU:HD21 | 1:A:59:ILE:HG23 | 4        | 0.34          |
| (1,2080) | 1:A:38:LEU:HD22 | 1:A:59:ILE:HG21 | 4        | 0.34          |
| (1,2080) | 1:A:38:LEU:HD22 | 1:A:59:ILE:HG22 | 4        | 0.34          |
| (1,2080) | 1:A:38:LEU:HD22 | 1:A:59:ILE:HG23 | 4        | 0.34          |
| (1,2080) | 1:A:38:LEU:HD23 | 1:A:59:ILE:HG21 | 4        | 0.34          |
| (1,2080) | 1:A:38:LEU:HD23 | 1:A:59:ILE:HG22 | 4        | 0.34          |
| (1,2080) | 1:A:38:LEU:HD23 | 1:A:59:ILE:HG23 | 4        | 0.34          |
| (1,2080) | 1:A:38:LEU:HD21 | 1:A:59:ILE:HG21 | 5        | 0.34          |
| (1,2080) | 1:A:38:LEU:HD21 | 1:A:59:ILE:HG22 | 5        | 0.34          |
| (1,2080) | 1:A:38:LEU:HD21 | 1:A:59:ILE:HG23 | 5        | 0.34          |
| (1,2080) | 1:A:38:LEU:HD22 | 1:A:59:ILE:HG21 | 5        | 0.34          |
| (1,2080) | 1:A:38:LEU:HD22 | 1:A:59:ILE:HG22 | 5        | 0.34          |
| (1,2080) | 1:A:38:LEU:HD22 | 1:A:59:ILE:HG23 | 5        | 0.34          |
| (1,2080) | 1:A:38:LEU:HD23 | 1:A:59:ILE:HG21 | 5        | 0.34          |
| (1,2080) | 1:A:38:LEU:HD23 | 1:A:59:ILE:HG22 | 5        | 0.34          |
| (1,2080) | 1:A:38:LEU:HD23 | 1:A:59:ILE:HG23 | 5        | 0.34          |
| (1,1978) | 1:A:38:LEU:HA   | 1:A:43:LEU:HD21 | 7        | 0.34          |
| (1,1978) | 1:A:38:LEU:HA   | 1:A:43:LEU:HD22 | 7        | 0.34          |
| (1,1978) | 1:A:38:LEU:HA   | 1:A:43:LEU:HD23 | 7        | 0.34          |
| (1,1724) | 1:A:56:TYR:HE1  | 1:A:38:LEU:HD21 | 3        | 0.34          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1724) | 1:A:56:TYR:HE1   | 1:A:38:LEU:HD22 | 3        | 0.34          |
| (1,1724) | 1:A:56:TYR:HE1   | 1:A:38:LEU:HD23 | 3        | 0.34          |
| (1,1724) | 1:A:56:TYR:HE2   | 1:A:38:LEU:HD21 | 3        | 0.34          |
| (1,1724) | 1:A:56:TYR:HE2   | 1:A:38:LEU:HD22 | 3        | 0.34          |
| (1,1724) | 1:A:56:TYR:HE2   | 1:A:38:LEU:HD23 | 3        | 0.34          |
| (1,1336) | 1:A:38:LEU:HA    | 1:A:43:LEU:HD21 | 1        | 0.34          |
| (1,1336) | 1:A:38:LEU:HA    | 1:A:43:LEU:HD22 | 1        | 0.34          |
| (1,1336) | 1:A:38:LEU:HA    | 1:A:43:LEU:HD23 | 1        | 0.34          |
| (1,1119) | 1:A:70:VAL:HG21  | 1:A:71:SER:HB3  | 1        | 0.34          |
| (1,1119) | 1:A:70:VAL:HG22  | 1:A:71:SER:HB3  | 1        | 0.34          |
| (1,1119) | 1:A:70:VAL:HG23  | 1:A:71:SER:HB3  | 1        | 0.34          |
| (1,1000) | 1:A:20:ALA:HB1   | 1:A:17:SER:HB3  | 6        | 0.34          |
| (1,1000) | 1:A:20:ALA:HB2   | 1:A:17:SER:HB3  | 6        | 0.34          |
| (1,1000) | 1:A:20:ALA:HB3   | 1:A:17:SER:HB3  | 6        | 0.34          |
| (3,149)  | 1:A:136:ASP:O    | 1:A:139:ALA:N   | 1        | 0.33          |
| (3,149)  | 1:A:136:ASP:O    | 1:A:139:ALA:N   | 11       | 0.33          |
| (3,139)  | 1:A:107:THR:O    | 1:A:111:MET:N   | 1        | 0.33          |
| (3,139)  | 1:A:107:THR:O    | 1:A:111:MET:N   | 10       | 0.33          |
| (3,120)  | 1:A:54:ALA:O     | 1:A:58:ALA:N    | 3        | 0.33          |
| (3,118)  | 1:A:38:LEU:O     | 1:A:44:ILE:N    | 7        | 0.33          |
| (3,115)  | 1:A:36:SER:O     | 1:A:40:SER:N    | 11       | 0.33          |
| (3,111)  | 1:A:31:LYS:O     | 1:A:35:ARG:N    | 9        | 0.33          |
| (3,101)  | 1:A:7:THR:O      | 1:A:11:MET:N    | 1        | 0.33          |
| (3,101)  | 1:A:7:THR:O      | 1:A:11:MET:N    | 5        | 0.33          |
| (3,101)  | 1:A:7:THR:O      | 1:A:11:MET:N    | 11       | 0.33          |
| (1,494)  | 1:A:10:GLN:HG2   | 1:A:13:GLU:H    | 3        | 0.33          |
| (1,2573) | 1:A:109:THR:HG21 | 1:A:113:LYS:HG2 | 1        | 0.33          |
| (1,2573) | 1:A:109:THR:HG22 | 1:A:113:LYS:HG2 | 1        | 0.33          |
| (1,2573) | 1:A:109:THR:HG23 | 1:A:113:LYS:HG2 | 1        | 0.33          |
| (1,2431) | 1:A:6:VAL:HG21   | 1:A:10:GLN:HG2  | 1        | 0.33          |
| (1,2431) | 1:A:6:VAL:HG22   | 1:A:10:GLN:HG2  | 1        | 0.33          |
| (1,2431) | 1:A:6:VAL:HG23   | 1:A:10:GLN:HG2  | 1        | 0.33          |
| (1,2327) | 1:A:113:LYS:HB3  | 1:A:113:LYS:HE3 | 1        | 0.33          |
| (1,2054) | 1:A:69:GLY:HA3   | 1:A:28:ILE:HB   | 12       | 0.33          |
| (1,1489) | 1:A:20:ALA:HB1   | 1:A:17:SER:HB3  | 5        | 0.33          |
| (1,1489) | 1:A:20:ALA:HB2   | 1:A:17:SER:HB3  | 5        | 0.33          |
| (1,1489) | 1:A:20:ALA:HB3   | 1:A:17:SER:HB3  | 5        | 0.33          |
| (3,149)  | 1:A:136:ASP:O    | 1:A:139:ALA:N   | 2        | 0.32          |
| (3,149)  | 1:A:136:ASP:O    | 1:A:139:ALA:N   | 7        | 0.32          |
| (3,149)  | 1:A:136:ASP:O    | 1:A:139:ALA:N   | 9        | 0.32          |
| (3,149)  | 1:A:136:ASP:O    | 1:A:139:ALA:N   | 10       | 0.32          |
| (3,144)  | 1:A:120:GLN:O    | 1:A:124:VAL:N   | 4        | 0.32          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (3,124)  | 1:A:29:LEU:O     | 1:A:70:VAL:N    | 5        | 0.32          |
| (3,123)  | 1:A:59:ILE:O     | 1:A:63:VAL:N    | 11       | 0.32          |
| (3,123)  | 1:A:59:ILE:O     | 1:A:63:VAL:N    | 12       | 0.32          |
| (3,118)  | 1:A:38:LEU:O     | 1:A:44:ILE:N    | 3        | 0.32          |
| (3,118)  | 1:A:38:LEU:O     | 1:A:44:ILE:N    | 12       | 0.32          |
| (3,113)  | 1:A:33:GLU:O     | 1:A:37:CYS:N    | 11       | 0.32          |
| (3,108)  | 1:A:16:GLN:O     | 1:A:20:ALA:N    | 2        | 0.32          |
| (3,108)  | 1:A:16:GLN:O     | 1:A:20:ALA:N    | 3        | 0.32          |
| (3,108)  | 1:A:16:GLN:O     | 1:A:20:ALA:N    | 11       | 0.32          |
| (3,107)  | 1:A:14:PHE:O     | 1:A:18:PHE:N    | 9        | 0.32          |
| (3,101)  | 1:A:7:THR:O      | 1:A:11:MET:N    | 9        | 0.32          |
| (1,2573) | 1:A:109:THR:HG21 | 1:A:113:LYS:HG2 | 12       | 0.32          |
| (1,2573) | 1:A:109:THR:HG22 | 1:A:113:LYS:HG2 | 12       | 0.32          |
| (1,2573) | 1:A:109:THR:HG23 | 1:A:113:LYS:HG2 | 12       | 0.32          |
| (1,2212) | 1:A:35:ARG:HD2   | 1:A:56:TYR:HE1  | 10       | 0.32          |
| (1,2212) | 1:A:35:ARG:HD2   | 1:A:56:TYR:HE2  | 10       | 0.32          |
| (1,1814) | 1:A:15:LYS:HD2   | 1:A:15:LYS:HA   | 12       | 0.32          |
| (1,1745) | 1:A:80:LYS:HE3   | 1:A:6:VAL:HG11  | 11       | 0.32          |
| (1,1745) | 1:A:80:LYS:HE3   | 1:A:6:VAL:HG12  | 11       | 0.32          |
| (1,1745) | 1:A:80:LYS:HE3   | 1:A:6:VAL:HG13  | 11       | 0.32          |
| (1,1721) | 1:A:15:LYS:HD2   | 1:A:15:LYS:HA   | 9        | 0.32          |
| (1,1081) | 1:A:6:VAL:HG21   | 1:A:11:MET:HG2  | 3        | 0.32          |
| (1,1081) | 1:A:6:VAL:HG22   | 1:A:11:MET:HG2  | 3        | 0.32          |
| (1,1081) | 1:A:6:VAL:HG23   | 1:A:11:MET:HG2  | 3        | 0.32          |
| (1,1081) | 1:A:6:VAL:HG21   | 1:A:11:MET:HG2  | 8        | 0.32          |
| (1,1081) | 1:A:6:VAL:HG22   | 1:A:11:MET:HG2  | 8        | 0.32          |
| (1,1081) | 1:A:6:VAL:HG23   | 1:A:11:MET:HG2  | 8        | 0.32          |
| (1,1000) | 1:A:20:ALA:HB1   | 1:A:17:SER:HB3  | 7        | 0.32          |
| (1,1000) | 1:A:20:ALA:HB2   | 1:A:17:SER:HB3  | 7        | 0.32          |
| (1,1000) | 1:A:20:ALA:HB3   | 1:A:17:SER:HB3  | 7        | 0.32          |
| (3,149)  | 1:A:136:ASP:O    | 1:A:139:ALA:N   | 12       | 0.31          |
| (3,147)  | 1:A:123:TYR:O    | 1:A:127:ASN:N   | 2        | 0.31          |
| (3,137)  | 1:A:100:ALA:O    | 1:A:103:LYS:N   | 4        | 0.31          |
| (3,132)  | 1:A:90:GLU:O     | 1:A:93:ASN:N    | 2        | 0.31          |
| (3,130)  | 1:A:79:MET:O     | 1:A:83:ASN:N    | 4        | 0.31          |
| (3,123)  | 1:A:59:ILE:O     | 1:A:63:VAL:N    | 2        | 0.31          |
| (3,123)  | 1:A:59:ILE:O     | 1:A:63:VAL:N    | 8        | 0.31          |
| (3,118)  | 1:A:38:LEU:O     | 1:A:44:ILE:N    | 8        | 0.31          |
| (3,118)  | 1:A:38:LEU:O     | 1:A:44:ILE:N    | 10       | 0.31          |
| (3,114)  | 1:A:34:PHE:O     | 1:A:38:LEU:N    | 2        | 0.31          |
| (3,114)  | 1:A:34:PHE:O     | 1:A:38:LEU:N    | 3        | 0.31          |
| (3,113)  | 1:A:33:GLU:O     | 1:A:37:CYS:N    | 12       | 0.31          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (3,110)  | 1:A:30:ASP:O     | 1:A:34:PHE:N    | 11       | 0.31          |
| (3,108)  | 1:A:16:GLN:O     | 1:A:20:ALA:N    | 5        | 0.31          |
| (3,107)  | 1:A:14:PHE:O     | 1:A:18:PHE:N    | 12       | 0.31          |
| (3,106)  | 1:A:13:GLU:O     | 1:A:17:SER:N    | 4        | 0.31          |
| (3,106)  | 1:A:13:GLU:O     | 1:A:17:SER:N    | 7        | 0.31          |
| (3,101)  | 1:A:7:THR:O      | 1:A:11:MET:N    | 4        | 0.31          |
| (1,1499) | 1:A:99:ILE:HG21  | 1:A:103:LYS:HE2 | 8        | 0.31          |
| (1,1499) | 1:A:99:ILE:HG22  | 1:A:103:LYS:HE2 | 8        | 0.31          |
| (1,1499) | 1:A:99:ILE:HG23  | 1:A:103:LYS:HE2 | 8        | 0.31          |
| (1,1439) | 1:A:141:VAL:HG11 | 1:A:137:TYR:HE1 | 7        | 0.31          |
| (1,1439) | 1:A:141:VAL:HG11 | 1:A:137:TYR:HE2 | 7        | 0.31          |
| (1,1439) | 1:A:141:VAL:HG12 | 1:A:137:TYR:HE1 | 7        | 0.31          |
| (1,1439) | 1:A:141:VAL:HG12 | 1:A:137:TYR:HE2 | 7        | 0.31          |
| (1,1439) | 1:A:141:VAL:HG13 | 1:A:137:TYR:HE1 | 7        | 0.31          |
| (1,1439) | 1:A:141:VAL:HG13 | 1:A:137:TYR:HE2 | 7        | 0.31          |
| (1,1119) | 1:A:70:VAL:HG21  | 1:A:71:SER:HB3  | 9        | 0.31          |
| (1,1119) | 1:A:70:VAL:HG22  | 1:A:71:SER:HB3  | 9        | 0.31          |
| (1,1119) | 1:A:70:VAL:HG23  | 1:A:71:SER:HB3  | 9        | 0.31          |
| (1,1000) | 1:A:20:ALA:HB1   | 1:A:17:SER:HB3  | 8        | 0.31          |
| (1,1000) | 1:A:20:ALA:HB2   | 1:A:17:SER:HB3  | 8        | 0.31          |
| (1,1000) | 1:A:20:ALA:HB3   | 1:A:17:SER:HB3  | 8        | 0.31          |
| (3,149)  | 1:A:136:ASP:O    | 1:A:139:ALA:N   | 3        | 0.3           |
| (3,133)  | 1:A:91:GLN:O     | 1:A:94:GLU:N    | 7        | 0.3           |
| (3,132)  | 1:A:90:GLU:O     | 1:A:93:ASN:N    | 5        | 0.3           |
| (3,131)  | 1:A:89:PRO:O     | 1:A:92:LEU:N    | 8        | 0.3           |
| (3,123)  | 1:A:59:ILE:O     | 1:A:63:VAL:N    | 9        | 0.3           |
| (3,120)  | 1:A:54:ALA:O     | 1:A:58:ALA:N    | 2        | 0.3           |
| (3,120)  | 1:A:54:ALA:O     | 1:A:58:ALA:N    | 10       | 0.3           |
| (3,119)  | 1:A:45:ASP:O     | 1:A:47:ASP:N    | 11       | 0.3           |
| (3,118)  | 1:A:38:LEU:O     | 1:A:44:ILE:N    | 1        | 0.3           |
| (3,118)  | 1:A:38:LEU:O     | 1:A:44:ILE:N    | 4        | 0.3           |
| (3,118)  | 1:A:38:LEU:O     | 1:A:44:ILE:N    | 5        | 0.3           |
| (3,115)  | 1:A:36:SER:O     | 1:A:40:SER:N    | 4        | 0.3           |
| (3,115)  | 1:A:36:SER:O     | 1:A:40:SER:N    | 6        | 0.3           |
| (3,115)  | 1:A:36:SER:O     | 1:A:40:SER:N    | 12       | 0.3           |
| (3,113)  | 1:A:33:GLU:O     | 1:A:37:CYS:N    | 2        | 0.3           |
| (3,111)  | 1:A:31:LYS:O     | 1:A:35:ARG:N    | 8        | 0.3           |
| (3,109)  | 1:A:29:LEU:N     | 1:A:70:VAL:O    | 11       | 0.3           |
| (3,108)  | 1:A:16:GLN:O     | 1:A:20:ALA:N    | 6        | 0.3           |
| (3,108)  | 1:A:16:GLN:O     | 1:A:20:ALA:N    | 8        | 0.3           |
| (3,108)  | 1:A:16:GLN:O     | 1:A:20:ALA:N    | 10       | 0.3           |
| (3,107)  | 1:A:14:PHE:O     | 1:A:18:PHE:N    | 11       | 0.3           |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (3,101)  | 1:A:7:THR:O      | 1:A:11:MET:N    | 2        | 0.3           |
| (3,101)  | 1:A:7:THR:O      | 1:A:11:MET:N    | 8        | 0.3           |
| (3,101)  | 1:A:7:THR:O      | 1:A:11:MET:N    | 12       | 0.3           |
| (1,1781) | 1:A:43:LEU:HD11  | 1:A:43:LEU:HA   | 1        | 0.3           |
| (1,1781) | 1:A:43:LEU:HD12  | 1:A:43:LEU:HA   | 1        | 0.3           |
| (1,1781) | 1:A:43:LEU:HD13  | 1:A:43:LEU:HA   | 1        | 0.3           |
| (1,1631) | 1:A:109:THR:HB   | 1:A:108:GLU:HG3 | 11       | 0.3           |
| (1,1439) | 1:A:141:VAL:HG11 | 1:A:137:TYR:HE1 | 3        | 0.3           |
| (1,1439) | 1:A:141:VAL:HG11 | 1:A:137:TYR:HE2 | 3        | 0.3           |
| (1,1439) | 1:A:141:VAL:HG12 | 1:A:137:TYR:HE1 | 3        | 0.3           |
| (1,1439) | 1:A:141:VAL:HG12 | 1:A:137:TYR:HE2 | 3        | 0.3           |
| (1,1439) | 1:A:141:VAL:HG13 | 1:A:137:TYR:HE1 | 3        | 0.3           |
| (1,1439) | 1:A:141:VAL:HG13 | 1:A:137:TYR:HE2 | 3        | 0.3           |
| (1,1024) | 1:A:15:LYS:HE3   | 1:A:15:LYS:HA   | 8        | 0.3           |
| (1,1000) | 1:A:20:ALA:HB1   | 1:A:17:SER:HB3  | 3        | 0.3           |
| (1,1000) | 1:A:20:ALA:HB2   | 1:A:17:SER:HB3  | 3        | 0.3           |
| (1,1000) | 1:A:20:ALA:HB3   | 1:A:17:SER:HB3  | 3        | 0.3           |
| (3,150)  | 1:A:138:ALA:O    | 1:A:142:LYS:N   | 3        | 0.29          |
| (3,149)  | 1:A:136:ASP:O    | 1:A:139:ALA:N   | 8        | 0.29          |
| (3,145)  | 1:A:121:ILE:O    | 1:A:125:LYS:N   | 6        | 0.29          |
| (3,145)  | 1:A:121:ILE:O    | 1:A:125:LYS:N   | 11       | 0.29          |
| (3,144)  | 1:A:120:GLN:O    | 1:A:124:VAL:N   | 10       | 0.29          |
| (3,139)  | 1:A:107:THR:O    | 1:A:111:MET:N   | 3        | 0.29          |
