



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2026 – 01:46 PM UTC

PDB ID : 2LVJ / pdb\_00002lvj  
BMRB ID : 18572  
Title : solution structure of hemi-Mg-bound Phl p 7  
Authors : Henzl, M.T.; Tanner, J.J.  
Deposited on : 2012-07-05

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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

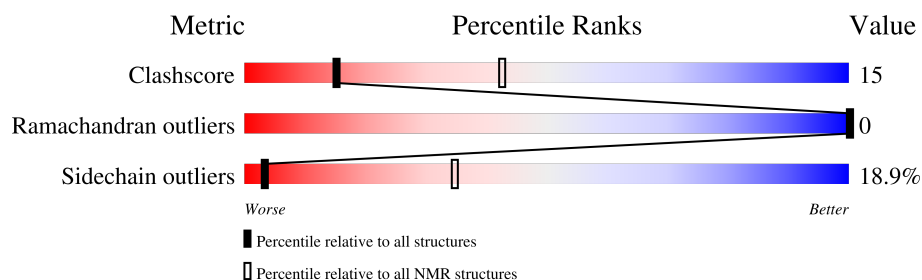
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 92%.

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



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

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 77     |                  |

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 8 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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

| Well-defined (core) protein residues |                          |                   |              |
|--------------------------------------|--------------------------|-------------------|--------------|
| Well-defined core                    | Residue range (total)    | Backbone RMSD (Å) | Medoid model |
| 1                                    | A:3-A:12, A:18-A:77 (70) | 0.25              | 8            |

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 4 clusters and 3 single-model clusters were found.

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

### 3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 1163 atoms, of which 566 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Polcalcin Phl p 7.

| Mol | Chain | Residues | Atoms |     |     |    |     |   | Trace |
|-----|-------|----------|-------|-----|-----|----|-----|---|-------|
| 1   | A     | 77       | Total | C   | H   | N  | O   | S | 0     |
|     |       |          | 1162  | 369 | 566 | 98 | 124 | 5 |       |

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

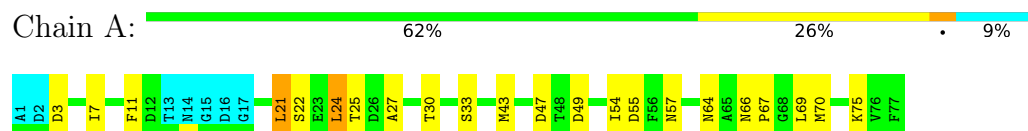
| Mol | Chain | Residues | Atoms |    |
|-----|-------|----------|-------|----|
| 2   | A     | 1        | Total | Mg |
|     |       |          | 1     | 1  |

## 4 Residue-property plots

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

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

- Molecule 1: Polcalcin Phl p 7

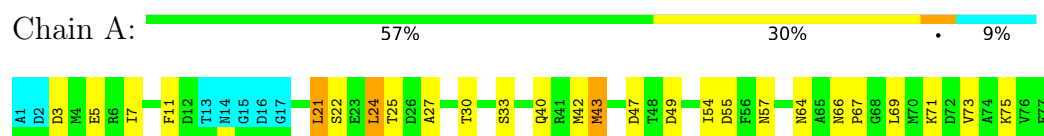


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

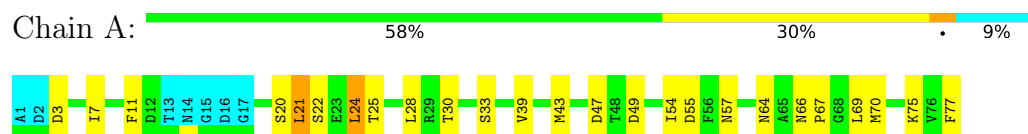
#### 4.2.1 Score per residue for model 1

- Molecule 1: Polcalcin Phl p 7



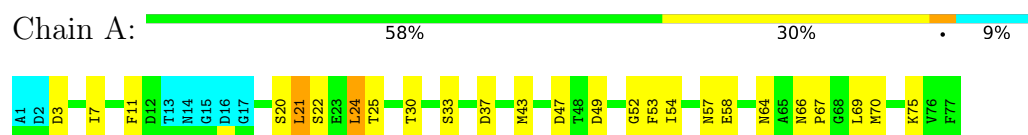
#### 4.2.2 Score per residue for model 2

- Molecule 1: Polcalcin Phl p 7



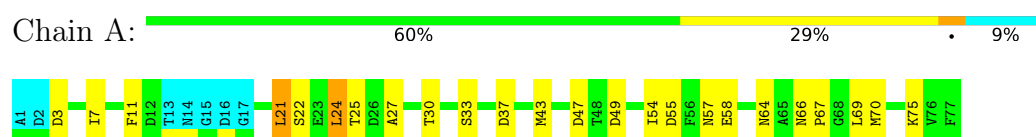
### 4.2.3 Score per residue for model 3

- Molecule 1: Polcalcin Phl p 7



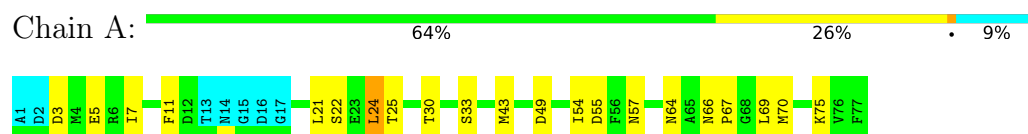
### 4.2.4 Score per residue for model 4

- Molecule 1: Polcalcin Phl p 7



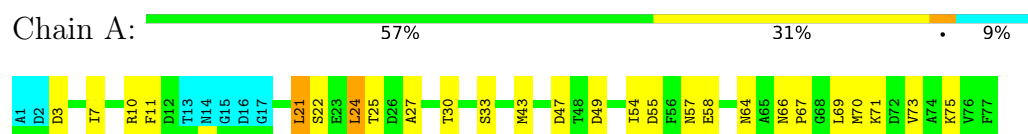
### 4.2.5 Score per residue for model 5

- Molecule 1: Polcalcin Phl p 7



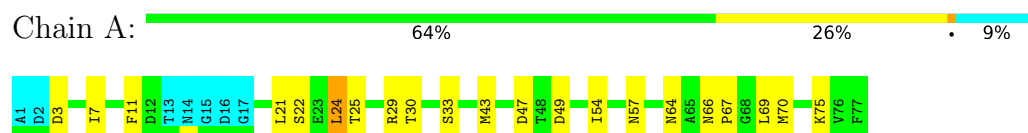
### 4.2.6 Score per residue for model 6

- Molecule 1: Polcalcin Phl p 7



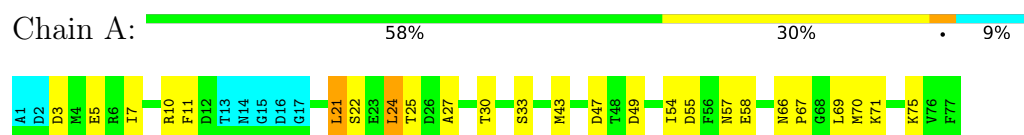
### 4.2.7 Score per residue for model 7

- Molecule 1: Polcalcin Phl p 7



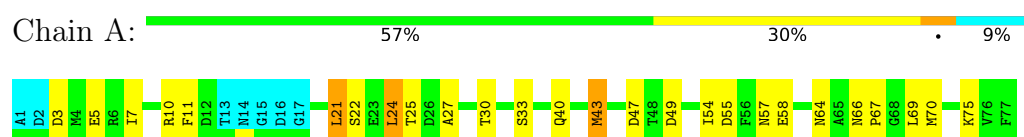
#### 4.2.8 Score per residue for model 8 (medoid)

- Molecule 1: Polcalcin Phl p 7



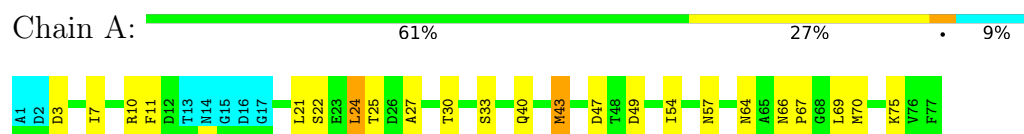
#### 4.2.9 Score per residue for model 9