| (3,132)  | 1:A:90:GLU:O     | 1:A:93:ASN:N    | 7        | 0.29          |
| (3,132)  | 1:A:90:GLU:O     | 1:A:93:ASN:N    | 8        | 0.29          |
| (3,118)  | 1:A:38:LEU:O     | 1:A:44:ILE:N    | 2        | 0.29          |
| (3,118)  | 1:A:38:LEU:O     | 1:A:44:ILE:N    | 11       | 0.29          |
| (3,110)  | 1:A:30:ASP:O     | 1:A:34:PHE:N    | 1        | 0.29          |
| (3,107)  | 1:A:14:PHE:O     | 1:A:18:PHE:N    | 6        | 0.29          |
| (3,103)  | 1:A:9:GLU:O      | 1:A:13:GLU:N    | 12       | 0.29          |
| (1,2543) | 1:A:59:ILE:HD11  | 1:A:55:GLN:HG3  | 6        | 0.29          |
| (1,2543) | 1:A:59:ILE:HD12  | 1:A:55:GLN:HG3  | 6        | 0.29          |
| (1,2543) | 1:A:59:ILE:HD13  | 1:A:55:GLN:HG3  | 6        | 0.29          |
| (1,2431) | 1:A:6:VAL:HG21   | 1:A:10:GLN:HG2  | 8        | 0.29          |
| (1,2431) | 1:A:6:VAL:HG22   | 1:A:10:GLN:HG2  | 8        | 0.29          |
| (1,2431) | 1:A:6:VAL:HG23   | 1:A:10:GLN:HG2  | 8        | 0.29          |
| (1,2399) | 1:A:103:LYS:HE2  | 1:A:100:ALA:HB1 | 8        | 0.29          |
| (1,2399) | 1:A:103:LYS:HE2  | 1:A:100:ALA:HB2 | 8        | 0.29          |
| (1,2399) | 1:A:103:LYS:HE2  | 1:A:100:ALA:HB3 | 8        | 0.29          |
| (1,2370) | 1:A:141:VAL:HG11 | 1:A:138:ALA:HA  | 1        | 0.29          |
| (1,2370) | 1:A:141:VAL:HG12 | 1:A:138:ALA:HA  | 1        | 0.29          |
| (1,2370) | 1:A:141:VAL:HG13 | 1:A:138:ALA:HA  | 1        | 0.29          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2300) | 1:A:57:ASP:HB3  | 1:A:54:ALA:HA   | 6        | 0.29          |
| (1,2083) | 1:A:89:PRO:HA   | 1:A:92:LEU:HD21 | 6        | 0.29          |
| (1,2083) | 1:A:89:PRO:HA   | 1:A:92:LEU:HD22 | 6        | 0.29          |
| (1,2083) | 1:A:89:PRO:HA   | 1:A:92:LEU:HD23 | 6        | 0.29          |
| (1,1847) | 1:A:6:VAL:HG11  | 1:A:80:LYS:HB3  | 5        | 0.29          |
| (1,1847) | 1:A:6:VAL:HG12  | 1:A:80:LYS:HB3  | 5        | 0.29          |
| (1,1847) | 1:A:6:VAL:HG13  | 1:A:80:LYS:HB3  | 5        | 0.29          |
| (1,1781) | 1:A:43:LEU:HD11 | 1:A:43:LEU:HA   | 2        | 0.29          |
| (1,1781) | 1:A:43:LEU:HD12 | 1:A:43:LEU:HA   | 2        | 0.29          |
| (1,1781) | 1:A:43:LEU:HD13 | 1:A:43:LEU:HA   | 2        | 0.29          |
| (1,1491) | 1:A:65:LYS:HE3  | 1:A:65:LYS:HB2  | 9        | 0.29          |
| (1,1491) | 1:A:65:LYS:HE3  | 1:A:65:LYS:HB2  | 11       | 0.29          |
| (1,1000) | 1:A:20:ALA:HB1  | 1:A:17:SER:HB3  | 1        | 0.29          |
| (1,1000) | 1:A:20:ALA:HB2  | 1:A:17:SER:HB3  | 1        | 0.29          |
| (1,1000) | 1:A:20:ALA:HB3  | 1:A:17:SER:HB3  | 1        | 0.29          |
| (1,1000) | 1:A:20:ALA:HB1  | 1:A:17:SER:HB3  | 4        | 0.29          |
| (1,1000) | 1:A:20:ALA:HB2  | 1:A:17:SER:HB3  | 4        | 0.29          |
| (1,1000) | 1:A:20:ALA:HB3  | 1:A:17:SER:HB3  | 4        | 0.29          |
| (3,147)  | 1:A:123:TYR:O   | 1:A:127:ASN:N   | 1        | 0.28          |
| (3,145)  | 1:A:121:ILE:O   | 1:A:125:LYS:N   | 10       | 0.28          |
| (3,145)  | 1:A:121:ILE:O   | 1:A:125:LYS:N   | 12       | 0.28          |
| (3,144)  | 1:A:120:GLN:O   | 1:A:124:VAL:N   | 8        | 0.28          |
| (3,139)  | 1:A:107:THR:O   | 1:A:111:MET:N   | 4        | 0.28          |
| (3,137)  | 1:A:100:ALA:O   | 1:A:103:LYS:N   | 3        | 0.28          |
| (3,136)  | 1:A:95:ILE:O    | 1:A:99:ILE:N    | 6        | 0.28          |
| (3,136)  | 1:A:95:ILE:O    | 1:A:99:ILE:N    | 12       | 0.28          |
| (3,132)  | 1:A:90:GLU:O    | 1:A:93:ASN:N    | 9        | 0.28          |
| (3,129)  | 1:A:76:VAL:O    | 1:A:80:LYS:N    | 2        | 0.28          |
| (3,124)  | 1:A:29:LEU:O    | 1:A:70:VAL:N    | 10       | 0.28          |
| (3,115)  | 1:A:36:SER:O    | 1:A:40:SER:N    | 8        | 0.28          |
| (3,115)  | 1:A:36:SER:O    | 1:A:40:SER:N    | 9        | 0.28          |
| (3,114)  | 1:A:34:PHE:O    | 1:A:38:LEU:N    | 1        | 0.28          |
| (3,114)  | 1:A:34:PHE:O    | 1:A:38:LEU:N    | 7        | 0.28          |
| (3,114)  | 1:A:34:PHE:O    | 1:A:38:LEU:N    | 10       | 0.28          |
| (3,114)  | 1:A:34:PHE:O    | 1:A:38:LEU:N    | 11       | 0.28          |
| (3,111)  | 1:A:31:LYS:O    | 1:A:35:ARG:N    | 10       | 0.28          |
| (3,108)  | 1:A:16:GLN:O    | 1:A:20:ALA:N    | 7        | 0.28          |
| (3,107)  | 1:A:14:PHE:O    | 1:A:18:PHE:N    | 1        | 0.28          |
| (3,107)  | 1:A:14:PHE:O    | 1:A:18:PHE:N    | 7        | 0.28          |
| (3,103)  | 1:A:9:GLU:O     | 1:A:13:GLU:N    | 4        | 0.28          |
| (2,318)  | 1:A:10:GLN:HB3  | 1:A:14:PHE:HZ   | 12       | 0.28          |
| (2,184)  | 1:A:92:LEU:HB2  | 1:A:95:ILE:H    | 10       | 0.28          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2444) | 1:A:121:ILE:HD11 | 1:A:112:GLN:HG2 | 9        | 0.28          |
| (1,2444) | 1:A:121:ILE:HD12 | 1:A:112:GLN:HG2 | 9        | 0.28          |
| (1,2444) | 1:A:121:ILE:HD13 | 1:A:112:GLN:HG2 | 9        | 0.28          |
| (1,2326) | 1:A:74:ASN:HA    | 1:A:77:GLN:HG3  | 8        | 0.28          |
| (1,2212) | 1:A:35:ARG:HD2   | 1:A:56:TYR:HE1  | 8        | 0.28          |
| (1,2212) | 1:A:35:ARG:HD2   | 1:A:56:TYR:HE2  | 8        | 0.28          |
| (1,2054) | 1:A:69:GLY:HA3   | 1:A:28:ILE:HB   | 11       | 0.28          |
| (1,2029) | 1:A:116:MET:HG2  | 1:A:114:ALA:HB1 | 1        | 0.28          |
| (1,2029) | 1:A:116:MET:HG2  | 1:A:114:ALA:HB2 | 1        | 0.28          |
| (1,2029) | 1:A:116:MET:HG2  | 1:A:114:ALA:HB3 | 1        | 0.28          |
| (1,1257) | 1:A:41:MET:HE1   | 1:A:38:LEU:HD11 | 8        | 0.28          |
| (1,1257) | 1:A:41:MET:HE1   | 1:A:38:LEU:HD12 | 8        | 0.28          |
| (1,1257) | 1:A:41:MET:HE1   | 1:A:38:LEU:HD13 | 8        | 0.28          |
| (1,1257) | 1:A:41:MET:HE2   | 1:A:38:LEU:HD11 | 8        | 0.28          |
| (1,1257) | 1:A:41:MET:HE2   | 1:A:38:LEU:HD12 | 8        | 0.28          |
| (1,1257) | 1:A:41:MET:HE2   | 1:A:38:LEU:HD13 | 8        | 0.28          |
| (1,1257) | 1:A:41:MET:HE3   | 1:A:38:LEU:HD11 | 8        | 0.28          |
| (1,1257) | 1:A:41:MET:HE3   | 1:A:38:LEU:HD12 | 8        | 0.28          |
| (1,1257) | 1:A:41:MET:HE3   | 1:A:38:LEU:HD13 | 8        | 0.28          |
| (3,147)  | 1:A:123:TYR:O    | 1:A:127:ASN:N   | 6        | 0.27          |
| (3,137)  | 1:A:100:ALA:O    | 1:A:103:LYS:N   | 5        | 0.27          |
| (3,137)  | 1:A:100:ALA:O    | 1:A:103:LYS:N   | 6        | 0.27          |
| (3,136)  | 1:A:95:ILE:O     | 1:A:99:ILE:N    | 11       | 0.27          |
| (3,130)  | 1:A:79:MET:O     | 1:A:83:ASN:N    | 10       | 0.27          |
| (3,128)  | 1:A:75:TYR:O     | 1:A:79:MET:N    | 3        | 0.27          |
| (3,128)  | 1:A:75:TYR:O     | 1:A:79:MET:N    | 11       | 0.27          |
| (3,123)  | 1:A:59:ILE:O     | 1:A:63:VAL:N    | 1        | 0.27          |
| (3,123)  | 1:A:59:ILE:O     | 1:A:63:VAL:N    | 10       | 0.27          |
| (3,115)  | 1:A:36:SER:O     | 1:A:40:SER:N    | 2        | 0.27          |
| (3,115)  | 1:A:36:SER:O     | 1:A:40:SER:N    | 5        | 0.27          |
| (3,113)  | 1:A:33:GLU:O     | 1:A:37:CYS:N    | 9        | 0.27          |
| (3,111)  | 1:A:31:LYS:O     | 1:A:35:ARG:N    | 2        | 0.27          |
| (1,494)  | 1:A:10:GLN:HG2   | 1:A:13:GLU:H    | 12       | 0.27          |
| (1,2602) | 1:A:141:VAL:HG11 | 1:A:137:TYR:HD1 | 7        | 0.27          |
| (1,2602) | 1:A:141:VAL:HG11 | 1:A:137:TYR:HD2 | 7        | 0.27          |
| (1,2602) | 1:A:141:VAL:HG12 | 1:A:137:TYR:HD1 | 7        | 0.27          |
| (1,2602) | 1:A:141:VAL:HG12 | 1:A:137:TYR:HD2 | 7        | 0.27          |
| (1,2602) | 1:A:141:VAL:HG13 | 1:A:137:TYR:HD1 | 7        | 0.27          |
| (1,2602) | 1:A:141:VAL:HG13 | 1:A:137:TYR:HD2 | 7        | 0.27          |
| (1,2560) | 1:A:37:CYS:HB2   | 1:A:21:PHE:HB3  | 11       | 0.27          |
| (1,2444) | 1:A:121:ILE:HD11 | 1:A:112:GLN:HG2 | 7        | 0.27          |
| (1,2444) | 1:A:121:ILE:HD12 | 1:A:112:GLN:HG2 | 7        | 0.27          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2444) | 1:A:121:ILE:HD13 | 1:A:112:GLN:HG2 | 7        | 0.27          |
| (1,2370) | 1:A:141:VAL:HG11 | 1:A:138:ALA:HA  | 7        | 0.27          |
| (1,2370) | 1:A:141:VAL:HG12 | 1:A:138:ALA:HA  | 7        | 0.27          |
| (1,2370) | 1:A:141:VAL:HG13 | 1:A:138:ALA:HA  | 7        | 0.27          |
| (1,2324) | 1:A:103:LYS:HB3  | 1:A:103:LYS:HE3 | 8        | 0.27          |
| (1,1814) | 1:A:15:LYS:HD2   | 1:A:15:LYS:HA   | 9        | 0.27          |
| (1,1631) | 1:A:109:THR:HB   | 1:A:108:GLU:HG3 | 6        | 0.27          |
| (3,149)  | 1:A:136:ASP:O    | 1:A:139:ALA:N   | 4        | 0.26          |
| (3,144)  | 1:A:120:GLN:O    | 1:A:124:VAL:N   | 5        | 0.26          |
| (3,139)  | 1:A:107:THR:O    | 1:A:111:MET:N   | 2        | 0.26          |
| (3,134)  | 1:A:94:GLU:O     | 1:A:97:SER:N    | 10       | 0.26          |
| (3,131)  | 1:A:89:PRO:O     | 1:A:92:LEU:N    | 2        | 0.26          |
| (3,128)  | 1:A:75:TYR:O     | 1:A:79:MET:N    | 1        | 0.26          |
| (3,124)  | 1:A:29:LEU:O     | 1:A:70:VAL:N    | 6        | 0.26          |
| (3,111)  | 1:A:31:LYS:O     | 1:A:35:ARG:N    | 3        | 0.26          |
| (3,111)  | 1:A:31:LYS:O     | 1:A:35:ARG:N    | 4        | 0.26          |
| (3,110)  | 1:A:30:ASP:O     | 1:A:34:PHE:N    | 12       | 0.26          |
| (3,108)  | 1:A:16:GLN:O     | 1:A:20:ALA:N    | 12       | 0.26          |
| (3,106)  | 1:A:13:GLU:O     | 1:A:17:SER:N    | 3        | 0.26          |
| (2,318)  | 1:A:10:GLN:HB3   | 1:A:14:PHE:HZ   | 6        | 0.26          |
| (2,318)  | 1:A:10:GLN:HB3   | 1:A:14:PHE:HZ   | 8        | 0.26          |
| (2,318)  | 1:A:10:GLN:HB3   | 1:A:14:PHE:HZ   | 9        | 0.26          |
| (1,2324) | 1:A:103:LYS:HB3  | 1:A:103:LYS:HE3 | 2        | 0.26          |
| (1,1847) | 1:A:6:VAL:HG11   | 1:A:80:LYS:HB3  | 12       | 0.26          |
| (1,1847) | 1:A:6:VAL:HG12   | 1:A:80:LYS:HB3  | 12       | 0.26          |
| (1,1847) | 1:A:6:VAL:HG13   | 1:A:80:LYS:HB3  | 12       | 0.26          |
| (1,1781) | 1:A:43:LEU:HD11  | 1:A:43:LEU:HA   | 10       | 0.26          |
| (1,1781) | 1:A:43:LEU:HD12  | 1:A:43:LEU:HA   | 10       | 0.26          |
| (1,1781) | 1:A:43:LEU:HD13  | 1:A:43:LEU:HA   | 10       | 0.26          |
| (1,1741) | 1:A:69:GLY:HA3   | 1:A:60:TYR:HE1  | 12       | 0.26          |
| (1,1741) | 1:A:69:GLY:HA3   | 1:A:60:TYR:HE2  | 12       | 0.26          |
| (1,1491) | 1:A:65:LYS:HE3   | 1:A:65:LYS:HB2  | 8        | 0.26          |
| (1,1145) | 1:A:6:VAL:HG21   | 1:A:11:MET:HA   | 2        | 0.26          |
| (1,1145) | 1:A:6:VAL:HG22   | 1:A:11:MET:HA   | 2        | 0.26          |
| (1,1145) | 1:A:6:VAL:HG23   | 1:A:11:MET:HA   | 2        | 0.26          |
| (1,1119) | 1:A:70:VAL:HG21  | 1:A:71:SER:HB3  | 5        | 0.26          |
| (1,1119) | 1:A:70:VAL:HG22  | 1:A:71:SER:HB3  | 5        | 0.26          |
| (1,1119) | 1:A:70:VAL:HG23  | 1:A:71:SER:HB3  | 5        | 0.26          |
| (1,1081) | 1:A:6:VAL:HG21   | 1:A:11:MET:HG2  | 11       | 0.26          |
| (1,1081) | 1:A:6:VAL:HG22   | 1:A:11:MET:HG2  | 11       | 0.26          |
| (1,1081) | 1:A:6:VAL:HG23   | 1:A:11:MET:HG2  | 11       | 0.26          |
| (1,1000) | 1:A:20:ALA:HB1   | 1:A:17:SER:HB3  | 2        | 0.26          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1000) | 1:A:20:ALA:HB2  | 1:A:17:SER:HB3  | 2        | 0.26          |
| (1,1000) | 1:A:20:ALA:HB3  | 1:A:17:SER:HB3  | 2        | 0.26          |
| (1,1000) | 1:A:20:ALA:HB1  | 1:A:17:SER:HB3  | 10       | 0.26          |
| (1,1000) | 1:A:20:ALA:HB2  | 1:A:17:SER:HB3  | 10       | 0.26          |
| (1,1000) | 1:A:20:ALA:HB3  | 1:A:17:SER:HB3  | 10       | 0.26          |
| (1,1000) | 1:A:20:ALA:HB1  | 1:A:17:SER:HB3  | 11       | 0.26          |
| (1,1000) | 1:A:20:ALA:HB2  | 1:A:17:SER:HB3  | 11       | 0.26          |
| (1,1000) | 1:A:20:ALA:HB3  | 1:A:17:SER:HB3  | 11       | 0.26          |
| (3,144)  | 1:A:120:GLN:O   | 1:A:124:VAL:N   | 2        | 0.25          |
| (3,144)  | 1:A:120:GLN:O   | 1:A:124:VAL:N   | 3        | 0.25          |
| (3,144)  | 1:A:120:GLN:O   | 1:A:124:VAL:N   | 6        | 0.25          |
| (3,144)  | 1:A:120:GLN:O   | 1:A:124:VAL:N   | 9        | 0.25          |
| (3,144)  | 1:A:120:GLN:O   | 1:A:124:VAL:N   | 11       | 0.25          |
| (3,132)  | 1:A:90:GLU:O    | 1:A:93:ASN:N    | 4        | 0.25          |
| (3,131)  | 1:A:89:PRO:O    | 1:A:92:LEU:N    | 11       | 0.25          |
| (3,130)  | 1:A:79:MET:O    | 1:A:83:ASN:N    | 3        | 0.25          |
| (3,123)  | 1:A:59:ILE:O    | 1:A:63:VAL:N    | 6        | 0.25          |
| (3,123)  | 1:A:59:ILE:O    | 1:A:63:VAL:N    | 7        | 0.25          |
| (3,120)  | 1:A:54:ALA:O    | 1:A:58:ALA:N    | 1        | 0.25          |
| (3,119)  | 1:A:45:ASP:O    | 1:A:47:ASP:N    | 5        | 0.25          |
| (3,113)  | 1:A:33:GLU:O    | 1:A:37:CYS:N    | 8        | 0.25          |
| (3,111)  | 1:A:31:LYS:O    | 1:A:35:ARG:N    | 6        | 0.25          |
| (3,111)  | 1:A:31:LYS:O    | 1:A:35:ARG:N    | 12       | 0.25          |
| (3,107)  | 1:A:14:PHE:O    | 1:A:18:PHE:N    | 8        | 0.25          |
| (3,106)  | 1:A:13:GLU:O    | 1:A:17:SER:N    | 6        | 0.25          |
| (2,318)  | 1:A:10:GLN:HB3  | 1:A:14:PHE:HZ   | 1        | 0.25          |
| (1,2642) | 1:A:81:GLU:HA   | 1:A:84:ASP:HB3  | 3        | 0.25          |
| (1,2212) | 1:A:35:ARG:HD2  | 1:A:56:TYR:HE1  | 5        | 0.25          |
| (1,2212) | 1:A:35:ARG:HD2  | 1:A:56:TYR:HE2  | 5        | 0.25          |
| (1,2054) | 1:A:69:GLY:HA3  | 1:A:28:ILE:HB   | 10       | 0.25          |
| (1,1978) | 1:A:38:LEU:HA   | 1:A:43:LEU:HD21 | 2        | 0.25          |
| (1,1978) | 1:A:38:LEU:HA   | 1:A:43:LEU:HD22 | 2        | 0.25          |
| (1,1978) | 1:A:38:LEU:HA   | 1:A:43:LEU:HD23 | 2        | 0.25          |
| (1,1762) | 1:A:6:VAL:HG21  | 1:A:14:PHE:HE1  | 7        | 0.25          |
| (1,1762) | 1:A:6:VAL:HG21  | 1:A:14:PHE:HE2  | 7        | 0.25          |
| (1,1762) | 1:A:6:VAL:HG22  | 1:A:14:PHE:HE1  | 7        | 0.25          |
| (1,1762) | 1:A:6:VAL:HG22  | 1:A:14:PHE:HE2  | 7        | 0.25          |
| (1,1762) | 1:A:6:VAL:HG23  | 1:A:14:PHE:HE1  | 7        | 0.25          |
| (1,1762) | 1:A:6:VAL:HG23  | 1:A:14:PHE:HE2  | 7        | 0.25          |
| (1,1499) | 1:A:99:ILE:HG21 | 1:A:103:LYS:HE2 | 11       | 0.25          |
| (1,1499) | 1:A:99:ILE:HG22 | 1:A:103:LYS:HE2 | 11       | 0.25          |
| (1,1499) | 1:A:99:ILE:HG23 | 1:A:103:LYS:HE2 | 11       | 0.25          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1491) | 1:A:65:LYS:HE3   | 1:A:65:LYS:HB2  | 5        | 0.25          |
| (1,1458) | 1:A:77:GLN:HB3   | 1:A:74:ASN:HA   | 10       | 0.25          |
| (1,1439) | 1:A:141:VAL:HG11 | 1:A:137:TYR:HE1 | 1        | 0.25          |
| (1,1439) | 1:A:141:VAL:HG11 | 1:A:137:TYR:HE2 | 1        | 0.25          |
| (1,1439) | 1:A:141:VAL:HG12 | 1:A:137:TYR:HE1 | 1        | 0.25          |
| (1,1439) | 1:A:141:VAL:HG12 | 1:A:137:TYR:HE2 | 1        | 0.25          |
| (1,1439) | 1:A:141:VAL:HG13 | 1:A:137:TYR:HE1 | 1        | 0.25          |
| (1,1439) | 1:A:141:VAL:HG13 | 1:A:137:TYR:HE2 | 1        | 0.25          |
| (1,1387) | 1:A:109:THR:HG21 | 1:A:113:LYS:HE3 | 7        | 0.25          |
| (1,1387) | 1:A:109:THR:HG22 | 1:A:113:LYS:HE3 | 7        | 0.25          |
| (1,1387) | 1:A:109:THR:HG23 | 1:A:113:LYS:HE3 | 7        | 0.25          |
| (1,1336) | 1:A:38:LEU:HA    | 1:A:43:LEU:HD21 | 10       | 0.25          |
| (1,1336) | 1:A:38:LEU:HA    | 1:A:43:LEU:HD22 | 10       | 0.25          |
| (1,1336) | 1:A:38:LEU:HA    | 1:A:43:LEU:HD23 | 10       | 0.25          |
| (3,145)  | 1:A:121:ILE:O    | 1:A:125:LYS:N   | 1        | 0.24          |
| (3,145)  | 1:A:121:ILE:O    | 1:A:125:LYS:N   | 5        | 0.24          |
| (3,145)  | 1:A:121:ILE:O    | 1:A:125:LYS:N   | 7        | 0.24          |
| (3,144)  | 1:A:120:GLN:O    | 1:A:124:VAL:N   | 12       | 0.24          |
| (3,137)  | 1:A:100:ALA:O    | 1:A:103:LYS:N   | 2        | 0.24          |
| (3,136)  | 1:A:95:ILE:O     | 1:A:99:ILE:N    | 2        | 0.24          |
| (3,132)  | 1:A:90:GLU:O     | 1:A:93:ASN:N    | 1        | 0.24          |
| (3,131)  | 1:A:89:PRO:O     | 1:A:92:LEU:N    | 1        | 0.24          |
| (3,131)  | 1:A:89:PRO:O     | 1:A:92:LEU:N    | 3        | 0.24          |
| (3,119)  | 1:A:45:ASP:O     | 1:A:47:ASP:N    | 7        | 0.24          |
| (3,119)  | 1:A:45:ASP:O     | 1:A:47:ASP:N    | 8        | 0.24          |
| (3,111)  | 1:A:31:LYS:O     | 1:A:35:ARG:N    | 5        | 0.24          |
| (3,108)  | 1:A:16:GLN:O     | 1:A:20:ALA:N    | 1        | 0.24          |
| (3,103)  | 1:A:9:GLU:O      | 1:A:13:GLU:N    | 3        | 0.24          |
| (2,318)  | 1:A:10:GLN:HB3   | 1:A:14:PHE:HZ   | 10       | 0.24          |
| (2,318)  | 1:A:10:GLN:HB3   | 1:A:14:PHE:HZ   | 11       | 0.24          |
| (1,2444) | 1:A:121:ILE:HD11 | 1:A:112:GLN:HG2 | 8        | 0.24          |
| (1,2444) | 1:A:121:ILE:HD12 | 1:A:112:GLN:HG2 | 8        | 0.24          |
| (1,2444) | 1:A:121:ILE:HD13 | 1:A:112:GLN:HG2 | 8        | 0.24          |
| (1,2370) | 1:A:141:VAL:HG11 | 1:A:138:ALA:HA  | 3        | 0.24          |
| (1,2370) | 1:A:141:VAL:HG12 | 1:A:138:ALA:HA  | 3        | 0.24          |
| (1,2370) | 1:A:141:VAL:HG13 | 1:A:138:ALA:HA  | 3        | 0.24          |
| (1,2212) | 1:A:35:ARG:HD2   | 1:A:56:TYR:HE1  | 4        | 0.24          |
| (1,2212) | 1:A:35:ARG:HD2   | 1:A:56:TYR:HE2  | 4        | 0.24          |
| (1,1781) | 1:A:43:LEU:HD11  | 1:A:43:LEU:HA   | 3        | 0.24          |
| (1,1781) | 1:A:43:LEU:HD12  | 1:A:43:LEU:HA   | 3        | 0.24          |
| (1,1781) | 1:A:43:LEU:HD13  | 1:A:43:LEU:HA   | 3        | 0.24          |
| (1,1781) | 1:A:43:LEU:HD11  | 1:A:43:LEU:HA   | 4        | 0.24          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1781) | 1:A:43:LEU:HD12  | 1:A:43:LEU:HA   | 4        | 0.24          |
| (1,1781) | 1:A:43:LEU:HD13  | 1:A:43:LEU:HA   | 4        | 0.24          |
| (1,1781) | 1:A:43:LEU:HD11  | 1:A:43:LEU:HA   | 7        | 0.24          |
| (1,1781) | 1:A:43:LEU:HD12  | 1:A:43:LEU:HA   | 7        | 0.24          |
| (1,1781) | 1:A:43:LEU:HD13  | 1:A:43:LEU:HA   | 7        | 0.24          |
| (1,1387) | 1:A:109:THR:HG21 | 1:A:113:LYS:HE3 | 12       | 0.24          |
| (1,1387) | 1:A:109:THR:HG22 | 1:A:113:LYS:HE3 | 12       | 0.24          |
| (1,1387) | 1:A:109:THR:HG23 | 1:A:113:LYS:HE3 | 12       | 0.24          |
| (3,146)  | 1:A:123:TYR:O    | 1:A:126:ALA:N   | 3        | 0.23          |
| (3,146)  | 1:A:123:TYR:O    | 1:A:126:ALA:N   | 9        | 0.23          |
| (3,141)  | 1:A:113:LYS:O    | 1:A:115:GLY:N   | 4        | 0.23          |
| (3,137)  | 1:A:100:ALA:O    | 1:A:103:LYS:N   | 8        | 0.23          |
| (3,136)  | 1:A:95:ILE:O     | 1:A:99:ILE:N    | 1        | 0.23          |
| (3,131)  | 1:A:89:PRO:O     | 1:A:92:LEU:N    | 10       | 0.23          |
| (3,118)  | 1:A:38:LEU:O     | 1:A:44:ILE:N    | 6        | 0.23          |
| (3,117)  | 1:A:38:LEU:O     | 1:A:43:LEU:N    | 7        | 0.23          |
| (3,115)  | 1:A:36:SER:O     | 1:A:40:SER:N    | 3        | 0.23          |
| (3,114)  | 1:A:34:PHE:O     | 1:A:38:LEU:N    | 12       | 0.23          |
| (3,113)  | 1:A:33:GLU:O     | 1:A:37:CYS:N    | 3        | 0.23          |
| (3,110)  | 1:A:30:ASP:O     | 1:A:34:PHE:N    | 4        | 0.23          |
| (3,107)  | 1:A:14:PHE:O     | 1:A:18:PHE:N    | 4        | 0.23          |
| (3,106)  | 1:A:13:GLU:O     | 1:A:17:SER:N    | 8        | 0.23          |
| (3,106)  | 1:A:13:GLU:O     | 1:A:17:SER:N    | 9        | 0.23          |
| (3,103)  | 1:A:9:GLU:O      | 1:A:13:GLU:N    | 11       | 0.23          |
| (3,102)  | 1:A:9:GLU:O      | 1:A:12:GLN:N    | 1        | 0.23          |
| (2,359)  | 1:A:109:THR:HA   | 1:A:113:LYS:HD3 | 5        | 0.23          |
| (2,318)  | 1:A:10:GLN:HB3   | 1:A:14:PHE:HZ   | 5        | 0.23          |
| (1,802)  | 1:A:54:ALA:HB1   | 1:A:57:ASP:HB3  | 7        | 0.23          |
| (1,802)  | 1:A:54:ALA:HB2   | 1:A:57:ASP:HB3  | 7        | 0.23          |
| (1,802)  | 1:A:54:ALA:HB3   | 1:A:57:ASP:HB3  | 7        | 0.23          |
| (1,793)  | 1:A:89:PRO:HA    | 1:A:92:LEU:HB3  | 9        | 0.23          |
| (1,2444) | 1:A:121:ILE:HD11 | 1:A:112:GLN:HG2 | 10       | 0.23          |
| (1,2444) | 1:A:121:ILE:HD12 | 1:A:112:GLN:HG2 | 10       | 0.23          |
| (1,2444) | 1:A:121:ILE:HD13 | 1:A:112:GLN:HG2 | 10       | 0.23          |
| (1,2326) | 1:A:74:ASN:HA    | 1:A:77:GLN:HG3  | 4        | 0.23          |
| (1,2164) | 1:A:121:ILE:HG21 | 1:A:108:GLU:HB3 | 12       | 0.23          |
| (1,2164) | 1:A:121:ILE:HG22 | 1:A:108:GLU:HB3 | 12       | 0.23          |
| (1,2164) | 1:A:121:ILE:HG23 | 1:A:108:GLU:HB3 | 12       | 0.23          |
| (1,2138) | 1:A:6:VAL:HG11   | 1:A:5:GLY:HA3   | 7        | 0.23          |
| (1,2138) | 1:A:6:VAL:HG12   | 1:A:5:GLY:HA3   | 7        | 0.23          |
| (1,2138) | 1:A:6:VAL:HG13   | 1:A:5:GLY:HA3   | 7        | 0.23          |
| (1,2054) | 1:A:69:GLY:HA3   | 1:A:28:ILE:HB   | 2        | 0.23          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1829) | 1:A:103:LYS:HE2 | 1:A:101:ALA:HB1 | 2        | 0.23          |
| (1,1829) | 1:A:103:LYS:HE2 | 1:A:101:ALA:HB2 | 2        | 0.23          |
| (1,1829) | 1:A:103:LYS:HE2 | 1:A:101:ALA:HB3 | 2        | 0.23          |
| (1,1724) | 1:A:56:TYR:HE1  | 1:A:38:LEU:HD21 | 2        | 0.23          |
| (1,1724) | 1:A:56:TYR:HE1  | 1:A:38:LEU:HD22 | 2        | 0.23          |
| (1,1724) | 1:A:56:TYR:HE1  | 1:A:38:LEU:HD23 | 2        | 0.23          |
| (1,1724) | 1:A:56:TYR:HE2  | 1:A:38:LEU:HD21 | 2        | 0.23          |
| (1,1724) | 1:A:56:TYR:HE2  | 1:A:38:LEU:HD22 | 2        | 0.23          |
| (1,1724) | 1:A:56:TYR:HE2  | 1:A:38:LEU:HD23 | 2        | 0.23          |
| (3,37)   | 1:A:45:ASP:O    | 1:A:47:ASP:H    | 12       | 0.22          |
| (3,146)  | 1:A:123:TYR:O   | 1:A:126:ALA:N   | 6        | 0.22          |
| (3,142)  | 1:A:117:SER:O   | 1:A:120:GLN:N   | 4        | 0.22          |
| (3,142)  | 1:A:117:SER:O   | 1:A:120:GLN:N   | 6        | 0.22          |
| (3,137)  | 1:A:100:ALA:O   | 1:A:103:LYS:N   | 7        | 0.22          |
| (3,137)  | 1:A:100:ALA:O   | 1:A:103:LYS:N   | 10       | 0.22          |
| (3,136)  | 1:A:95:ILE:O    | 1:A:99:ILE:N    | 7        | 0.22          |
| (3,136)  | 1:A:95:ILE:O    | 1:A:99:ILE:N    | 10       | 0.22          |
| (3,134)  | 1:A:94:GLU:O    | 1:A:97:SER:N    | 5        | 0.22          |
| (3,132)  | 1:A:90:GLU:O    | 1:A:93:ASN:N    | 12       | 0.22          |
| (3,131)  | 1:A:89:PRO:O    | 1:A:92:LEU:N    | 6        | 0.22          |
| (3,126)  | 1:A:73:ASP:O    | 1:A:77:GLN:N    | 7        | 0.22          |
| (3,124)  | 1:A:29:LEU:O    | 1:A:70:VAL:N    | 4        | 0.22          |
| (3,117)  | 1:A:38:LEU:O    | 1:A:43:LEU:N    | 4        | 0.22          |
| (3,116)  | 1:A:37:CYS:O    | 1:A:41:MET:N    | 9        | 0.22          |
| (3,115)  | 1:A:36:SER:O    | 1:A:40:SER:N    | 7        | 0.22          |
| (3,114)  | 1:A:34:PHE:O    | 1:A:38:LEU:N    | 5        | 0.22          |
| (3,102)  | 1:A:9:GLU:O     | 1:A:12:GLN:N    | 11       | 0.22          |
| (3,102)  | 1:A:9:GLU:O     | 1:A:12:GLN:N    | 12       | 0.22          |
| (2,318)  | 1:A:10:GLN:HB3  | 1:A:14:PHE:HZ   | 4        | 0.22          |
| (2,318)  | 1:A:10:GLN:HB3  | 1:A:14:PHE:HZ   | 7        | 0.22          |
| (2,267)  | 1:A:63:VAL:HG11 | 1:A:69:GLY:H    | 6        | 0.22          |
| (2,267)  | 1:A:63:VAL:HG12 | 1:A:69:GLY:H    | 6        | 0.22          |
| (2,267)  | 1:A:63:VAL:HG13 | 1:A:69:GLY:H    | 6        | 0.22          |
| (1,952)  | 1:A:29:LEU:HD21 | 1:A:70:VAL:HB   | 4        | 0.22          |
| (1,952)  | 1:A:29:LEU:HD22 | 1:A:70:VAL:HB   | 4        | 0.22          |
| (1,952)  | 1:A:29:LEU:HD23 | 1:A:70:VAL:HB   | 4        | 0.22          |
| (1,2631) | 1:A:10:GLN:HA   | 1:A:13:GLU:HG2  | 1        | 0.22          |
| (1,2290) | 1:A:40:SER:HB3  | 1:A:37:CYS:HA   | 5        | 0.22          |
| (1,2167) | 1:A:81:GLU:HA   | 1:A:84:ASP:HB3  | 10       | 0.22          |
| (1,2124) | 1:A:38:LEU:HD11 | 1:A:43:LEU:HD21 | 8        | 0.22          |
| (1,2124) | 1:A:38:LEU:HD11 | 1:A:43:LEU:HD22 | 8        | 0.22          |
| (1,2124) | 1:A:38:LEU:HD11 | 1:A:43:LEU:HD23 | 8        | 0.22          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2124) | 1:A:38:LEU:HD12  | 1:A:43:LEU:HD21 | 8        | 0.22          |
| (1,2124) | 1:A:38:LEU:HD12  | 1:A:43:LEU:HD22 | 8        | 0.22          |
| (1,2124) | 1:A:38:LEU:HD12  | 1:A:43:LEU:HD23 | 8        | 0.22          |
| (1,2124) | 1:A:38:LEU:HD13  | 1:A:43:LEU:HD21 | 8        | 0.22          |
| (1,2124) | 1:A:38:LEU:HD13  | 1:A:43:LEU:HD22 | 8        | 0.22          |
| (1,2124) | 1:A:38:LEU:HD13  | 1:A:43:LEU:HD23 | 8        | 0.22          |
| (1,1941) | 1:A:44:ILE:HG21  | 1:A:38:LEU:HD21 | 12       | 0.22          |
| (1,1941) | 1:A:44:ILE:HG21  | 1:A:38:LEU:HD22 | 12       | 0.22          |
| (1,1941) | 1:A:44:ILE:HG21  | 1:A:38:LEU:HD23 | 12       | 0.22          |
| (1,1941) | 1:A:44:ILE:HG22  | 1:A:38:LEU:HD21 | 12       | 0.22          |
| (1,1941) | 1:A:44:ILE:HG22  | 1:A:38:LEU:HD22 | 12       | 0.22          |
| (1,1941) | 1:A:44:ILE:HG22  | 1:A:38:LEU:HD23 | 12       | 0.22          |
| (1,1941) | 1:A:44:ILE:HG23  | 1:A:38:LEU:HD21 | 12       | 0.22          |
| (1,1941) | 1:A:44:ILE:HG23  | 1:A:38:LEU:HD22 | 12       | 0.22          |
| (1,1941) | 1:A:44:ILE:HG23  | 1:A:38:LEU:HD23 | 12       | 0.22          |
| (1,1933) | 1:A:78:TYR:HB3   | 1:A:63:VAL:HA   | 10       | 0.22          |
| (3,146)  | 1:A:123:TYR:O    | 1:A:126:ALA:N   | 11       | 0.21          |
| (3,142)  | 1:A:117:SER:O    | 1:A:120:GLN:N   | 10       | 0.21          |
| (3,137)  | 1:A:100:ALA:O    | 1:A:103:LYS:N   | 11       | 0.21          |
| (3,137)  | 1:A:100:ALA:O    | 1:A:103:LYS:N   | 12       | 0.21          |
| (3,136)  | 1:A:95:ILE:O     | 1:A:99:ILE:N    | 5        | 0.21          |
| (3,134)  | 1:A:94:GLU:O     | 1:A:97:SER:N    | 7        | 0.21          |
| (3,133)  | 1:A:91:GLN:O     | 1:A:94:GLU:N    | 1        | 0.21          |
| (3,133)  | 1:A:91:GLN:O     | 1:A:94:GLU:N    | 3        | 0.21          |
| (3,130)  | 1:A:79:MET:O     | 1:A:83:ASN:N    | 9        | 0.21          |
| (3,124)  | 1:A:29:LEU:O     | 1:A:70:VAL:N    | 1        | 0.21          |
| (3,123)  | 1:A:59:ILE:O     | 1:A:63:VAL:N    | 4        | 0.21          |