- Molecule 1: Polcalcin Phl p 7



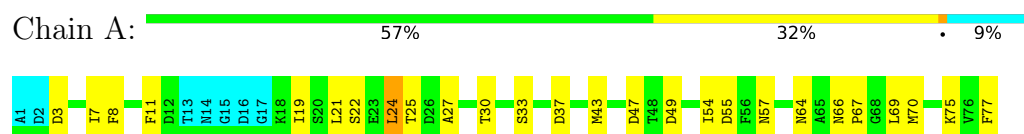
#### 4.2.10 Score per residue for model 10

- Molecule 1: Polcalcin Phl p 7



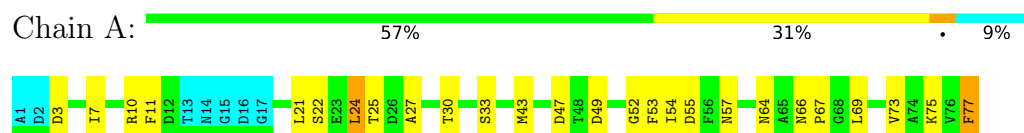
#### 4.2.11 Score per residue for model 11

- Molecule 1: Polcalcin Phl p 7



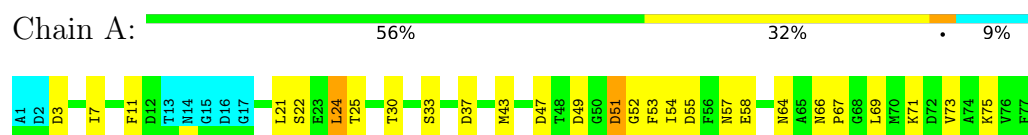
#### 4.2.12 Score per residue for model 12

- Molecule 1: Polcalcin Phl p 7



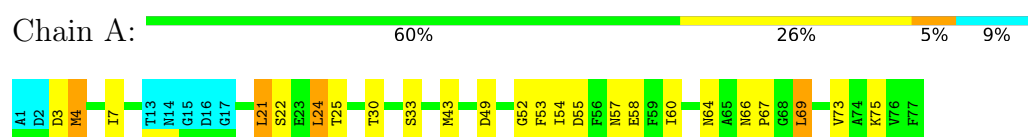
### 4.2.13 Score per residue for model 13

- Molecule 1: Polcalcin Phl p 7



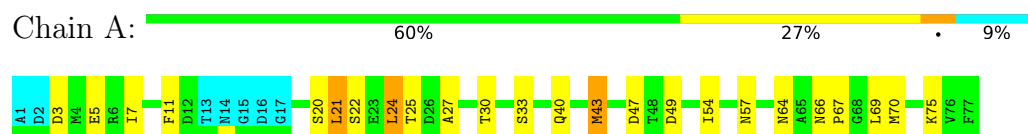
### 4.2.14 Score per residue for model 14

- Molecule 1: Polcalcin Phl p 7



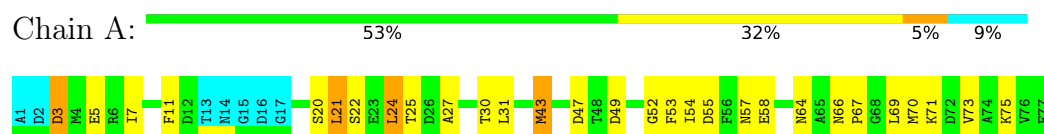
### 4.2.15 Score per residue for model 15

- Molecule 1: Polcalcin Phl p 7



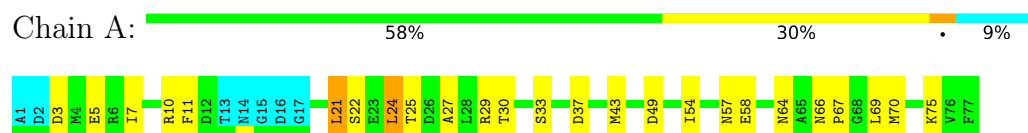
### 4.2.16 Score per residue for model 16

- Molecule 1: Polcalcin Phl p 7



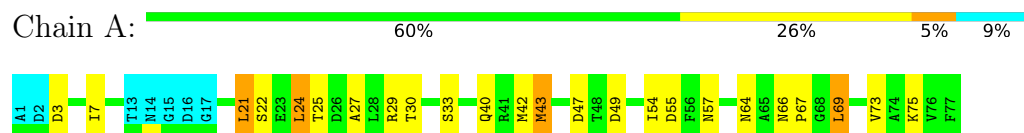
### 4.2.17 Score per residue for model 17

- Molecule 1: Polcalcin Phl p 7



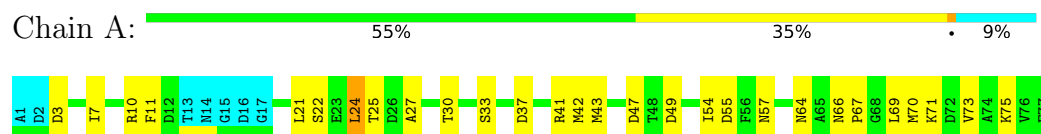
#### 4.2.18 Score per residue for model 18

- Molecule 1: Polcalcin Phl p 7



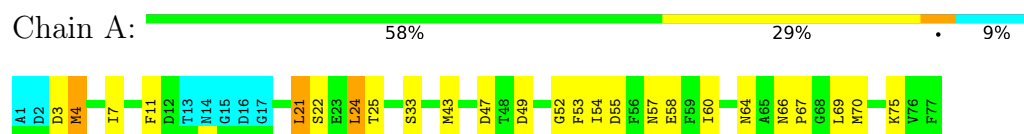
#### 4.2.19 Score per residue for model 19

- Molecule 1: Polcalcin Phl p 7



#### 4.2.20 Score per residue for model 20

- Molecule 1: Polcalcin Phl p 7



## 5 Refinement protocol and experimental data overview

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

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

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

| Software name | Classification     | Version |
|---------------|--------------------|---------|
| CYANA         | structure solution |         |
| CYANA         | 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                       | 923            |
| Number of shifts mapped to atoms             | 923            |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 92%            |

## 6 Model quality

### 6.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 6.2 Too-close contacts

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     | 552   | 534      | 534      | 16±2    |
| All | All   | 11060 | 10680    | 10680    | 324     |

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 15.