| (3,117)  | 1:A:38:LEU:O     | 1:A:43:LEU:N    | 10       | 0.21          |
| (3,116)  | 1:A:37:CYS:O     | 1:A:41:MET:N    | 3        | 0.21          |
| (3,110)  | 1:A:30:ASP:O     | 1:A:34:PHE:N    | 10       | 0.21          |
| (3,109)  | 1:A:29:LEU:N     | 1:A:70:VAL:O    | 2        | 0.21          |
| (3,103)  | 1:A:9:GLU:O      | 1:A:13:GLU:N    | 5        | 0.21          |
| (3,103)  | 1:A:9:GLU:O      | 1:A:13:GLU:N    | 7        | 0.21          |
| (2,318)  | 1:A:10:GLN:HB3   | 1:A:14:PHE:HZ   | 2        | 0.21          |
| (2,318)  | 1:A:10:GLN:HB3   | 1:A:14:PHE:HZ   | 3        | 0.21          |
| (1,2370) | 1:A:141:VAL:HG11 | 1:A:138:ALA:HA  | 11       | 0.21          |
| (1,2370) | 1:A:141:VAL:HG12 | 1:A:138:ALA:HA  | 11       | 0.21          |
| (1,2370) | 1:A:141:VAL:HG13 | 1:A:138:ALA:HA  | 11       | 0.21          |
| (1,2326) | 1:A:74:ASN:HA    | 1:A:77:GLN:HG3  | 9        | 0.21          |
| (1,2253) | 1:A:79:MET:HE1   | 1:A:43:LEU:HD21 | 11       | 0.21          |
| (1,2253) | 1:A:79:MET:HE1   | 1:A:43:LEU:HD22 | 11       | 0.21          |
| (1,2253) | 1:A:79:MET:HE1   | 1:A:43:LEU:HD23 | 11       | 0.21          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2253) | 1:A:79:MET:HE2   | 1:A:43:LEU:HD21 | 11       | 0.21          |
| (1,2253) | 1:A:79:MET:HE2   | 1:A:43:LEU:HD22 | 11       | 0.21          |
| (1,2253) | 1:A:79:MET:HE2   | 1:A:43:LEU:HD23 | 11       | 0.21          |
| (1,2253) | 1:A:79:MET:HE3   | 1:A:43:LEU:HD21 | 11       | 0.21          |
| (1,2253) | 1:A:79:MET:HE3   | 1:A:43:LEU:HD22 | 11       | 0.21          |
| (1,2253) | 1:A:79:MET:HE3   | 1:A:43:LEU:HD23 | 11       | 0.21          |
| (1,2212) | 1:A:35:ARG:HD2   | 1:A:56:TYR:HE1  | 1        | 0.21          |
| (1,2212) | 1:A:35:ARG:HD2   | 1:A:56:TYR:HE2  | 1        | 0.21          |
| (1,2174) | 1:A:99:ILE:HG21  | 1:A:100:ALA:HB1 | 2        | 0.21          |
| (1,2174) | 1:A:99:ILE:HG21  | 1:A:100:ALA:HB2 | 2        | 0.21          |
| (1,2174) | 1:A:99:ILE:HG21  | 1:A:100:ALA:HB3 | 2        | 0.21          |
| (1,2174) | 1:A:99:ILE:HG22  | 1:A:100:ALA:HB1 | 2        | 0.21          |
| (1,2174) | 1:A:99:ILE:HG22  | 1:A:100:ALA:HB2 | 2        | 0.21          |
| (1,2174) | 1:A:99:ILE:HG22  | 1:A:100:ALA:HB3 | 2        | 0.21          |
| (1,2174) | 1:A:99:ILE:HG23  | 1:A:100:ALA:HB1 | 2        | 0.21          |
| (1,2174) | 1:A:99:ILE:HG23  | 1:A:100:ALA:HB2 | 2        | 0.21          |
| (1,2174) | 1:A:99:ILE:HG23  | 1:A:100:ALA:HB3 | 2        | 0.21          |
| (1,2164) | 1:A:121:ILE:HG21 | 1:A:108:GLU:HB3 | 8        | 0.21          |
| (1,2164) | 1:A:121:ILE:HG22 | 1:A:108:GLU:HB3 | 8        | 0.21          |
| (1,2164) | 1:A:121:ILE:HG23 | 1:A:108:GLU:HB3 | 8        | 0.21          |
| (1,2164) | 1:A:121:ILE:HG21 | 1:A:108:GLU:HB3 | 11       | 0.21          |
| (1,2164) | 1:A:121:ILE:HG22 | 1:A:108:GLU:HB3 | 11       | 0.21          |
| (1,2164) | 1:A:121:ILE:HG23 | 1:A:108:GLU:HB3 | 11       | 0.21          |
| (1,2124) | 1:A:38:LEU:HD11  | 1:A:43:LEU:HD21 | 5        | 0.21          |
| (1,2124) | 1:A:38:LEU:HD11  | 1:A:43:LEU:HD22 | 5        | 0.21          |
| (1,2124) | 1:A:38:LEU:HD11  | 1:A:43:LEU:HD23 | 5        | 0.21          |
| (1,2124) | 1:A:38:LEU:HD12  | 1:A:43:LEU:HD21 | 5        | 0.21          |
| (1,2124) | 1:A:38:LEU:HD12  | 1:A:43:LEU:HD22 | 5        | 0.21          |
| (1,2124) | 1:A:38:LEU:HD12  | 1:A:43:LEU:HD23 | 5        | 0.21          |
| (1,2124) | 1:A:38:LEU:HD13  | 1:A:43:LEU:HD21 | 5        | 0.21          |
| (1,2124) | 1:A:38:LEU:HD13  | 1:A:43:LEU:HD22 | 5        | 0.21          |
| (1,2124) | 1:A:38:LEU:HD13  | 1:A:43:LEU:HD23 | 5        | 0.21          |
| (1,2080) | 1:A:38:LEU:HD21  | 1:A:59:ILE:HG21 | 6        | 0.21          |
| (1,2080) | 1:A:38:LEU:HD21  | 1:A:59:ILE:HG22 | 6        | 0.21          |
| (1,2080) | 1:A:38:LEU:HD21  | 1:A:59:ILE:HG23 | 6        | 0.21          |
| (1,2080) | 1:A:38:LEU:HD22  | 1:A:59:ILE:HG21 | 6        | 0.21          |
| (1,2080) | 1:A:38:LEU:HD22  | 1:A:59:ILE:HG22 | 6        | 0.21          |
| (1,2080) | 1:A:38:LEU:HD22  | 1:A:59:ILE:HG23 | 6        | 0.21          |
| (1,2080) | 1:A:38:LEU:HD23  | 1:A:59:ILE:HG21 | 6        | 0.21          |
| (1,2080) | 1:A:38:LEU:HD23  | 1:A:59:ILE:HG22 | 6        | 0.21          |
| (1,2080) | 1:A:38:LEU:HD23  | 1:A:59:ILE:HG23 | 6        | 0.21          |
| (1,2029) | 1:A:116:MET:HG2  | 1:A:114:ALA:HB1 | 7        | 0.21          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2029) | 1:A:116:MET:HG2  | 1:A:114:ALA:HB2 | 7        | 0.21          |
| (1,2029) | 1:A:116:MET:HG2  | 1:A:114:ALA:HB3 | 7        | 0.21          |
| (1,1847) | 1:A:6:VAL:HG11   | 1:A:80:LYS:HB3  | 9        | 0.21          |
| (1,1847) | 1:A:6:VAL:HG12   | 1:A:80:LYS:HB3  | 9        | 0.21          |
| (1,1847) | 1:A:6:VAL:HG13   | 1:A:80:LYS:HB3  | 9        | 0.21          |
| (1,1439) | 1:A:141:VAL:HG11 | 1:A:137:TYR:HE1 | 9        | 0.21          |
| (1,1439) | 1:A:141:VAL:HG11 | 1:A:137:TYR:HE2 | 9        | 0.21          |
| (1,1439) | 1:A:141:VAL:HG12 | 1:A:137:TYR:HE1 | 9        | 0.21          |
| (1,1439) | 1:A:141:VAL:HG12 | 1:A:137:TYR:HE2 | 9        | 0.21          |
| (1,1439) | 1:A:141:VAL:HG13 | 1:A:137:TYR:HE1 | 9        | 0.21          |
| (1,1439) | 1:A:141:VAL:HG13 | 1:A:137:TYR:HE2 | 9        | 0.21          |
| (3,139)  | 1:A:107:THR:O    | 1:A:111:MET:N   | 6        | 0.2           |
| (3,139)  | 1:A:107:THR:O    | 1:A:111:MET:N   | 9        | 0.2           |
| (3,137)  | 1:A:100:ALA:O    | 1:A:103:LYS:N   | 9        | 0.2           |
| (3,134)  | 1:A:94:GLU:O     | 1:A:97:SER:N    | 4        | 0.2           |
| (3,134)  | 1:A:94:GLU:O     | 1:A:97:SER:N    | 8        | 0.2           |
| (3,133)  | 1:A:91:GLN:O     | 1:A:94:GLU:N    | 8        | 0.2           |
| (3,133)  | 1:A:91:GLN:O     | 1:A:94:GLU:N    | 10       | 0.2           |
| (3,127)  | 1:A:75:TYR:O     | 1:A:78:TYR:N    | 3        | 0.2           |
| (3,126)  | 1:A:73:ASP:O     | 1:A:77:GLN:N    | 10       | 0.2           |
| (3,110)  | 1:A:30:ASP:O     | 1:A:34:PHE:N    | 9        | 0.2           |
| (3,106)  | 1:A:13:GLU:O     | 1:A:17:SER:N    | 12       | 0.2           |
| (3,105)  | 1:A:13:GLU:O     | 1:A:16:GLN:N    | 10       | 0.2           |
| (3,102)  | 1:A:9:GLU:O      | 1:A:12:GLN:N    | 5        | 0.2           |
| (2,184)  | 1:A:92:LEU:HB2   | 1:A:95:ILE:H    | 4        | 0.2           |
| (1,2408) | 1:A:6:VAL:HG21   | 1:A:14:PHE:HD1  | 3        | 0.2           |
| (1,2408) | 1:A:6:VAL:HG21   | 1:A:14:PHE:HD2  | 3        | 0.2           |
| (1,2408) | 1:A:6:VAL:HG22   | 1:A:14:PHE:HD1  | 3        | 0.2           |
| (1,2408) | 1:A:6:VAL:HG22   | 1:A:14:PHE:HD2  | 3        | 0.2           |
| (1,2408) | 1:A:6:VAL:HG23   | 1:A:14:PHE:HD1  | 3        | 0.2           |
| (1,2408) | 1:A:6:VAL:HG23   | 1:A:14:PHE:HD2  | 3        | 0.2           |
| (1,2393) | 1:A:6:VAL:HG11   | 1:A:80:LYS:HD3  | 7        | 0.2           |
| (1,2393) | 1:A:6:VAL:HG12   | 1:A:80:LYS:HD3  | 7        | 0.2           |
| (1,2393) | 1:A:6:VAL:HG13   | 1:A:80:LYS:HD3  | 7        | 0.2           |
| (1,2326) | 1:A:74:ASN:HA    | 1:A:77:GLN:HG3  | 1        | 0.2           |
| (1,2164) | 1:A:121:ILE:HG21 | 1:A:108:GLU:HB3 | 1        | 0.2           |
| (1,2164) | 1:A:121:ILE:HG22 | 1:A:108:GLU:HB3 | 1        | 0.2           |
| (1,2164) | 1:A:121:ILE:HG23 | 1:A:108:GLU:HB3 | 1        | 0.2           |
| (1,2164) | 1:A:121:ILE:HG21 | 1:A:108:GLU:HB3 | 4        | 0.2           |
| (1,2164) | 1:A:121:ILE:HG22 | 1:A:108:GLU:HB3 | 4        | 0.2           |
| (1,2164) | 1:A:121:ILE:HG23 | 1:A:108:GLU:HB3 | 4        | 0.2           |
| (1,2124) | 1:A:38:LEU:HD11  | 1:A:43:LEU:HD21 | 9        | 0.2           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2124) | 1:A:38:LEU:HD11 | 1:A:43:LEU:HD22 | 9        | 0.2           |
| (1,2124) | 1:A:38:LEU:HD11 | 1:A:43:LEU:HD23 | 9        | 0.2           |
| (1,2124) | 1:A:38:LEU:HD12 | 1:A:43:LEU:HD21 | 9        | 0.2           |
| (1,2124) | 1:A:38:LEU:HD12 | 1:A:43:LEU:HD22 | 9        | 0.2           |
| (1,2124) | 1:A:38:LEU:HD12 | 1:A:43:LEU:HD23 | 9        | 0.2           |
| (1,2124) | 1:A:38:LEU:HD13 | 1:A:43:LEU:HD21 | 9        | 0.2           |
| (1,2124) | 1:A:38:LEU:HD13 | 1:A:43:LEU:HD22 | 9        | 0.2           |
| (1,2124) | 1:A:38:LEU:HD13 | 1:A:43:LEU:HD23 | 9        | 0.2           |
| (1,2054) | 1:A:69:GLY:HA3  | 1:A:28:ILE:HB   | 6        | 0.2           |
| (1,1829) | 1:A:103:LYS:HE2 | 1:A:101:ALA:HB1 | 9        | 0.2           |
| (1,1829) | 1:A:103:LYS:HE2 | 1:A:101:ALA:HB2 | 9        | 0.2           |
| (1,1829) | 1:A:103:LYS:HE2 | 1:A:101:ALA:HB3 | 9        | 0.2           |
| (1,1447) | 1:A:89:PRO:HA   | 1:A:92:LEU:HD21 | 10       | 0.2           |
| (1,1447) | 1:A:89:PRO:HA   | 1:A:92:LEU:HD22 | 10       | 0.2           |
| (1,1447) | 1:A:89:PRO:HA   | 1:A:92:LEU:HD23 | 10       | 0.2           |
| (1,1144) | 1:A:44:ILE:HG21 | 1:A:56:TYR:HB3  | 1        | 0.2           |
| (1,1144) | 1:A:44:ILE:HG22 | 1:A:56:TYR:HB3  | 1        | 0.2           |
| (1,1144) | 1:A:44:ILE:HG23 | 1:A:56:TYR:HB3  | 1        | 0.2           |
| (3,97)   | 1:A:136:ASP:O   | 1:A:139:ALA:H   | 6        | 0.19          |
| (3,37)   | 1:A:45:ASP:O    | 1:A:47:ASP:H    | 3        | 0.19          |
| (3,150)  | 1:A:138:ALA:O   | 1:A:142:LYS:N   | 11       | 0.19          |
| (3,148)  | 1:A:124:VAL:O   | 1:A:128:LEU:N   | 3        | 0.19          |
| (3,146)  | 1:A:123:TYR:O   | 1:A:126:ALA:N   | 1        | 0.19          |
| (3,146)  | 1:A:123:TYR:O   | 1:A:126:ALA:N   | 4        | 0.19          |
| (3,146)  | 1:A:123:TYR:O   | 1:A:126:ALA:N   | 5        | 0.19          |
| (3,142)  | 1:A:117:SER:O   | 1:A:120:GLN:N   | 7        | 0.19          |
| (3,142)  | 1:A:117:SER:O   | 1:A:120:GLN:N   | 8        | 0.19          |
| (3,139)  | 1:A:107:THR:O   | 1:A:111:MET:N   | 8        | 0.19          |
| (3,135)  | 1:A:95:ILE:O    | 1:A:98:THR:N    | 11       | 0.19          |
| (3,135)  | 1:A:95:ILE:O    | 1:A:98:THR:N    | 12       | 0.19          |
| (3,133)  | 1:A:91:GLN:O    | 1:A:94:GLU:N    | 4        | 0.19          |
| (3,132)  | 1:A:90:GLU:O    | 1:A:93:ASN:N    | 6        | 0.19          |
| (3,131)  | 1:A:89:PRO:O    | 1:A:92:LEU:N    | 4        | 0.19          |
| (3,127)  | 1:A:75:TYR:O    | 1:A:78:TYR:N    | 6        | 0.19          |
| (3,126)  | 1:A:73:ASP:O    | 1:A:77:GLN:N    | 8        | 0.19          |
| (3,124)  | 1:A:29:LEU:O    | 1:A:70:VAL:N    | 8        | 0.19          |
| (3,114)  | 1:A:34:PHE:O    | 1:A:38:LEU:N    | 4        | 0.19          |
| (3,111)  | 1:A:31:LYS:O    | 1:A:35:ARG:N    | 7        | 0.19          |
| (3,110)  | 1:A:30:ASP:O    | 1:A:34:PHE:N    | 5        | 0.19          |
| (3,109)  | 1:A:29:LEU:N    | 1:A:70:VAL:O    | 12       | 0.19          |
| (3,106)  | 1:A:13:GLU:O    | 1:A:17:SER:N    | 10       | 0.19          |
| (3,103)  | 1:A:9:GLU:O     | 1:A:13:GLU:N    | 1        | 0.19          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (3,102)  | 1:A:9:GLU:O      | 1:A:12:GLN:N    | 9        | 0.19          |
| (2,267)  | 1:A:63:VAL:HG11  | 1:A:69:GLY:H    | 10       | 0.19          |
| (2,267)  | 1:A:63:VAL:HG12  | 1:A:69:GLY:H    | 10       | 0.19          |
| (2,267)  | 1:A:63:VAL:HG13  | 1:A:69:GLY:H    | 10       | 0.19          |
| (1,947)  | 1:A:6:VAL:HG11   | 1:A:80:LYS:HD3  | 7        | 0.19          |
| (1,947)  | 1:A:6:VAL:HG12   | 1:A:80:LYS:HD3  | 7        | 0.19          |
| (1,947)  | 1:A:6:VAL:HG13   | 1:A:80:LYS:HD3  | 7        | 0.19          |
| (1,2370) | 1:A:141:VAL:HG11 | 1:A:138:ALA:HA  | 2        | 0.19          |
| (1,2370) | 1:A:141:VAL:HG12 | 1:A:138:ALA:HA  | 2        | 0.19          |
| (1,2370) | 1:A:141:VAL:HG13 | 1:A:138:ALA:HA  | 2        | 0.19          |
| (1,2300) | 1:A:57:ASP:HB3   | 1:A:54:ALA:HA   | 11       | 0.19          |
| (1,2290) | 1:A:40:SER:HB3   | 1:A:37:CYS:HA   | 8        | 0.19          |
| (1,2273) | 1:A:109:THR:HG21 | 1:A:108:GLU:HG3 | 12       | 0.19          |
| (1,2273) | 1:A:109:THR:HG22 | 1:A:108:GLU:HG3 | 12       | 0.19          |
| (1,2273) | 1:A:109:THR:HG23 | 1:A:108:GLU:HG3 | 12       | 0.19          |
| (1,2054) | 1:A:69:GLY:HA3   | 1:A:28:ILE:HB   | 5        | 0.19          |
| (1,1938) | 1:A:6:VAL:HB     | 1:A:5:GLY:HA3   | 1        | 0.19          |
| (1,1499) | 1:A:99:ILE:HG21  | 1:A:103:LYS:HE2 | 6        | 0.19          |
| (1,1499) | 1:A:99:ILE:HG22  | 1:A:103:LYS:HE2 | 6        | 0.19          |
| (1,1499) | 1:A:99:ILE:HG23  | 1:A:103:LYS:HE2 | 6        | 0.19          |
| (1,1493) | 1:A:14:PHE:HE1   | 1:A:79:MET:HE1  | 8        | 0.19          |
| (1,1493) | 1:A:14:PHE:HE1   | 1:A:79:MET:HE2  | 8        | 0.19          |
| (1,1493) | 1:A:14:PHE:HE1   | 1:A:79:MET:HE3  | 8        | 0.19          |
| (1,1493) | 1:A:14:PHE:HE2   | 1:A:79:MET:HE1  | 8        | 0.19          |
| (1,1493) | 1:A:14:PHE:HE2   | 1:A:79:MET:HE2  | 8        | 0.19          |
| (1,1493) | 1:A:14:PHE:HE2   | 1:A:79:MET:HE3  | 8        | 0.19          |
| (1,1265) | 1:A:92:LEU:HD11  | 1:A:92:LEU:HA   | 7        | 0.19          |
| (1,1265) | 1:A:92:LEU:HD12  | 1:A:92:LEU:HA   | 7        | 0.19          |
| (1,1265) | 1:A:92:LEU:HD13  | 1:A:92:LEU:HA   | 7        | 0.19          |