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

| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:21:LEU:HD23 | 1:A:54:ILE:CG2  | 0.79     | 2.08        | 5      | 19    |
| 1:A:24:LEU:HD13 | 1:A:25:THR:N    | 0.78     | 1.93        | 12     | 20    |
| 1:A:24:LEU:HD22 | 1:A:24:LEU:C    | 0.73     | 2.08        | 1      | 19    |
| 1:A:24:LEU:C    | 1:A:24:LEU:HD22 | 0.71     | 2.10        | 16     | 1     |
| 1:A:54:ILE:HG22 | 1:A:58:GLU:OE1  | 0.68     | 1.89        | 3      | 10    |
| 1:A:21:LEU:HD23 | 1:A:54:ILE:HG23 | 0.64     | 1.69        | 13     | 15    |
| 1:A:24:LEU:HD22 | 1:A:24:LEU:O    | 0.63     | 1.93        | 1      | 20    |
| 1:A:69:LEU:O    | 1:A:73:VAL:HG23 | 0.62     | 1.95        | 18     | 8     |
| 1:A:11:PHE:CZ   | 1:A:24:LEU:HD23 | 0.62     | 2.30        | 15     | 18    |
| 1:A:3:ASP:O     | 1:A:7:ILE:HD12  | 0.61     | 1.95        | 17     | 20    |
| 1:A:69:LEU:N    | 1:A:69:LEU:HD22 | 0.59     | 2.12        | 9      | 17    |
| 1:A:11:PHE:CE2  | 1:A:24:LEU:HD23 | 0.59     | 2.33        | 2      | 14    |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:28:LEU:HD12 | 1:A:39:VAL:HG11 | 0.59     | 1.72        | 2      | 1     |
| 1:A:21:LEU:HD12 | 1:A:22:SER:N    | 0.58     | 2.13        | 15     | 20    |
| 1:A:67:PRO:HB2  | 1:A:69:LEU:CD2  | 0.55     | 2.31        | 14     | 8     |
| 1:A:21:LEU:HD21 | 1:A:47:ASP:OD2  | 0.53     | 2.03        | 7      | 13    |
| 1:A:21:LEU:HD21 | 1:A:47:ASP:CG   | 0.52     | 2.30        | 20     | 7     |
| 1:A:69:LEU:HD22 | 1:A:69:LEU:N    | 0.51     | 2.20        | 16     | 1     |
| 1:A:67:PRO:HB2  | 1:A:69:LEU:HD23 | 0.51     | 1.81        | 8      | 15    |
| 1:A:42:MET:HE3  | 1:A:69:LEU:HD21 | 0.50     | 1.83        | 1      | 1     |
| 1:A:52:GLY:O    | 1:A:53:PHE:CG   | 0.47     | 2.68        | 13     | 6     |
| 1:A:24:LEU:C    | 1:A:24:LEU:CD2  | 0.46     | 2.81        | 15     | 8     |
| 1:A:66:ASN:N    | 1:A:67:PRO:CD   | 0.46     | 2.78        | 16     | 20    |
| 1:A:69:LEU:N    | 1:A:69:LEU:CD2  | 0.45     | 2.79        | 9      | 7     |
| 1:A:24:LEU:HD13 | 1:A:24:LEU:C    | 0.45     | 2.37        | 2      | 6     |
| 1:A:25:THR:HG21 | 1:A:43:MET:HE2  | 0.45     | 1.88        | 9      | 4     |
| 1:A:40:GLN:O    | 1:A:43:MET:HE3  | 0.44     | 2.11        | 18     | 5     |
| 1:A:51:ASP:OD2  | 1:A:53:PHE:HB2  | 0.44     | 2.13        | 13     | 1     |
| 1:A:27:ALA:O    | 1:A:30:THR:HG22 | 0.43     | 2.13        | 6      | 13    |
| 1:A:77:PHE:CD1  | 1:A:77:PHE:C    | 0.43     | 2.97        | 12     | 1     |
| 1:A:4:MET:HG2   | 1:A:60:ILE:HD13 | 0.42     | 1.91        | 14     | 2     |
| 1:A:30:THR:HG23 | 1:A:31:LEU:HD22 | 0.41     | 1.92        | 16     | 1     |
| 1:A:41:ARG:NH1  | 1:A:42:MET:HE2  | 0.41     | 2.31        | 19     | 1     |
| 1:A:67:PRO:HB2  | 1:A:69:LEU:HD22 | 0.40     | 1.92        | 14     | 1     |
| 1:A:8:PHE:O     | 1:A:19:ILE:HG21 | 0.40     | 2.16        | 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     | 69/77 (90%)     | 67±1 (97±2%) | 2±1 (3±2%) | 0±0 (0±0%) | 100         | 100 |
| All | All   | 1380/1540 (90%) | 1335 (97%)   | 45 (3%)    | 0 (0%)     | 100         | 100 |

There are no Ramachandran outliers.

### 6.3.2 Protein sidechains ⓘ

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

| Mol | Chain | Analysed        | Rotameric    | Outliers     | Percentiles |
|-----|-------|-----------------|--------------|--------------|-------------|
| 1   | A     | 61/65 (94%)     | 50±1 (81±2%) | 12±1 (19±2%) | <b>3</b> 35 |
| All | All   | 1220/1300 (94%) | 990 (81%)    | 230 (19%)    | <b>3</b> 35 |

All 23 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 24  | LEU  | 20             |
| 1   | A     | 43  | MET  | 20             |
| 1   | A     | 49  | ASP  | 20             |
| 1   | A     | 57  | ASN  | 20             |
| 1   | A     | 75  | LYS  | 20             |
| 1   | A     | 33  | SER  | 19             |
| 1   | A     | 64  | ASN  | 19             |
| 1   | A     | 55  | ASP  | 15             |
| 1   | A     | 70  | MET  | 15             |
| 1   | A     | 21  | LEU  | 13             |
| 1   | A     | 5   | GLU  | 7              |
| 1   | A     | 10  | ARG  | 7              |
| 1   | A     | 71  | LYS  | 6              |
| 1   | A     | 30  | THR  | 6              |
| 1   | A     | 37  | ASP  | 6              |
| 1   | A     | 20  | SER  | 4              |
| 1   | A     | 77  | PHE  | 3              |
| 1   | A     | 29  | ARG  | 3              |
| 1   | A     | 4   | MET  | 2              |
| 1   | A     | 69  | LEU  | 2              |
| 1   | A     | 51  | ASP  | 1              |
| 1   | A     | 3   | ASP  | 1              |
| 1   | A     | 42  | MET  | 1              |

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

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

There are no chain breaks in this entry.

## 7 Chemical shift validation [i](#)

The completeness of assignment taking into account all chemical shift lists is 92% for the well-defined parts and 92% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

Chemical shift list name: *assigned\_chem\_shift\_list\_1*

#### 7.1.1 Bookkeeping [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                  | 923 |
| Number of shifts mapped to atoms        | 923 |
| Number of unparsed shifts               | 0   |
| Number of shifts with mapping errors    | 0   |
| Number of shifts with mapping warnings  | 0   |
| Number of shift outliers (ShiftChecker) | 34  |

#### 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           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 77       | $-0.23 \pm 0.14$                | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}_\beta$  | 71       | $0.14 \pm 0.06$                 | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}'$       | 77       | $-0.45 \pm 0.17$                | None needed ( $< 0.5$ ppm) |
| $^{15}\text{N}$        | 76       | $0.64 \pm 0.39$                 | None needed (imprecise)    |

#### 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 92%, i.e. 864 atoms were assigned a chemical shift out of a possible 940. 0 out of 8 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total          | $^1\text{H}$   | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|----------------|----------------|-----------------|-----------------|
| Backbone  | 352/352 (100%) | 143/143 (100%) | 140/140 (100%)  | 69/69 (100%)    |
| Sidechain | 484/518 (93%)  | 326/334 (98%)  | 142/164 (87%)   | 16/20 (80%)     |

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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 | 28/70 (40%)   | 28/35 (80%)          | 0/35 (0%)             | 0/0 (—%)              |
| Overall  | 864/940 (92%) | 497/512 (97%)        | 282/339 (83%)         | 85/89 (96%)           |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 92%, i.e. 922 atoms were assigned a chemical shift out of a possible 1002. 0 out of 8 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  | 388/389 (100%) | 158/159 (99%)        | 154/154 (100%)        | 76/76 (100%)          |
| Sidechain | 506/543 (93%)  | 341/349 (98%)        | 148/173 (86%)         | 17/21 (81%)           |
| Aromatic  | 28/70 (40%)    | 28/35 (80%)          | 0/35 (0%)             | 0/0 (—%)              |
| Overall   | 922/1002 (92%) | 527/543 (97%)        | 302/362 (83%)         | 93/97 (96%)           |

#### 7.1.4 Statistically unusual chemical shifts ⓘ

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

| List Id | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|---------|-------|-----|------|------|------------|---------------------|---------|
| 1       | A     | 1   | ALA  | C    | 0.00       | 167.61 – 188.05     | -87.0   |
| 1       | A     | 6   | ARG  | NE   | 0.00       | 76.53 – 92.65       | -52.5   |
| 1       | A     | 10  | ARG  | NE   | 0.00       | 76.53 – 92.65       | -52.5   |
| 1       | A     | 29  | ARG  | NE   | 0.00       | 76.53 – 92.65       | -52.5   |
| 1       | A     | 41  | ARG  | NE   | 0.00       | 76.53 – 92.65       | -52.5   |
| 1       | A     | 1   | ALA  | N    | 0.00       | 106.13 – 140.55     | -35.8   |
| 1       | A     | 2   | ASP  | N    | 0.00       | 102.08 – 139.36     | -32.4   |
| 1       | A     | 1   | ALA  | CA   | 0.00       | 43.52 – 62.81       | -27.6   |
| 1       | A     | 6   | ARG  | NH2  | 0.00       | 57.68 – 87.89       | -24.1   |
| 1       | A     | 10  | ARG  | NH2  | 0.00       | 57.68 – 87.89       | -24.1   |
| 1       | A     | 29  | ARG  | NH2  | 0.00       | 57.68 – 87.89       | -24.1   |
| 1       | A     | 41  | ARG  | NH2  | 0.00       | 57.68 – 87.89       | -24.1   |
| 1       | A     | 6   | ARG  | HH22 | 0.00       | 5.04 – 8.54         | -19.4   |
| 1       | A     | 10  | ARG  | HH22 | 0.00       | 5.04 – 8.54         | -19.4   |
| 1       | A     | 29  | ARG  | HH22 | 0.00       | 5.04 – 8.54         | -19.4   |
| 1       | A     | 41  | ARG  | HH22 | 0.00       | 5.04 – 8.54         | -19.4   |
| 1       | A     | 6   | ARG  | HH21 | 0.00       | 4.81 – 8.80         | -17.1   |
| 1       | A     | 10  | ARG  | HH21 | 0.00       | 4.81 – 8.80         | -17.1   |
| 1       | A     | 29  | ARG  | HH21 | 0.00       | 4.81 – 8.80         | -17.1   |
| 1       | A     | 41  | ARG  | HH21 | 0.00       | 4.81 – 8.80         | -17.1   |
| 1       | A     | 2   | ASP  | H    | 0.00       | 5.52 – 11.08        | -14.9   |
| 1       | A     | 6   | ARG  | NH1  | 0.00       | 49.05 – 99.42       | -14.7   |