| (1,1149) | 1:A:82:LYS:HA    | 1:A:85:GLU:HG3  | 11       | 0.19          |
| (3,53)   | 1:A:75:TYR:O     | 1:A:78:TYR:H    | 11       | 0.18          |
| (3,148)  | 1:A:124:VAL:O    | 1:A:128:LEU:N   | 5        | 0.18          |
| (3,146)  | 1:A:123:TYR:O    | 1:A:126:ALA:N   | 12       | 0.18          |
| (3,143)  | 1:A:120:GLN:O    | 1:A:123:TYR:N   | 9        | 0.18          |
| (3,142)  | 1:A:117:SER:O    | 1:A:120:GLN:N   | 2        | 0.18          |
| (3,142)  | 1:A:117:SER:O    | 1:A:120:GLN:N   | 5        | 0.18          |
| (3,142)  | 1:A:117:SER:O    | 1:A:120:GLN:N   | 12       | 0.18          |
| (3,138)  | 1:A:107:THR:O    | 1:A:110:ASP:N   | 3        | 0.18          |
| (3,135)  | 1:A:95:ILE:O     | 1:A:98:THR:N    | 2        | 0.18          |
| (3,135)  | 1:A:95:ILE:O     | 1:A:98:THR:N    | 6        | 0.18          |
| (3,133)  | 1:A:91:GLN:O     | 1:A:94:GLU:N    | 11       | 0.18          |
| (3,132)  | 1:A:90:GLU:O     | 1:A:93:ASN:N    | 3        | 0.18          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,132)  | 1:A:90:GLU:O    | 1:A:93:ASN:N    | 10       | 0.18          |
| (3,132)  | 1:A:90:GLU:O    | 1:A:93:ASN:N    | 11       | 0.18          |
| (3,131)  | 1:A:89:PRO:O    | 1:A:92:LEU:N    | 5        | 0.18          |
| (3,130)  | 1:A:79:MET:O    | 1:A:83:ASN:N    | 1        | 0.18          |
| (3,130)  | 1:A:79:MET:O    | 1:A:83:ASN:N    | 11       | 0.18          |
| (3,128)  | 1:A:75:TYR:O    | 1:A:79:MET:N    | 7        | 0.18          |
| (3,127)  | 1:A:75:TYR:O    | 1:A:78:TYR:N    | 2        | 0.18          |
| (3,127)  | 1:A:75:TYR:O    | 1:A:78:TYR:N    | 7        | 0.18          |
| (3,117)  | 1:A:38:LEU:O    | 1:A:43:LEU:N    | 12       | 0.18          |
| (3,113)  | 1:A:33:GLU:O    | 1:A:37:CYS:N    | 6        | 0.18          |
| (3,111)  | 1:A:31:LYS:O    | 1:A:35:ARG:N    | 1        | 0.18          |
| (3,110)  | 1:A:30:ASP:O    | 1:A:34:PHE:N    | 2        | 0.18          |
| (3,110)  | 1:A:30:ASP:O    | 1:A:34:PHE:N    | 8        | 0.18          |
| (3,107)  | 1:A:14:PHE:O    | 1:A:18:PHE:N    | 3        | 0.18          |
| (3,107)  | 1:A:14:PHE:O    | 1:A:18:PHE:N    | 10       | 0.18          |
| (3,105)  | 1:A:13:GLU:O    | 1:A:16:GLN:N    | 9        | 0.18          |
| (3,103)  | 1:A:9:GLU:O     | 1:A:13:GLU:N    | 6        | 0.18          |
| (3,103)  | 1:A:9:GLU:O     | 1:A:13:GLU:N    | 8        | 0.18          |
| (3,103)  | 1:A:9:GLU:O     | 1:A:13:GLU:N    | 9        | 0.18          |
| (1,952)  | 1:A:29:LEU:HD21 | 1:A:70:VAL:HB   | 12       | 0.18          |
| (1,952)  | 1:A:29:LEU:HD22 | 1:A:70:VAL:HB   | 12       | 0.18          |
| (1,952)  | 1:A:29:LEU:HD23 | 1:A:70:VAL:HB   | 12       | 0.18          |
| (1,2641) | 1:A:122:GLU:HB2 | 1:A:126:ALA:HB1 | 1        | 0.18          |
| (1,2641) | 1:A:122:GLU:HB2 | 1:A:126:ALA:HB2 | 1        | 0.18          |
| (1,2641) | 1:A:122:GLU:HB2 | 1:A:126:ALA:HB3 | 1        | 0.18          |
| (1,2292) | 1:A:113:LYS:HB3 | 1:A:113:LYS:HE3 | 1        | 0.18          |
| (1,2253) | 1:A:79:MET:HE1  | 1:A:43:LEU:HD21 | 5        | 0.18          |
| (1,2253) | 1:A:79:MET:HE1  | 1:A:43:LEU:HD22 | 5        | 0.18          |
| (1,2253) | 1:A:79:MET:HE1  | 1:A:43:LEU:HD23 | 5        | 0.18          |
| (1,2253) | 1:A:79:MET:HE2  | 1:A:43:LEU:HD21 | 5        | 0.18          |
| (1,2253) | 1:A:79:MET:HE2  | 1:A:43:LEU:HD22 | 5        | 0.18          |
| (1,2253) | 1:A:79:MET:HE2  | 1:A:43:LEU:HD23 | 5        | 0.18          |
| (1,2253) | 1:A:79:MET:HE3  | 1:A:43:LEU:HD21 | 5        | 0.18          |
| (1,2253) | 1:A:79:MET:HE3  | 1:A:43:LEU:HD22 | 5        | 0.18          |
| (1,2253) | 1:A:79:MET:HE3  | 1:A:43:LEU:HD23 | 5        | 0.18          |
| (1,2182) | 1:A:79:MET:HB2  | 1:A:79:MET:HE1  | 11       | 0.18          |
| (1,2182) | 1:A:79:MET:HB2  | 1:A:79:MET:HE2  | 11       | 0.18          |
| (1,2182) | 1:A:79:MET:HB2  | 1:A:79:MET:HE3  | 11       | 0.18          |
| (1,1978) | 1:A:38:LEU:HA   | 1:A:43:LEU:HD21 | 3        | 0.18          |
| (1,1978) | 1:A:38:LEU:HA   | 1:A:43:LEU:HD22 | 3        | 0.18          |
| (1,1978) | 1:A:38:LEU:HA   | 1:A:43:LEU:HD23 | 3        | 0.18          |
| (1,1716) | 1:A:40:SER:HB3  | 1:A:37:CYS:HA   | 5        | 0.18          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1510) | 1:A:78:TYR:HB2  | 1:A:79:MET:HE1  | 11       | 0.18          |
| (1,1510) | 1:A:78:TYR:HB2  | 1:A:79:MET:HE2  | 11       | 0.18          |
| (1,1510) | 1:A:78:TYR:HB2  | 1:A:79:MET:HE3  | 11       | 0.18          |
| (1,1424) | 1:A:87:PRO:HD3  | 1:A:86:ASN:HB3  | 12       | 0.18          |
| (3,53)   | 1:A:75:TYR:O    | 1:A:78:TYR:H    | 5        | 0.17          |
| (3,23)   | 1:A:33:GLU:O    | 1:A:36:SER:H    | 1        | 0.17          |
| (3,147)  | 1:A:123:TYR:O   | 1:A:127:ASN:N   | 11       | 0.17          |
| (3,146)  | 1:A:123:TYR:O   | 1:A:126:ALA:N   | 7        | 0.17          |
| (3,143)  | 1:A:120:GLN:O   | 1:A:123:TYR:N   | 5        | 0.17          |
| (3,142)  | 1:A:117:SER:O   | 1:A:120:GLN:N   | 1        | 0.17          |
| (3,142)  | 1:A:117:SER:O   | 1:A:120:GLN:N   | 9        | 0.17          |
| (3,141)  | 1:A:113:LYS:O   | 1:A:115:GLY:N   | 1        | 0.17          |
| (3,141)  | 1:A:113:LYS:O   | 1:A:115:GLY:N   | 7        | 0.17          |
| (3,138)  | 1:A:107:THR:O   | 1:A:110:ASP:N   | 7        | 0.17          |
| (3,135)  | 1:A:95:ILE:O    | 1:A:98:THR:N    | 7        | 0.17          |
| (3,131)  | 1:A:89:PRO:O    | 1:A:92:LEU:N    | 9        | 0.17          |
| (3,127)  | 1:A:75:TYR:O    | 1:A:78:TYR:N    | 8        | 0.17          |
| (3,126)  | 1:A:73:ASP:O    | 1:A:77:GLN:N    | 6        | 0.17          |
| (3,119)  | 1:A:45:ASP:O    | 1:A:47:ASP:N    | 6        | 0.17          |
| (3,111)  | 1:A:31:LYS:O    | 1:A:35:ARG:N    | 11       | 0.17          |
| (3,109)  | 1:A:29:LEU:N    | 1:A:70:VAL:O    | 3        | 0.17          |
| (3,106)  | 1:A:13:GLU:O    | 1:A:17:SER:N    | 11       | 0.17          |
| (3,102)  | 1:A:9:GLU:O     | 1:A:12:GLN:N    | 4        | 0.17          |
| (3,102)  | 1:A:9:GLU:O     | 1:A:12:GLN:N    | 6        | 0.17          |
| (3,102)  | 1:A:9:GLU:O     | 1:A:12:GLN:N    | 8        | 0.17          |
| (1,872)  | 1:A:138:ALA:HB1 | 1:A:104:ASP:HB3 | 3        | 0.17          |
| (1,872)  | 1:A:138:ALA:HB2 | 1:A:104:ASP:HB3 | 3        | 0.17          |
| (1,872)  | 1:A:138:ALA:HB3 | 1:A:104:ASP:HB3 | 3        | 0.17          |
| (1,2639) | 1:A:43:LEU:HD11 | 1:A:43:LEU:HA   | 1        | 0.17          |
| (1,2639) | 1:A:43:LEU:HD12 | 1:A:43:LEU:HA   | 1        | 0.17          |
| (1,2639) | 1:A:43:LEU:HD13 | 1:A:43:LEU:HA   | 1        | 0.17          |
| (1,2174) | 1:A:99:ILE:HG21 | 1:A:100:ALA:HB1 | 4        | 0.17          |
| (1,2174) | 1:A:99:ILE:HG21 | 1:A:100:ALA:HB2 | 4        | 0.17          |
| (1,2174) | 1:A:99:ILE:HG21 | 1:A:100:ALA:HB3 | 4        | 0.17          |
| (1,2174) | 1:A:99:ILE:HG22 | 1:A:100:ALA:HB1 | 4        | 0.17          |
| (1,2174) | 1:A:99:ILE:HG22 | 1:A:100:ALA:HB2 | 4        | 0.17          |
| (1,2174) | 1:A:99:ILE:HG22 | 1:A:100:ALA:HB3 | 4        | 0.17          |
| (1,2174) | 1:A:99:ILE:HG23 | 1:A:100:ALA:HB1 | 4        | 0.17          |
| (1,2174) | 1:A:99:ILE:HG23 | 1:A:100:ALA:HB2 | 4        | 0.17          |
| (1,2174) | 1:A:99:ILE:HG23 | 1:A:100:ALA:HB3 | 4        | 0.17          |
| (1,2142) | 1:A:79:MET:HA   | 1:A:82:LYS:HB3  | 10       | 0.17          |
| (1,1675) | 1:A:15:LYS:HB2  | 1:A:15:LYS:HE3  | 8        | 0.17          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1257) | 1:A:41:MET:HE1  | 1:A:38:LEU:HD11 | 4        | 0.17          |
| (1,1257) | 1:A:41:MET:HE1  | 1:A:38:LEU:HD12 | 4        | 0.17          |
| (1,1257) | 1:A:41:MET:HE1  | 1:A:38:LEU:HD13 | 4        | 0.17          |
| (1,1257) | 1:A:41:MET:HE2  | 1:A:38:LEU:HD11 | 4        | 0.17          |
| (1,1257) | 1:A:41:MET:HE2  | 1:A:38:LEU:HD12 | 4        | 0.17          |
| (1,1257) | 1:A:41:MET:HE2  | 1:A:38:LEU:HD13 | 4        | 0.17          |
| (1,1257) | 1:A:41:MET:HE3  | 1:A:38:LEU:HD11 | 4        | 0.17          |
| (1,1257) | 1:A:41:MET:HE3  | 1:A:38:LEU:HD12 | 4        | 0.17          |
| (1,1257) | 1:A:41:MET:HE3  | 1:A:38:LEU:HD13 | 4        | 0.17          |
| (1,1144) | 1:A:44:ILE:HG21 | 1:A:56:TYR:HB3  | 10       | 0.17          |
| (1,1144) | 1:A:44:ILE:HG22 | 1:A:56:TYR:HB3  | 10       | 0.17          |
| (1,1144) | 1:A:44:ILE:HG23 | 1:A:56:TYR:HB3  | 10       | 0.17          |
| (3,97)   | 1:A:136:ASP:O   | 1:A:139:ALA:H   | 11       | 0.16          |
| (3,81)   | 1:A:113:LYS:O   | 1:A:115:GLY:H   | 4        | 0.16          |
| (3,59)   | 1:A:79:MET:O    | 1:A:83:ASN:H    | 4        | 0.16          |
| (3,59)   | 1:A:79:MET:O    | 1:A:83:ASN:H    | 12       | 0.16          |
| (3,53)   | 1:A:75:TYR:O    | 1:A:78:TYR:H    | 7        | 0.16          |
| (3,147)  | 1:A:123:TYR:O   | 1:A:127:ASN:N   | 4        | 0.16          |
| (3,146)  | 1:A:123:TYR:O   | 1:A:126:ALA:N   | 8        | 0.16          |
| (3,143)  | 1:A:120:GLN:O   | 1:A:123:TYR:N   | 11       | 0.16          |
| (3,141)  | 1:A:113:LYS:O   | 1:A:115:GLY:N   | 2        | 0.16          |
| (3,138)  | 1:A:107:THR:O   | 1:A:110:ASP:N   | 1        | 0.16          |
| (3,138)  | 1:A:107:THR:O   | 1:A:110:ASP:N   | 5        | 0.16          |
| (3,138)  | 1:A:107:THR:O   | 1:A:110:ASP:N   | 8        | 0.16          |
| (3,138)  | 1:A:107:THR:O   | 1:A:110:ASP:N   | 9        | 0.16          |
| (3,135)  | 1:A:95:ILE:O    | 1:A:98:THR:N    | 10       | 0.16          |
| (3,134)  | 1:A:94:GLU:O    | 1:A:97:SER:N    | 12       | 0.16          |
| (3,130)  | 1:A:79:MET:O    | 1:A:83:ASN:N    | 6        | 0.16          |
| (3,128)  | 1:A:75:TYR:O    | 1:A:79:MET:N    | 9        | 0.16          |
| (3,127)  | 1:A:75:TYR:O    | 1:A:78:TYR:N    | 9        | 0.16          |
| (3,123)  | 1:A:59:ILE:O    | 1:A:63:VAL:N    | 5        | 0.16          |
| (3,119)  | 1:A:45:ASP:O    | 1:A:47:ASP:N    | 1        | 0.16          |
| (3,117)  | 1:A:38:LEU:O    | 1:A:43:LEU:N    | 11       | 0.16          |
| (3,116)  | 1:A:37:CYS:O    | 1:A:41:MET:N    | 12       | 0.16          |
| (3,113)  | 1:A:33:GLU:O    | 1:A:37:CYS:N    | 5        | 0.16          |
| (3,105)  | 1:A:13:GLU:O    | 1:A:16:GLN:N    | 3        | 0.16          |
| (3,102)  | 1:A:9:GLU:O     | 1:A:12:GLN:N    | 2        | 0.16          |
| (3,102)  | 1:A:9:GLU:O     | 1:A:12:GLN:N    | 7        | 0.16          |
| (2,335)  | 1:A:71:SER:HB3  | 1:A:28:ILE:HG12 | 4        | 0.16          |
| (1,56)   | 1:A:52:GLU:HA   | 1:A:50:GLY:H    | 1        | 0.16          |
| (1,2639) | 1:A:43:LEU:HD11 | 1:A:43:LEU:HA   | 2        | 0.16          |
| (1,2639) | 1:A:43:LEU:HD12 | 1:A:43:LEU:HA   | 2        | 0.16          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2639) | 1:A:43:LEU:HD13  | 1:A:43:LEU:HA   | 2        | 0.16          |
| (1,2602) | 1:A:141:VAL:HG11 | 1:A:137:TYR:HD1 | 2        | 0.16          |
| (1,2602) | 1:A:141:VAL:HG11 | 1:A:137:TYR:HD2 | 2        | 0.16          |
| (1,2602) | 1:A:141:VAL:HG12 | 1:A:137:TYR:HD1 | 2        | 0.16          |
| (1,2602) | 1:A:141:VAL:HG12 | 1:A:137:TYR:HD2 | 2        | 0.16          |
| (1,2602) | 1:A:141:VAL:HG13 | 1:A:137:TYR:HD1 | 2        | 0.16          |
| (1,2602) | 1:A:141:VAL:HG13 | 1:A:137:TYR:HD2 | 2        | 0.16          |
| (1,2326) | 1:A:74:ASN:HA    | 1:A:77:GLN:HG3  | 2        | 0.16          |
| (1,1595) | 1:A:78:TYR:HE1   | 1:A:82:LYS:HE3  | 4        | 0.16          |
| (1,1595) | 1:A:78:TYR:HE2   | 1:A:82:LYS:HE3  | 4        | 0.16          |
| (1,1519) | 1:A:6:VAL:HG21   | 1:A:11:MET:HE1  | 2        | 0.16          |
| (1,1519) | 1:A:6:VAL:HG21   | 1:A:11:MET:HE2  | 2        | 0.16          |
| (1,1519) | 1:A:6:VAL:HG21   | 1:A:11:MET:HE3  | 2        | 0.16          |
| (1,1519) | 1:A:6:VAL:HG22   | 1:A:11:MET:HE1  | 2        | 0.16          |
| (1,1519) | 1:A:6:VAL:HG22   | 1:A:11:MET:HE2  | 2        | 0.16          |
| (1,1519) | 1:A:6:VAL:HG22   | 1:A:11:MET:HE3  | 2        | 0.16          |
| (1,1519) | 1:A:6:VAL:HG23   | 1:A:11:MET:HE1  | 2        | 0.16          |
| (1,1519) | 1:A:6:VAL:HG23   | 1:A:11:MET:HE2  | 2        | 0.16          |
| (1,1519) | 1:A:6:VAL:HG23   | 1:A:11:MET:HE3  | 2        | 0.16          |
| (1,1510) | 1:A:78:TYR:HB2   | 1:A:79:MET:HE1  | 7        | 0.16          |
| (1,1510) | 1:A:78:TYR:HB2   | 1:A:79:MET:HE2  | 7        | 0.16          |
| (1,1510) | 1:A:78:TYR:HB2   | 1:A:79:MET:HE3  | 7        | 0.16          |
| (1,1489) | 1:A:20:ALA:HB1   | 1:A:17:SER:HB3  | 6        | 0.16          |
| (1,1489) | 1:A:20:ALA:HB2   | 1:A:17:SER:HB3  | 6        | 0.16          |
| (1,1489) | 1:A:20:ALA:HB3   | 1:A:17:SER:HB3  | 6        | 0.16          |
| (1,1387) | 1:A:109:THR:HG21 | 1:A:113:LYS:HE3 | 11       | 0.16          |
| (1,1387) | 1:A:109:THR:HG22 | 1:A:113:LYS:HE3 | 11       | 0.16          |
| (1,1387) | 1:A:109:THR:HG23 | 1:A:113:LYS:HE3 | 11       | 0.16          |
| (1,1276) | 1:A:28:ILE:HA    | 1:A:14:PHE:HZ   | 4        | 0.16          |
| (3,9)    | 1:A:13:GLU:O     | 1:A:16:GLN:H    | 11       | 0.15          |
| (3,77)   | 1:A:107:THR:O    | 1:A:111:MET:H   | 5        | 0.15          |
| (3,59)   | 1:A:79:MET:O     | 1:A:83:ASN:H    | 7        | 0.15          |
| (3,53)   | 1:A:75:TYR:O     | 1:A:78:TYR:H    | 1        | 0.15          |
| (3,148)  | 1:A:124:VAL:O    | 1:A:128:LEU:N   | 11       | 0.15          |
| (3,146)  | 1:A:123:TYR:O    | 1:A:126:ALA:N   | 10       | 0.15          |
| (3,145)  | 1:A:121:ILE:O    | 1:A:125:LYS:N   | 8        | 0.15          |
| (3,144)  | 1:A:120:GLN:O    | 1:A:124:VAL:N   | 7        | 0.15          |
| (3,143)  | 1:A:120:GLN:O    | 1:A:123:TYR:N   | 2        | 0.15          |
| (3,143)  | 1:A:120:GLN:O    | 1:A:123:TYR:N   | 4        | 0.15          |
| (3,143)  | 1:A:120:GLN:O    | 1:A:123:TYR:N   | 6        | 0.15          |
| (3,143)  | 1:A:120:GLN:O    | 1:A:123:TYR:N   | 10       | 0.15          |
| (3,141)  | 1:A:113:LYS:O    | 1:A:115:GLY:N   | 8        | 0.15          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,141)  | 1:A:113:LYS:O   | 1:A:115:GLY:N   | 9        | 0.15          |
| (3,141)  | 1:A:113:LYS:O   | 1:A:115:GLY:N   | 10       | 0.15          |
| (3,141)  | 1:A:113:LYS:O   | 1:A:115:GLY:N   | 11       | 0.15          |
| (3,138)  | 1:A:107:THR:O   | 1:A:110:ASP:N   | 2        | 0.15          |
| (3,138)  | 1:A:107:THR:O   | 1:A:110:ASP:N   | 6        | 0.15          |
| (3,138)  | 1:A:107:THR:O   | 1:A:110:ASP:N   | 10       | 0.15          |
| (3,136)  | 1:A:95:ILE:O    | 1:A:99:ILE:N    | 8        | 0.15          |
| (3,135)  | 1:A:95:ILE:O    | 1:A:98:THR:N    | 1        | 0.15          |
| (3,135)  | 1:A:95:ILE:O    | 1:A:98:THR:N    | 3        | 0.15          |
| (3,135)  | 1:A:95:ILE:O    | 1:A:98:THR:N    | 5        | 0.15          |
| (3,135)  | 1:A:95:ILE:O    | 1:A:98:THR:N    | 8        | 0.15          |
| (3,135)  | 1:A:95:ILE:O    | 1:A:98:THR:N    | 9        | 0.15          |
| (3,134)  | 1:A:94:GLU:O    | 1:A:97:SER:N    | 6        | 0.15          |
| (3,133)  | 1:A:91:GLN:O    | 1:A:94:GLU:N    | 6        | 0.15          |
| (3,128)  | 1:A:75:TYR:O    | 1:A:79:MET:N    | 4        | 0.15          |
| (3,128)  | 1:A:75:TYR:O    | 1:A:79:MET:N    | 10       | 0.15          |
| (3,120)  | 1:A:54:ALA:O    | 1:A:58:ALA:N    | 7        | 0.15          |
| (3,117)  | 1:A:38:LEU:O    | 1:A:43:LEU:N    | 5        | 0.15          |
| (3,102)  | 1:A:9:GLU:O     | 1:A:12:GLN:N    | 10       | 0.15          |
| (2,320)  | 1:A:32:LEU:HA   | 1:A:35:ARG:HD2  | 6        | 0.15          |
| (1,418)  | 1:A:117:SER:H   | 1:A:120:GLN:HB3 | 5        | 0.15          |
| (1,2253) | 1:A:79:MET:HE1  | 1:A:43:LEU:HD21 | 8        | 0.15          |
| (1,2253) | 1:A:79:MET:HE1  | 1:A:43:LEU:HD22 | 8        | 0.15          |
| (1,2253) | 1:A:79:MET:HE1  | 1:A:43:LEU:HD23 | 8        | 0.15          |
| (1,2253) | 1:A:79:MET:HE2  | 1:A:43:LEU:HD21 | 8        | 0.15          |
| (1,2253) | 1:A:79:MET:HE2  | 1:A:43:LEU:HD22 | 8        | 0.15          |
| (1,2253) | 1:A:79:MET:HE2  | 1:A:43:LEU:HD23 | 8        | 0.15          |
| (1,2253) | 1:A:79:MET:HE3  | 1:A:43:LEU:HD21 | 8        | 0.15          |
| (1,2253) | 1:A:79:MET:HE3  | 1:A:43:LEU:HD22 | 8        | 0.15          |
| (1,2253) | 1:A:79:MET:HE3  | 1:A:43:LEU:HD23 | 8        | 0.15          |
| (1,2156) | 1:A:44:ILE:HG21 | 1:A:56:TYR:HA   | 9        | 0.15          |
| (1,2156) | 1:A:44:ILE:HG22 | 1:A:56:TYR:HA   | 9        | 0.15          |
| (1,2156) | 1:A:44:ILE:HG23 | 1:A:56:TYR:HA   | 9        | 0.15          |
| (1,1716) | 1:A:40:SER:HB3  | 1:A:37:CYS:HA   | 8        | 0.15          |
| (1,1653) | 1:A:76:VAL:HG21 | 1:A:75:TYR:HE1  | 12       | 0.15          |
| (1,1653) | 1:A:76:VAL:HG21 | 1:A:75:TYR:HE2  | 12       | 0.15          |
| (1,1653) | 1:A:76:VAL:HG22 | 1:A:75:TYR:HE1  | 12       | 0.15          |
| (1,1653) | 1:A:76:VAL:HG22 | 1:A:75:TYR:HE2  | 12       | 0.15          |
| (1,1653) | 1:A:76:VAL:HG23 | 1:A:75:TYR:HE1  | 12       | 0.15          |
| (1,1653) | 1:A:76:VAL:HG23 | 1:A:75:TYR:HE2  | 12       | 0.15          |
| (1,1645) | 1:A:68:ASN:HB2  | 1:A:67:GLU:HA   | 2        | 0.15          |
| (1,1595) | 1:A:78:TYR:HE1  | 1:A:82:LYS:HE3  | 8        | 0.15          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1595) | 1:A:78:TYR:HE2  | 1:A:82:LYS:HE3  | 8        | 0.15          |
| (1,1580) | 1:A:44:ILE:HB   | 1:A:43:LEU:HB3  | 7        | 0.15          |
| (1,1510) | 1:A:78:TYR:HB2  | 1:A:79:MET:HE1  | 9        | 0.15          |
| (1,1510) | 1:A:78:TYR:HB2  | 1:A:79:MET:HE2  | 9        | 0.15          |
| (1,1510) | 1:A:78:TYR:HB2  | 1:A:79:MET:HE3  | 9        | 0.15          |
| (1,1491) | 1:A:65:LYS:HE3  | 1:A:65:LYS:HB2  | 7        | 0.15          |
| (1,1447) | 1:A:89:PRO:HA   | 1:A:92:LEU:HD21 | 6        | 0.15          |
| (1,1447) | 1:A:89:PRO:HA   | 1:A:92:LEU:HD22 | 6        | 0.15          |
| (1,1447) | 1:A:89:PRO:HA   | 1:A:92:LEU:HD23 | 6        | 0.15          |
| (1,1276) | 1:A:28:ILE:HA   | 1:A:14:PHE:HZ   | 2        | 0.15          |
| (1,1138) | 1:A:70:VAL:HG21 | 1:A:74:ASN:HB2  | 4        | 0.15          |
| (1,1138) | 1:A:70:VAL:HG22 | 1:A:74:ASN:HB2  | 4        | 0.15          |
| (1,1138) | 1:A:70:VAL:HG23 | 1:A:74:ASN:HB2  | 4        | 0.15          |
| (3,9)    | 1:A:13:GLU:O    | 1:A:16:GLN:H    | 5        | 0.14          |
| (3,65)   | 1:A:91:GLN:O    | 1:A:94:GLU:H    | 4        | 0.14          |
| (3,61)   | 1:A:89:PRO:O    | 1:A:92:LEU:H    | 4        | 0.14          |
| (3,150)  | 1:A:138:ALA:O   | 1:A:142:LYS:N   | 6        | 0.14          |
| (3,146)  | 1:A:123:TYR:O   | 1:A:126:ALA:N   | 2        | 0.14          |
| (3,142)  | 1:A:117:SER:O   | 1:A:120:GLN:N   | 3        | 0.14          |
| (3,142)  | 1:A:117:SER:O   | 1:A:120:GLN:N   | 11       | 0.14          |
| (3,141)  | 1:A:113:LYS:O   | 1:A:115:GLY:N   | 3        | 0.14          |
| (3,141)  | 1:A:113:LYS:O   | 1:A:115:GLY:N   | 5        | 0.14          |
| (3,134)  | 1:A:94:GLU:O    | 1:A:97:SER:N    | 9        | 0.14          |
| (3,130)  | 1:A:79:MET:O    | 1:A:83:ASN:N    | 8        | 0.14          |
| (3,129)  | 1:A:76:VAL:O    | 1:A:80:LYS:N    | 12       | 0.14          |
| (3,127)  | 1:A:75:TYR:O    | 1:A:78:TYR:N    | 12       | 0.14          |
| (3,121)  | 1:A:56:TYR:O    | 1:A:60:TYR:N    | 11       | 0.14          |
| (3,119)  | 1:A:45:ASP:O    | 1:A:47:ASP:N    | 10       | 0.14          |
| (3,117)  | 1:A:38:LEU:O    | 1:A:43:LEU:N    | 6        | 0.14          |
| (3,116)  | 1:A:37:CYS:O    | 1:A:41:MET:N    | 2        | 0.14          |
| (3,116)  | 1:A:37:CYS:O    | 1:A:41:MET:N    | 11       | 0.14          |
| (3,114)  | 1:A:34:PHE:O    | 1:A:38:LEU:N    | 6        | 0.14          |
| (3,105)  | 1:A:13:GLU:O    | 1:A:16:GLN:N    | 8        | 0.14          |
| (3,104)  | 1:A:10:GLN:O    | 1:A:14:PHE:N    | 3        | 0.14          |
| (3,103)  | 1:A:9:GLU:O     | 1:A:13:GLU:N    | 2        | 0.14          |
| (2,267)  | 1:A:63:VAL:HG11 | 1:A:69:GLY:H    | 4        | 0.14          |
| (2,267)  | 1:A:63:VAL:HG12 | 1:A:69:GLY:H    | 4        | 0.14          |
| (2,267)  | 1:A:63:VAL:HG13 | 1:A:69:GLY:H    | 4        | 0.14          |
| (2,267)  | 1:A:63:VAL:HG11 | 1:A:69:GLY:H    | 9        | 0.14          |
| (2,267)  | 1:A:63:VAL:HG12 | 1:A:69:GLY:H    | 9        | 0.14          |
| (2,267)  | 1:A:63:VAL:HG13 | 1:A:69:GLY:H    | 9        | 0.14          |
| (1,952)  | 1:A:29:LEU:HD21 | 1:A:70:VAL:HB   | 1        | 0.14          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,952)  | 1:A:29:LEU:HD22  | 1:A:70:VAL:HB    | 1        | 0.14          |
| (1,952)  | 1:A:29:LEU:HD23  | 1:A:70:VAL:HB    | 1        | 0.14          |
| (1,952)  | 1:A:29:LEU:HD21  | 1:A:70:VAL:HB    | 2        | 0.14          |
| (1,952)  | 1:A:29:LEU:HD22  | 1:A:70:VAL:HB    | 2        | 0.14          |
| (1,952)  | 1:A:29:LEU:HD23  | 1:A:70:VAL:HB    | 2        | 0.14          |
| (1,952)  | 1:A:29:LEU:HD21  | 1:A:70:VAL:HB    | 3        | 0.14          |
| (1,952)  | 1:A:29:LEU:HD22  | 1:A:70:VAL:HB    | 3        | 0.14          |
| (1,952)  | 1:A:29:LEU:HD23  | 1:A:70:VAL:HB    | 3        | 0.14          |
| (1,934)  | 1:A:39:SER:HB2   | 1:A:44:ILE:HG12  | 9        | 0.14          |
| (1,786)  | 1:A:63:VAL:HB    | 1:A:60:TYR:HD1   | 9        | 0.14          |
| (1,786)  | 1:A:63:VAL:HB    | 1:A:60:TYR:HD2   | 9        | 0.14          |
| (1,2653) | 1:A:61:ASN:HB3   | 1:A:58:ALA:HB1   | 10       | 0.14          |
| (1,2653) | 1:A:61:ASN:HB3   | 1:A:58:ALA:HB2   | 10       | 0.14          |
| (1,2653) | 1:A:61:ASN:HB3   | 1:A:58:ALA:HB3   | 10       | 0.14          |
| (1,2602) | 1:A:141:VAL:HG11 | 1:A:137:TYR:HD1  | 9        | 0.14          |
| (1,2602) | 1:A:141:VAL:HG11 | 1:A:137:TYR:HD2  | 9        | 0.14          |
| (1,2602) | 1:A:141:VAL:HG12 | 1:A:137:TYR:HD1  | 9        | 0.14          |
| (1,2602) | 1:A:141:VAL:HG12 | 1:A:137:TYR:HD2  | 9        | 0.14          |
| (1,2602) | 1:A:141:VAL:HG13 | 1:A:137:TYR:HD1  | 9        | 0.14          |
| (1,2602) | 1:A:141:VAL:HG13 | 1:A:137:TYR:HD2  | 9        | 0.14          |
| (1,2594) | 1:A:70:VAL:HG21  | 1:A:74:ASN:HB3   | 10       | 0.14          |
| (1,2594) | 1:A:70:VAL:HG22  | 1:A:74:ASN:HB3   | 10       | 0.14          |
| (1,2594) | 1:A:70:VAL:HG23  | 1:A:74:ASN:HB3   | 10       | 0.14          |
| (1,2436) | 1:A:6:VAL:HG11   | 1:A:80:LYS:HB3   | 3        | 0.14          |
| (1,2436) | 1:A:6:VAL:HG12   | 1:A:80:LYS:HB3   | 3        | 0.14          |
| (1,2436) | 1:A:6:VAL:HG13   | 1:A:80:LYS:HB3   | 3        | 0.14          |
| (1,2327) | 1:A:113:LYS:HB3  | 1:A:113:LYS:HE3  | 7        | 0.14          |
| (1,2290) | 1:A:40:SER:HB3   | 1:A:37:CYS:HA    | 7        | 0.14          |
| (1,2226) | 1:A:100:ALA:HA   | 1:A:106:ILE:HG21 | 1        | 0.14          |
| (1,2226) | 1:A:100:ALA:HA   | 1:A:106:ILE:HG22 | 1        | 0.14          |
| (1,2226) | 1:A:100:ALA:HA   | 1:A:106:ILE:HG23 | 1        | 0.14          |
| (1,1978) | 1:A:38:LEU:HA    | 1:A:43:LEU:HD21  | 1        | 0.14          |
| (1,1978) | 1:A:38:LEU:HA    | 1:A:43:LEU:HD22  | 1        | 0.14          |
| (1,1978) | 1:A:38:LEU:HA    | 1:A:43:LEU:HD23  | 1        | 0.14          |
| (1,1930) | 1:A:63:VAL:HG11  | 1:A:34:PHE:HZ    | 4        | 0.14          |
| (1,1930) | 1:A:63:VAL:HG12  | 1:A:34:PHE:HZ    | 4        | 0.14          |
| (1,1930) | 1:A:63:VAL:HG13  | 1:A:34:PHE:HZ    | 4        | 0.14          |
| (1,1580) | 1:A:44:ILE:HB    | 1:A:43:LEU:HB3   | 10       | 0.14          |
| (1,1539) | 1:A:6:VAL:HG21   | 1:A:11:MET:HE1   | 12       | 0.14          |
| (1,1539) | 1:A:6:VAL:HG21   | 1:A:11:MET:HE2   | 12       | 0.14          |
| (1,1539) | 1:A:6:VAL:HG21   | 1:A:11:MET:HE3   | 12       | 0.14          |
| (1,1539) | 1:A:6:VAL:HG22   | 1:A:11:MET:HE1   | 12       | 0.14          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1539) | 1:A:6:VAL:HG22   | 1:A:11:MET:HE2   | 12       | 0.14          |
| (1,1539) | 1:A:6:VAL:HG22   | 1:A:11:MET:HE3   | 12       | 0.14          |
| (1,1539) | 1:A:6:VAL:HG23   | 1:A:11:MET:HE1   | 12       | 0.14          |
| (1,1539) | 1:A:6:VAL:HG23   | 1:A:11:MET:HE2   | 12       | 0.14          |
| (1,1539) | 1:A:6:VAL:HG23   | 1:A:11:MET:HE3   | 12       | 0.14          |
| (1,1493) | 1:A:14:PHE:HE1   | 1:A:79:MET:HE1   | 1        | 0.14          |
| (1,1493) | 1:A:14:PHE:HE1   | 1:A:79:MET:HE2   | 1        | 0.14          |
| (1,1493) | 1:A:14:PHE:HE1   | 1:A:79:MET:HE3   | 1        | 0.14          |
| (1,1493) | 1:A:14:PHE:HE2   | 1:A:79:MET:HE1   | 1        | 0.14          |
| (1,1493) | 1:A:14:PHE:HE2   | 1:A:79:MET:HE2   | 1        | 0.14          |
| (1,1493) | 1:A:14:PHE:HE2   | 1:A:79:MET:HE3   | 1        | 0.14          |
| (1,1493) | 1:A:14:PHE:HE1   | 1:A:79:MET:HE1   | 4        | 0.14          |
| (1,1493) | 1:A:14:PHE:HE1   | 1:A:79:MET:HE2   | 4        | 0.14          |
| (1,1493) | 1:A:14:PHE:HE1   | 1:A:79:MET:HE3   | 4        | 0.14          |
| (1,1493) | 1:A:14:PHE:HE2   | 1:A:79:MET:HE1   | 4        | 0.14          |
| (1,1493) | 1:A:14:PHE:HE2   | 1:A:79:MET:HE2   | 4        | 0.14          |
| (1,1493) | 1:A:14:PHE:HE2   | 1:A:79:MET:HE3   | 4        | 0.14          |
| (1,1489) | 1:A:20:ALA:HB1   | 1:A:17:SER:HB3   | 7        | 0.14          |
| (1,1489) | 1:A:20:ALA:HB2   | 1:A:17:SER:HB3   | 7        | 0.14          |
| (1,1489) | 1:A:20:ALA:HB3   | 1:A:17:SER:HB3   | 7        | 0.14          |
| (1,1468) | 1:A:79:MET:HE1   | 1:A:38:LEU:HD11  | 6        | 0.14          |
| (1,1468) | 1:A:79:MET:HE1   | 1:A:38:LEU:HD12  | 6        | 0.14          |
| (1,1468) | 1:A:79:MET:HE1   | 1:A:38:LEU:HD13  | 6        | 0.14          |
| (1,1468) | 1:A:79:MET:HE2   | 1:A:38:LEU:HD11  | 6        | 0.14          |
| (1,1468) | 1:A:79:MET:HE2   | 1:A:38:LEU:HD12  | 6        | 0.14          |
| (1,1468) | 1:A:79:MET:HE2   | 1:A:38:LEU:HD13  | 6        | 0.14          |
| (1,1468) | 1:A:79:MET:HE3   | 1:A:38:LEU:HD11  | 6        | 0.14          |
| (1,1468) | 1:A:79:MET:HE3   | 1:A:38:LEU:HD12  | 6        | 0.14          |
| (1,1468) | 1:A:79:MET:HE3   | 1:A:38:LEU:HD13  | 6        | 0.14          |
| (1,1419) | 1:A:128:LEU:HB2  | 1:A:106:ILE:HG21 | 7        | 0.14          |
| (1,1419) | 1:A:128:LEU:HB2  | 1:A:106:ILE:HG22 | 7        | 0.14          |
| (1,1419) | 1:A:128:LEU:HB2  | 1:A:106:ILE:HG23 | 7        | 0.14          |
| (1,1276) | 1:A:28:ILE:HA    | 1:A:14:PHE:HZ    | 6        | 0.14          |
| (1,1186) | 1:A:135:TYR:HB3  | 1:A:106:ILE:HG12 | 10       | 0.14          |
| (1,1138) | 1:A:70:VAL:HG21  | 1:A:74:ASN:HB2   | 10       | 0.14          |
| (1,1138) | 1:A:70:VAL:HG22  | 1:A:74:ASN:HB2   | 10       | 0.14          |
| (1,1138) | 1:A:70:VAL:HG23  | 1:A:74:ASN:HB2   | 10       | 0.14          |
| (1,1080) | 1:A:106:ILE:HG21 | 1:A:110:ASP:HB3  | 7        | 0.14          |
| (1,1080) | 1:A:106:ILE:HG22 | 1:A:110:ASP:HB3  | 7        | 0.14          |
| (1,1080) | 1:A:106:ILE:HG23 | 1:A:110:ASP:HB3  | 7        | 0.14          |
| (1,1045) | 1:A:41:MET:HB3   | 1:A:43:LEU:HD21  | 4        | 0.14          |
| (1,1045) | 1:A:41:MET:HB3   | 1:A:43:LEU:HD22  | 4        | 0.14          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1045) | 1:A:41:MET:HB3  | 1:A:43:LEU:HD23 | 4        | 0.14          |
| (1,1002) | 1:A:41:MET:HE1  | 1:A:17:SER:HB3  | 3        | 0.14          |
| (1,1002) | 1:A:41:MET:HE2  | 1:A:17:SER:HB3  | 3        | 0.14          |
| (1,1002) | 1:A:41:MET:HE3  | 1:A:17:SER:HB3  | 3        | 0.14          |
| (4,40)   | 1:A:108:GLU:O   | 1:A:112:GLN:H   | 5        | 0.13          |
| (3,97)   | 1:A:136:ASP:O   | 1:A:139:ALA:H   | 3        | 0.13          |
| (3,97)   | 1:A:136:ASP:O   | 1:A:139:ALA:H   | 5        | 0.13          |
| (3,9)    | 1:A:13:GLU:O    | 1:A:16:GLN:H    | 1        | 0.13          |
| (3,9)    | 1:A:13:GLU:O    | 1:A:16:GLN:H    | 4        | 0.13          |
| (3,85)   | 1:A:120:GLN:O   | 1:A:123:TYR:H   | 9        | 0.13          |
| (3,81)   | 1:A:113:LYS:O   | 1:A:115:GLY:H   | 7        | 0.13          |
| (3,65)   | 1:A:91:GLN:O    | 1:A:94:GLU:H    | 1        | 0.13          |
| (3,59)   | 1:A:79:MET:O    | 1:A:83:ASN:H    | 1        | 0.13          |
| (3,53)   | 1:A:75:TYR:O    | 1:A:78:TYR:H    | 8        | 0.13          |
| (3,5)    | 1:A:9:GLU:O     | 1:A:13:GLU:H    | 12       | 0.13          |
| (3,45)   | 1:A:59:ILE:O    | 1:A:63:VAL:H    | 9        | 0.13          |
| (3,35)   | 1:A:38:LEU:O    | 1:A:44:ILE:H    | 9        | 0.13          |
| (3,23)   | 1:A:33:GLU:O    | 1:A:36:SER:H    | 10       | 0.13          |
| (3,147)  | 1:A:123:TYR:O   | 1:A:127:ASN:N   | 9        | 0.13          |
| (3,145)  | 1:A:121:ILE:O   | 1:A:125:LYS:N   | 2        | 0.13          |
| (3,145)  | 1:A:121:ILE:O   | 1:A:125:LYS:N   | 3        | 0.13          |
| (3,143)  | 1:A:120:GLN:O   | 1:A:123:TYR:N   | 1        | 0.13          |
| (3,143)  | 1:A:120:GLN:O   | 1:A:123:TYR:N   | 7        | 0.13          |
| (3,141)  | 1:A:113:LYS:O   | 1:A:115:GLY:N   | 6        | 0.13          |
| (3,138)  | 1:A:107:THR:O   | 1:A:110:ASP:N   | 4        | 0.13          |
| (3,135)  | 1:A:95:ILE:O    | 1:A:98:THR:N    | 4        | 0.13          |
| (3,134)  | 1:A:94:GLU:O    | 1:A:97:SER:N    | 2        | 0.13          |
| (3,133)  | 1:A:91:GLN:O    | 1:A:94:GLU:N    | 12       | 0.13          |
| (3,128)  | 1:A:75:TYR:O    | 1:A:79:MET:N    | 6        | 0.13          |
| (3,127)  | 1:A:75:TYR:O    | 1:A:78:TYR:N    | 10       | 0.13          |
| (3,125)  | 1:A:71:SER:O    | 1:A:75:TYR:N    | 4        | 0.13          |
| (3,122)  | 1:A:57:ASP:O    | 1:A:61:ASN:N    | 8        | 0.13          |
| (3,116)  | 1:A:37:CYS:O    | 1:A:41:MET:N    | 1        | 0.13          |
| (3,115)  | 1:A:36:SER:O    | 1:A:40:SER:N    | 10       | 0.13          |
| (3,114)  | 1:A:34:PHE:O    | 1:A:38:LEU:N    | 8        | 0.13          |
| (3,113)  | 1:A:33:GLU:O    | 1:A:37:CYS:N    | 10       | 0.13          |
| (3,112)  | 1:A:33:GLU:O    | 1:A:36:SER:N    | 8        | 0.13          |
| (3,105)  | 1:A:13:GLU:O    | 1:A:16:GLN:N    | 5        | 0.13          |
| (2,52)   | 1:A:88:SER:H    | 1:A:91:GLN:H    | 12       | 0.13          |
| (2,342)  | 1:A:34:PHE:HB3  | 1:A:29:LEU:HB2  | 3        | 0.13          |
| (2,267)  | 1:A:63:VAL:HG11 | 1:A:69:GLY:H    | 5        | 0.13          |
| (2,267)  | 1:A:63:VAL:HG12 | 1:A:69:GLY:H    | 5        | 0.13          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,267)  | 1:A:63:VAL:HG13 | 1:A:69:GLY:H     | 5        | 0.13          |
| (1,952)  | 1:A:29:LEU:HD21 | 1:A:70:VAL:HB    | 10       | 0.13          |
| (1,952)  | 1:A:29:LEU:HD22 | 1:A:70:VAL:HB    | 10       | 0.13          |
| (1,952)  | 1:A:29:LEU:HD23 | 1:A:70:VAL:HB    | 10       | 0.13          |
| (1,583)  | 1:A:87:PRO:HB3  | 1:A:90:GLU:H     | 8        | 0.13          |
| (1,2639) | 1:A:43:LEU:HD11 | 1:A:43:LEU:HA    | 10       | 0.13          |
| (1,2639) | 1:A:43:LEU:HD12 | 1:A:43:LEU:HA    | 10       | 0.13          |
| (1,2639) | 1:A:43:LEU:HD13 | 1:A:43:LEU:HA    | 10       | 0.13          |
| (1,2459) | 1:A:41:MET:HB3  | 1:A:43:LEU:HG    | 3        | 0.13          |
| (1,2314) | 1:A:6:VAL:HG21  | 1:A:11:MET:HA    | 4        | 0.13          |
| (1,2314) | 1:A:6:VAL:HG22  | 1:A:11:MET:HA    | 4        | 0.13          |
| (1,2314) | 1:A:6:VAL:HG23  | 1:A:11:MET:HA    | 4        | 0.13          |
| (1,2224) | 1:A:108:GLU:HG2 | 1:A:121:ILE:HG21 | 4        | 0.13          |
| (1,2224) | 1:A:108:GLU:HG2 | 1:A:121:ILE:HG22 | 4        | 0.13          |
| (1,2224) | 1:A:108:GLU:HG2 | 1:A:121:ILE:HG23 | 4        | 0.13          |
| (1,2182) | 1:A:79:MET:HB2  | 1:A:79:MET:HE1   | 8        | 0.13          |
| (1,2182) | 1:A:79:MET:HB2  | 1:A:79:MET:HE2   | 8        | 0.13          |
| (1,2182) | 1:A:79:MET:HB2  | 1:A:79:MET:HE3   | 8        | 0.13          |
| (1,2047) | 1:A:43:LEU:HD11 | 1:A:82:LYS:HE3   | 2        | 0.13          |
| (1,2047) | 1:A:43:LEU:HD12 | 1:A:82:LYS:HE3   | 2        | 0.13          |
| (1,2047) | 1:A:43:LEU:HD13 | 1:A:82:LYS:HE3   | 2        | 0.13          |
| (1,2025) | 1:A:63:VAL:HG11 | 1:A:78:TYR:HA    | 7        | 0.13          |
| (1,2025) | 1:A:63:VAL:HG12 | 1:A:78:TYR:HA    | 7        | 0.13          |
| (1,2025) | 1:A:63:VAL:HG13 | 1:A:78:TYR:HA    | 7        | 0.13          |
| (1,1941) | 1:A:44:ILE:HG21 | 1:A:38:LEU:HD21  | 7        | 0.13          |
| (1,1941) | 1:A:44:ILE:HG21 | 1:A:38:LEU:HD22  | 7        | 0.13          |
| (1,1941) | 1:A:44:ILE:HG21 | 1:A:38:LEU:HD23  | 7        | 0.13          |
| (1,1941) | 1:A:44:ILE:HG22 | 1:A:38:LEU:HD21  | 7        | 0.13          |
| (1,1941) | 1:A:44:ILE:HG22 | 1:A:38:LEU:HD22  | 7        | 0.13          |
| (1,1941) | 1:A:44:ILE:HG22 | 1:A:38:LEU:HD23  | 7        | 0.13          |
| (1,1941) | 1:A:44:ILE:HG23 | 1:A:38:LEU:HD21  | 7        | 0.13          |
| (1,1941) | 1:A:44:ILE:HG23 | 1:A:38:LEU:HD22  | 7        | 0.13          |
| (1,1941) | 1:A:44:ILE:HG23 | 1:A:38:LEU:HD23  | 7        | 0.13          |
| (1,1625) | 1:A:29:LEU:HB3  | 1:A:70:VAL:HB    | 11       | 0.13          |
| (1,1580) | 1:A:44:ILE:HB   | 1:A:43:LEU:HB3   | 4        | 0.13          |
| (1,1493) | 1:A:14:PHE:HE1  | 1:A:79:MET:HE1   | 2        | 0.13          |
| (1,1493) | 1:A:14:PHE:HE1  | 1:A:79:MET:HE2   | 2        | 0.13          |
| (1,1493) | 1:A:14:PHE:HE1  | 1:A:79:MET:HE3   | 2        | 0.13          |
| (1,1493) | 1:A:14:PHE:HE2  | 1:A:79:MET:HE1   | 2        | 0.13          |
| (1,1493) | 1:A:14:PHE:HE2  | 1:A:79:MET:HE2   | 2        | 0.13          |
| (1,1493) | 1:A:14:PHE:HE2  | 1:A:79:MET:HE3   | 2        | 0.13          |
| (1,1489) | 1:A:20:ALA:HB1  | 1:A:17:SER:HB3   | 8        | 0.13          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1489) | 1:A:20:ALA:HB2   | 1:A:17:SER:HB3  | 8        | 0.13          |
| (1,1489) | 1:A:20:ALA:HB3   | 1:A:17:SER:HB3  | 8        | 0.13          |
| (1,1387) | 1:A:109:THR:HG21 | 1:A:113:LYS:HE3 | 4        | 0.13          |
| (1,1387) | 1:A:109:THR:HG22 | 1:A:113:LYS:HE3 | 4        | 0.13          |
| (1,1387) | 1:A:109:THR:HG23 | 1:A:113:LYS:HE3 | 4        | 0.13          |
| (1,1276) | 1:A:28:ILE:HA    | 1:A:14:PHE:HZ   | 9        | 0.13          |
| (1,1276) | 1:A:28:ILE:HA    | 1:A:14:PHE:HZ   | 11       | 0.13          |
| (3,9)    | 1:A:13:GLU:O     | 1:A:16:GLN:H    | 7        | 0.12          |
| (3,85)   | 1:A:120:GLN:O    | 1:A:123:TYR:H   | 6        | 0.12          |
| (3,85)   | 1:A:120:GLN:O    | 1:A:123:TYR:H   | 12       | 0.12          |
| (3,81)   | 1:A:113:LYS:O    | 1:A:115:GLY:H   | 1        | 0.12          |
| (3,65)   | 1:A:91:GLN:O     | 1:A:94:GLU:H    | 5        | 0.12          |
| (3,5)    | 1:A:9:GLU:O      | 1:A:13:GLU:H    | 4        | 0.12          |
| (3,37)   | 1:A:45:ASP:O     | 1:A:47:ASP:H    | 4        | 0.12          |
| (3,23)   | 1:A:33:GLU:O     | 1:A:36:SER:H    | 2        | 0.12          |
| (3,150)  | 1:A:138:ALA:O    | 1:A:142:LYS:N   | 12       | 0.12          |
| (3,143)  | 1:A:120:GLN:O    | 1:A:123:TYR:N   | 3        | 0.12          |
| (3,143)  | 1:A:120:GLN:O    | 1:A:123:TYR:N   | 8        | 0.12          |
| (3,143)  | 1:A:120:GLN:O    | 1:A:123:TYR:N   | 12       | 0.12          |
| (3,138)  | 1:A:107:THR:O    | 1:A:110:ASP:N   | 11       | 0.12          |
| (3,136)  | 1:A:95:ILE:O     | 1:A:99:ILE:N    | 4        | 0.12          |
| (3,134)  | 1:A:94:GLU:O     | 1:A:97:SER:N    | 11       | 0.12          |
| (3,128)  | 1:A:75:TYR:O     | 1:A:79:MET:N    | 12       | 0.12          |
| (3,124)  | 1:A:29:LEU:O     | 1:A:70:VAL:N    | 3        | 0.12          |
| (3,124)  | 1:A:29:LEU:O     | 1:A:70:VAL:N    | 12       | 0.12          |
| (3,120)  | 1:A:54:ALA:O     | 1:A:58:ALA:N    | 11       | 0.12          |
| (3,120)  | 1:A:54:ALA:O     | 1:A:58:ALA:N    | 12       | 0.12          |
| (3,118)  | 1:A:38:LEU:O     | 1:A:44:ILE:N    | 9        | 0.12          |
| (3,116)  | 1:A:37:CYS:O     | 1:A:41:MET:N    | 6        | 0.12          |
| (3,116)  | 1:A:37:CYS:O     | 1:A:41:MET:N    | 8        | 0.12          |
| (3,113)  | 1:A:33:GLU:O     | 1:A:37:CYS:N    | 7        | 0.12          |
| (3,109)  | 1:A:29:LEU:N     | 1:A:70:VAL:O    | 6        | 0.12          |
| (3,106)  | 1:A:13:GLU:O     | 1:A:17:SER:N    | 2        | 0.12          |
| (3,103)  | 1:A:9:GLU:O      | 1:A:13:GLU:N    | 10       | 0.12          |
| (2,304)  | 1:A:46:ILE:HD11  | 1:A:47:ASP:HA   | 5        | 0.12          |
| (2,304)  | 1:A:46:ILE:HD12  | 1:A:47:ASP:HA   | 5        | 0.12          |
| (2,304)  | 1:A:46:ILE:HD13  | 1:A:47:ASP:HA   | 5        | 0.12          |
| (1,882)  | 1:A:80:LYS:HE3   | 1:A:6:VAL:HG11  | 2        | 0.12          |
| (1,882)  | 1:A:80:LYS:HE3   | 1:A:6:VAL:HG12  | 2        | 0.12          |
| (1,882)  | 1:A:80:LYS:HE3   | 1:A:6:VAL:HG13  | 2        | 0.12          |
| (1,56)   | 1:A:52:GLU:HA    | 1:A:50:GLY:H    | 8        | 0.12          |
| (1,2631) | 1:A:10:GLN:HA    | 1:A:13:GLU:HG2  | 5        | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2593) | 1:A:62:ASN:HB3  | 1:A:59:ILE:HA   | 1        | 0.12          |
| (1,2327) | 1:A:113:LYS:HB3 | 1:A:113:LYS:HE3 | 8        | 0.12          |
| (1,2174) | 1:A:99:ILE:HG21 | 1:A:100:ALA:HB1 | 6        | 0.12          |
| (1,2174) | 1:A:99:ILE:HG21 | 1:A:100:ALA:HB2 | 6        | 0.12          |
| (1,2174) | 1:A:99:ILE:HG21 | 1:A:100:ALA:HB3 | 6        | 0.12          |
| (1,2174) | 1:A:99:ILE:HG22 | 1:A:100:ALA:HB1 | 6        | 0.12          |
| (1,2174) | 1:A:99:ILE:HG22 | 1:A:100:ALA:HB2 | 6        | 0.12          |
| (1,2174) | 1:A:99:ILE:HG22 | 1:A:100:ALA:HB3 | 6        | 0.12          |
| (1,2174) | 1:A:99:ILE:HG23 | 1:A:100:ALA:HB1 | 6        | 0.12          |
| (1,2174) | 1:A:99:ILE:HG23 | 1:A:100:ALA:HB2 | 6        | 0.12          |
| (1,2174) | 1:A:99:ILE:HG23 | 1:A:100:ALA:HB3 | 6        | 0.12          |
| (1,2118) | 1:A:89:PRO:HA   | 1:A:92:LEU:HB2  | 12       | 0.12          |
| (1,2052) | 1:A:13:GLU:HA   | 1:A:13:GLU:HG2  | 8        | 0.12          |
| (1,1939) | 1:A:10:GLN:HG2  | 1:A:7:THR:HG21  | 8        | 0.12          |
| (1,1939) | 1:A:10:GLN:HG2  | 1:A:7:THR:HG22  | 8        | 0.12          |
| (1,1939) | 1:A:10:GLN:HG2  | 1:A:7:THR:HG23  | 8        | 0.12          |
| (1,1863) | 1:A:14:PHE:HE1  | 1:A:14:PHE:HA   | 2        | 0.12          |
| (1,1863) | 1:A:14:PHE:HE2  | 1:A:14:PHE:HA   | 2        | 0.12          |
| (1,1542) | 1:A:38:LEU:HD21 | 1:A:43:LEU:HD21 | 2        | 0.12          |
| (1,1542) | 1:A:38:LEU:HD21 | 1:A:43:LEU:HD22 | 2        | 0.12          |
| (1,1542) | 1:A:38:LEU:HD21 | 1:A:43:LEU:HD23 | 2        | 0.12          |
| (1,1542) | 1:A:38:LEU:HD22 | 1:A:43:LEU:HD21 | 2        | 0.12          |
| (1,1542) | 1:A:38:LEU:HD22 | 1:A:43:LEU:HD22 | 2        | 0.12          |
| (1,1542) | 1:A:38:LEU:HD22 | 1:A:43:LEU:HD23 | 2        | 0.12          |
| (1,1542) | 1:A:38:LEU:HD23 | 1:A:43:LEU:HD21 | 2        | 0.12          |
| (1,1542) | 1:A:38:LEU:HD23 | 1:A:43:LEU:HD22 | 2        | 0.12          |
| (1,1542) | 1:A:38:LEU:HD23 | 1:A:43:LEU:HD23 | 2        | 0.12          |
| (1,1517) | 1:A:70:VAL:HG21 | 1:A:75:TYR:HB3  | 11       | 0.12          |
| (1,1517) | 1:A:70:VAL:HG22 | 1:A:75:TYR:HB3  | 11       | 0.12          |
| (1,1517) | 1:A:70:VAL:HG23 | 1:A:75:TYR:HB3  | 11       | 0.12          |
| (1,1493) | 1:A:14:PHE:HE1  | 1:A:79:MET:HE1  | 5        | 0.12          |
| (1,1493) | 1:A:14:PHE:HE1  | 1:A:79:MET:HE2  | 5        | 0.12          |
| (1,1493) | 1:A:14:PHE:HE1  | 1:A:79:MET:HE3  | 5        | 0.12          |
| (1,1493) | 1:A:14:PHE:HE2  | 1:A:79:MET:HE1  | 5        | 0.12          |
| (1,1493) | 1:A:14:PHE:HE2  | 1:A:79:MET:HE2  | 5        | 0.12          |
| (1,1493) | 1:A:14:PHE:HE2  | 1:A:79:MET:HE3  | 5        | 0.12          |
| (1,1493) | 1:A:14:PHE:HE1  | 1:A:79:MET:HE1  | 7        | 0.12          |
| (1,1493) | 1:A:14:PHE:HE1  | 1:A:79:MET:HE2  | 7        | 0.12          |
| (1,1493) | 1:A:14:PHE:HE1  | 1:A:79:MET:HE3  | 7        | 0.12          |
| (1,1493) | 1:A:14:PHE:HE2  | 1:A:79:MET:HE1  | 7        | 0.12          |
| (1,1493) | 1:A:14:PHE:HE2  | 1:A:79:MET:HE2  | 7        | 0.12          |
| (1,1493) | 1:A:14:PHE:HE2  | 1:A:79:MET:HE3  | 7        | 0.12          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1493) | 1:A:14:PHE:HE1  | 1:A:79:MET:HE1 | 10       | 0.12          |
| (1,1493) | 1:A:14:PHE:HE1  | 1:A:79:MET:HE2 | 10       | 0.12          |
| (1,1493) | 1:A:14:PHE:HE1  | 1:A:79:MET:HE3 | 10       | 0.12          |
| (1,1493) | 1:A:14:PHE:HE2  | 1:A:79:MET:HE1 | 10       | 0.12          |
| (1,1493) | 1:A:14:PHE:HE2  | 1:A:79:MET:HE2 | 10       | 0.12          |
| (1,1493) | 1:A:14:PHE:HE2  | 1:A:79:MET:HE3 | 10       | 0.12          |
| (1,1489) | 1:A:20:ALA:HB1  | 1:A:17:SER:HB3 | 3        | 0.12          |
| (1,1489) | 1:A:20:ALA:HB2  | 1:A:17:SER:HB3 | 3        | 0.12          |
| (1,1489) | 1:A:20:ALA:HB3  | 1:A:17:SER:HB3 | 3        | 0.12          |
| (1,1276) | 1:A:28:ILE:HA   | 1:A:14:PHE:HZ  | 3        | 0.12          |
| (1,1253) | 1:A:7:THR:HB    | 1:A:9:GLU:HB2  | 12       | 0.12          |
| (1,1064) | 1:A:63:VAL:HG11 | 1:A:78:TYR:HB3 | 11       | 0.12          |
| (1,1064) | 1:A:63:VAL:HG12 | 1:A:78:TYR:HB3 | 11       | 0.12          |
| (1,1064) | 1:A:63:VAL:HG13 | 1:A:78:TYR:HB3 | 11       | 0.12          |
| (4,21)   | 1:A:56:TYR:O    | 1:A:60:TYR:H   | 6        | 0.11          |
| (3,9)    | 1:A:13:GLU:O    | 1:A:16:GLN:H   | 12       | 0.11          |
| (3,85)   | 1:A:120:GLN:O   | 1:A:123:TYR:H  | 1        | 0.11          |
| (3,85)   | 1:A:120:GLN:O   | 1:A:123:TYR:H  | 3        | 0.11          |
| (3,85)   | 1:A:120:GLN:O   | 1:A:123:TYR:H  | 5        | 0.11          |
| (3,85)   | 1:A:120:GLN:O   | 1:A:123:TYR:H  | 10       | 0.11          |
| (3,85)   | 1:A:120:GLN:O   | 1:A:123:TYR:H  | 11       | 0.11          |
| (3,81)   | 1:A:113:LYS:O   | 1:A:115:GLY:H  | 8        | 0.11          |
| (3,81)   | 1:A:113:LYS:O   | 1:A:115:GLY:H  | 10       | 0.11          |
| (3,77)   | 1:A:107:THR:O   | 1:A:111:MET:H  | 7        | 0.11          |
| (3,77)   | 1:A:107:THR:O   | 1:A:111:MET:H  | 10       | 0.11          |
| (3,75)   | 1:A:107:THR:O   | 1:A:110:ASP:H  | 7        | 0.11          |
| (3,67)   | 1:A:94:GLU:O    | 1:A:97:SER:H   | 4        | 0.11          |
| (3,67)   | 1:A:94:GLU:O    | 1:A:97:SER:H   | 10       | 0.11          |
| (3,65)   | 1:A:91:GLN:O    | 1:A:94:GLU:H   | 6        | 0.11          |
| (3,59)   | 1:A:79:MET:O    | 1:A:83:ASN:H   | 3        | 0.11          |
| (3,53)   | 1:A:75:TYR:O    | 1:A:78:TYR:H   | 6        | 0.11          |
| (3,47)   | 1:A:29:LEU:O    | 1:A:70:VAL:H   | 4        | 0.11          |
| (3,45)   | 1:A:59:ILE:O    | 1:A:63:VAL:H   | 3        | 0.11          |
| (3,37)   | 1:A:45:ASP:O    | 1:A:47:ASP:H   | 11       | 0.11          |
| (3,23)   | 1:A:33:GLU:O    | 1:A:36:SER:H   | 8        | 0.11          |
| (3,21)   | 1:A:31:LYS:O    | 1:A:35:ARG:H   | 9        | 0.11          |
| (3,148)  | 1:A:124:VAL:O   | 1:A:128:LEU:N  | 7        | 0.11          |
| (3,147)  | 1:A:123:TYR:O   | 1:A:127:ASN:N  | 3        | 0.11          |
| (3,140)  | 1:A:108:GLU:O   | 1:A:112:GLN:N  | 4        | 0.11          |
| (3,140)  | 1:A:108:GLU:O   | 1:A:112:GLN:N  | 6        | 0.11          |
| (3,138)  | 1:A:107:THR:O   | 1:A:110:ASP:N  | 12       | 0.11          |
| (3,137)  | 1:A:100:ALA:O   | 1:A:103:LYS:N  | 1        | 0.11          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (3,136)  | 1:A:95:ILE:O     | 1:A:99:ILE:N    | 3        | 0.11          |
| (3,134)  | 1:A:94:GLU:O     | 1:A:97:SER:N    | 1        | 0.11          |
| (3,134)  | 1:A:94:GLU:O     | 1:A:97:SER:N    | 3        | 0.11          |
| (3,128)  | 1:A:75:TYR:O     | 1:A:79:MET:N    | 8        | 0.11          |
| (3,127)  | 1:A:75:TYR:O     | 1:A:78:TYR:N    | 1        | 0.11          |
| (3,127)  | 1:A:75:TYR:O     | 1:A:78:TYR:N    | 4        | 0.11          |
| (3,126)  | 1:A:73:ASP:O     | 1:A:77:GLN:N    | 9        | 0.11          |
| (3,119)  | 1:A:45:ASP:O     | 1:A:47:ASP:N    | 9        | 0.11          |
| (3,117)  | 1:A:38:LEU:O     | 1:A:43:LEU:N    | 2        | 0.11          |
| (3,114)  | 1:A:34:PHE:O     | 1:A:38:LEU:N    | 9        | 0.11          |
| (3,113)  | 1:A:33:GLU:O     | 1:A:37:CYS:N    | 1        | 0.11          |
| (3,112)  | 1:A:33:GLU:O     | 1:A:36:SER:N    | 4        | 0.11          |
| (3,112)  | 1:A:33:GLU:O     | 1:A:36:SER:N    | 10       | 0.11          |
| (3,110)  | 1:A:30:ASP:O     | 1:A:34:PHE:N    | 3        | 0.11          |
| (3,107)  | 1:A:14:PHE:O     | 1:A:18:PHE:N    | 2        | 0.11          |
| (3,105)  | 1:A:13:GLU:O     | 1:A:16:GLN:N    | 6        | 0.11          |
| (3,105)  | 1:A:13:GLU:O     | 1:A:16:GLN:N    | 7        | 0.11          |
| (3,1)    | 1:A:7:THR:O      | 1:A:11:MET:H    | 3        | 0.11          |
| (3,1)    | 1:A:7:THR:O      | 1:A:11:MET:H    | 7        | 0.11          |
| (3,1)    | 1:A:7:THR:O      | 1:A:11:MET:H    | 10       | 0.11          |
| (1,784)  | 1:A:70:VAL:HG21  | 1:A:63:VAL:HG21 | 5        | 0.11          |
| (1,784)  | 1:A:70:VAL:HG21  | 1:A:63:VAL:HG22 | 5        | 0.11          |
| (1,784)  | 1:A:70:VAL:HG21  | 1:A:63:VAL:HG23 | 5        | 0.11          |
| (1,784)  | 1:A:70:VAL:HG22  | 1:A:63:VAL:HG21 | 5        | 0.11          |
| (1,784)  | 1:A:70:VAL:HG22  | 1:A:63:VAL:HG22 | 5        | 0.11          |
| (1,784)  | 1:A:70:VAL:HG22  | 1:A:63:VAL:HG23 | 5        | 0.11          |
| (1,784)  | 1:A:70:VAL:HG23  | 1:A:63:VAL:HG21 | 5        | 0.11          |
| (1,784)  | 1:A:70:VAL:HG23  | 1:A:63:VAL:HG22 | 5        | 0.11          |
| (1,784)  | 1:A:70:VAL:HG23  | 1:A:63:VAL:HG23 | 5        | 0.11          |
| (1,2639) | 1:A:43:LEU:HD11  | 1:A:43:LEU:HA   | 3        | 0.11          |
| (1,2639) | 1:A:43:LEU:HD12  | 1:A:43:LEU:HA   | 3        | 0.11          |
| (1,2639) | 1:A:43:LEU:HD13  | 1:A:43:LEU:HA   | 3        | 0.11          |
| (1,2639) | 1:A:43:LEU:HD11  | 1:A:43:LEU:HA   | 4        | 0.11          |
| (1,2639) | 1:A:43:LEU:HD12  | 1:A:43:LEU:HA   | 4        | 0.11          |
| (1,2639) | 1:A:43:LEU:HD13  | 1:A:43:LEU:HA   | 4        | 0.11          |
| (1,2639) | 1:A:43:LEU:HD11  | 1:A:43:LEU:HA   | 7        | 0.11          |
| (1,2639) | 1:A:43:LEU:HD12  | 1:A:43:LEU:HA   | 7        | 0.11          |
| (1,2639) | 1:A:43:LEU:HD13  | 1:A:43:LEU:HA   | 7        | 0.11          |
| (1,2631) | 1:A:10:GLN:HA    | 1:A:13:GLU:HG2  | 2        | 0.11          |
| (1,2460) | 1:A:62:ASN:HB3   | 1:A:59:ILE:HA   | 1        | 0.11          |
| (1,2370) | 1:A:141:VAL:HG11 | 1:A:138:ALA:HA  | 10       | 0.11          |
| (1,2370) | 1:A:141:VAL:HG12 | 1:A:138:ALA:HA  | 10       | 0.11          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2370) | 1:A:141:VAL:HG13 | 1:A:138:ALA:HA   | 10       | 0.11          |
| (1,2174) | 1:A:99:ILE:HG21  | 1:A:100:ALA:HB1  | 9        | 0.11          |
| (1,2174) | 1:A:99:ILE:HG21  | 1:A:100:ALA:HB2  | 9        | 0.11          |
| (1,2174) | 1:A:99:ILE:HG21  | 1:A:100:ALA:HB3  | 9        | 0.11          |
| (1,2174) | 1:A:99:ILE:HG22  | 1:A:100:ALA:HB1  | 9        | 0.11          |
| (1,2174) | 1:A:99:ILE:HG22  | 1:A:100:ALA:HB2  | 9        | 0.11          |
| (1,2174) | 1:A:99:ILE:HG22  | 1:A:100:ALA:HB3  | 9        | 0.11          |
| (1,2174) | 1:A:99:ILE:HG23  | 1:A:100:ALA:HB1  | 9        | 0.11          |
| (1,2174) | 1:A:99:ILE:HG23  | 1:A:100:ALA:HB2  | 9        | 0.11          |
| (1,2174) | 1:A:99:ILE:HG23  | 1:A:100:ALA:HB3  | 9        | 0.11          |
| (1,2167) | 1:A:81:GLU:HA    | 1:A:84:ASP:HB3   | 5        | 0.11          |
| (1,2167) | 1:A:81:GLU:HA    | 1:A:84:ASP:HB3   | 7        | 0.11          |
| (1,2012) | 1:A:54:ALA:HB1   | 1:A:57:ASP:HA    | 10       | 0.11          |
| (1,2012) | 1:A:54:ALA:HB2   | 1:A:57:ASP:HA    | 10       | 0.11          |
| (1,2012) | 1:A:54:ALA:HB3   | 1:A:57:ASP:HA    | 10       | 0.11          |
| (1,1717) | 1:A:111:MET:HG2  | 1:A:106:ILE:HG21 | 11       | 0.11          |
| (1,1717) | 1:A:111:MET:HG2  | 1:A:106:ILE:HG22 | 11       | 0.11          |
| (1,1717) | 1:A:111:MET:HG2  | 1:A:106:ILE:HG23 | 11       | 0.11          |
| (1,1656) | 1:A:8:ALA:HB1    | 1:A:11:MET:HG2   | 2        | 0.11          |
| (1,1656) | 1:A:8:ALA:HB2    | 1:A:11:MET:HG2   | 2        | 0.11          |
| (1,1656) | 1:A:8:ALA:HB3    | 1:A:11:MET:HG2   | 2        | 0.11          |
| (1,1653) | 1:A:76:VAL:HG21  | 1:A:75:TYR:HE1   | 5        | 0.11          |
| (1,1653) | 1:A:76:VAL:HG21  | 1:A:75:TYR:HE2   | 5        | 0.11          |
| (1,1653) | 1:A:76:VAL:HG22  | 1:A:75:TYR:HE1   | 5        | 0.11          |
| (1,1653) | 1:A:76:VAL:HG22  | 1:A:75:TYR:HE2   | 5        | 0.11          |
| (1,1653) | 1:A:76:VAL:HG23  | 1:A:75:TYR:HE1   | 5        | 0.11          |
| (1,1653) | 1:A:76:VAL:HG23  | 1:A:75:TYR:HE2   | 5        | 0.11          |
| (1,1565) | 1:A:38:LEU:HD11  | 1:A:43:LEU:HD21  | 8        | 0.11          |
| (1,1565) | 1:A:38:LEU:HD11  | 1:A:43:LEU:HD22  | 8        | 0.11          |
| (1,1565) | 1:A:38:LEU:HD11  | 1:A:43:LEU:HD23  | 8        | 0.11          |
| (1,1565) | 1:A:38:LEU:HD12  | 1:A:43:LEU:HD21  | 8        | 0.11          |
| (1,1565) | 1:A:38:LEU:HD12  | 1:A:43:LEU:HD22  | 8        | 0.11          |
| (1,1565) | 1:A:38:LEU:HD12  | 1:A:43:LEU:HD23  | 8        | 0.11          |
| (1,1565) | 1:A:38:LEU:HD13  | 1:A:43:LEU:HD21  | 8        | 0.11          |
| (1,1565) | 1:A:38:LEU:HD13  | 1:A:43:LEU:HD22  | 8        | 0.11          |
| (1,1565) | 1:A:38:LEU:HD13  | 1:A:43:LEU:HD23  | 8        | 0.11          |
| (1,1493) | 1:A:14:PHE:HE1   | 1:A:79:MET:HE1   | 9        | 0.11          |
| (1,1493) | 1:A:14:PHE:HE1   | 1:A:79:MET:HE2   | 9        | 0.11          |
| (1,1493) | 1:A:14:PHE:HE1   | 1:A:79:MET:HE3   | 9        | 0.11          |
| (1,1493) | 1:A:14:PHE:HE2   | 1:A:79:MET:HE1   | 9        | 0.11          |
| (1,1493) | 1:A:14:PHE:HE2   | 1:A:79:MET:HE2   | 9        | 0.11          |
| (1,1493) | 1:A:14:PHE:HE2   | 1:A:79:MET:HE3   | 9        | 0.11          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1489) | 1:A:20:ALA:HB1  | 1:A:17:SER:HB3   | 1        | 0.11          |
| (1,1489) | 1:A:20:ALA:HB2  | 1:A:17:SER:HB3   | 1        | 0.11          |
| (1,1489) | 1:A:20:ALA:HB3  | 1:A:17:SER:HB3   | 1        | 0.11          |
| (1,1489) | 1:A:20:ALA:HB1  | 1:A:17:SER:HB3   | 4        | 0.11          |
| (1,1489) | 1:A:20:ALA:HB2  | 1:A:17:SER:HB3   | 4        | 0.11          |
| (1,1489) | 1:A:20:ALA:HB3  | 1:A:17:SER:HB3   | 4        | 0.11          |
| (1,1468) | 1:A:79:MET:HE1  | 1:A:38:LEU:HD11  | 9        | 0.11          |
| (1,1468) | 1:A:79:MET:HE1  | 1:A:38:LEU:HD12  | 9        | 0.11          |
| (1,1468) | 1:A:79:MET:HE1  | 1:A:38:LEU:HD13  | 9        | 0.11          |
| (1,1468) | 1:A:79:MET:HE2  | 1:A:38:LEU:HD11  | 9        | 0.11          |
| (1,1468) | 1:A:79:MET:HE2  | 1:A:38:LEU:HD12  | 9        | 0.11          |
| (1,1468) | 1:A:79:MET:HE2  | 1:A:38:LEU:HD13  | 9        | 0.11          |
| (1,1468) | 1:A:79:MET:HE3  | 1:A:38:LEU:HD11  | 9        | 0.11          |
| (1,1468) | 1:A:79:MET:HE3  | 1:A:38:LEU:HD12  | 9        | 0.11          |
| (1,1468) | 1:A:79:MET:HE3  | 1:A:38:LEU:HD13  | 9        | 0.11          |
| (1,1395) | 1:A:25:HIS:HB2  | 1:A:18:PHE:HD1   | 2        | 0.11          |
| (1,1395) | 1:A:25:HIS:HB2  | 1:A:18:PHE:HD2   | 2        | 0.11          |
| (1,1395) | 1:A:25:HIS:HB2  | 1:A:18:PHE:HD1   | 10       | 0.11          |
| (1,1395) | 1:A:25:HIS:HB2  | 1:A:18:PHE:HD2   | 10       | 0.11          |
| (1,1276) | 1:A:28:ILE:HA   | 1:A:14:PHE:HZ    | 5        | 0.11          |
| (1,1276) | 1:A:28:ILE:HA   | 1:A:14:PHE:HZ    | 10       | 0.11          |
| (1,1186) | 1:A:135:TYR:HB3 | 1:A:106:ILE:HG12 | 4        | 0.11          |
| (1,1186) | 1:A:135:TYR:HB3 | 1:A:106:ILE:HG12 | 6        | 0.11          |
| (1,1186) | 1:A:135:TYR:HB3 | 1:A:106:ILE:HG12 | 11       | 0.11          |
| (1,1122) | 1:A:29:LEU:HD11 | 1:A:38:LEU:HD11  | 11       | 0.11          |
| (1,1122) | 1:A:29:LEU:HD11 | 1:A:38:LEU:HD12  | 11       | 0.11          |
| (1,1122) | 1:A:29:LEU:HD11 | 1:A:38:LEU:HD13  | 11       | 0.11          |
| (1,1122) | 1:A:29:LEU:HD12 | 1:A:38:LEU:HD11  | 11       | 0.11          |
| (1,1122) | 1:A:29:LEU:HD12 | 1:A:38:LEU:HD12  | 11       | 0.11          |
| (1,1122) | 1:A:29:LEU:HD12 | 1:A:38:LEU:HD13  | 11       | 0.11          |
| (1,1122) | 1:A:29:LEU:HD13 | 1:A:38:LEU:HD11  | 11       | 0.11          |
| (1,1122) | 1:A:29:LEU:HD13 | 1:A:38:LEU:HD12  | 11       | 0.11          |
| (1,1122) | 1:A:29:LEU:HD13 | 1:A:38:LEU:HD13  | 11       | 0.11          |
| (1,1037) | 1:A:103:LYS:HG2 | 1:A:100:ALA:HA   | 10       | 0.11          |

## 10 Dihedral-angle violation analysis

Dihedral angle analysis failed due to data error in the dihedral angle restraints, possibly missing target value