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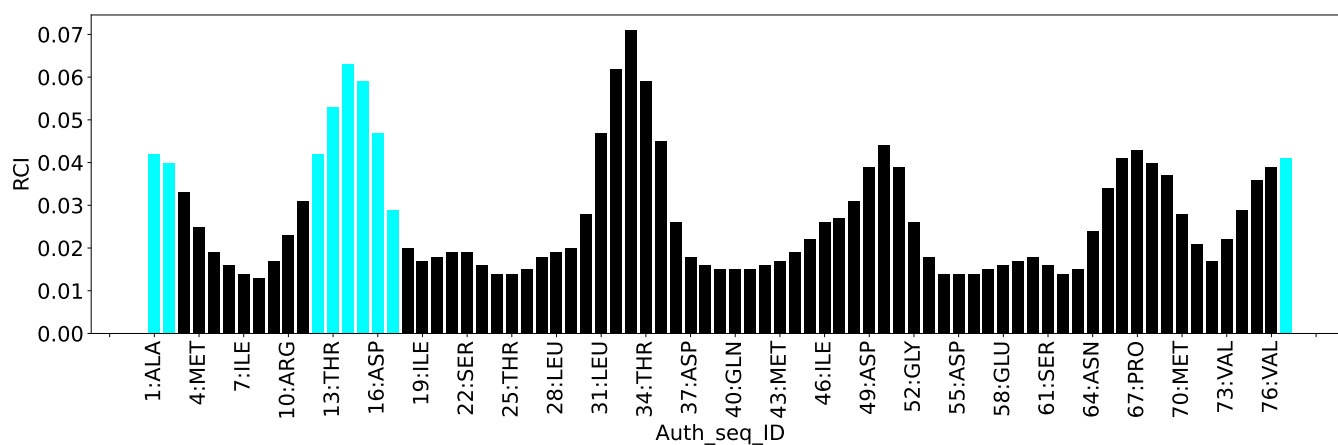
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| List Id | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|---------|-------|-----|------|------|------------|---------------------|---------|
| 1       | A     | 10  | ARG  | NH1  | 0.00       | 49.05 – 99.42       | -14.7   |
| 1       | A     | 29  | ARG  | NH1  | 0.00       | 49.05 – 99.42       | -14.7   |
| 1       | A     | 41  | ARG  | NH1  | 0.00       | 49.05 – 99.42       | -14.7   |
| 1       | A     | 6   | ARG  | HE   | 0.00       | 4.52 – 10.19        | -13.0   |
| 1       | A     | 10  | ARG  | HE   | 0.00       | 4.52 – 10.19        | -13.0   |
| 1       | A     | 29  | ARG  | HE   | 0.00       | 4.52 – 10.19        | -13.0   |
| 1       | A     | 41  | ARG  | HE   | 0.00       | 4.52 – 10.19        | -13.0   |
| 1       | A     | 1   | ALA  | CB   | 0.00       | 10.19 – 27.75       | -10.8   |
| 1       | A     | 1   | ALA  | HA   | 0.00       | 2.13 – 6.34         | -10.1   |
| 1       | A     | 1   | ALA  | HB1  | 0.00       | 0.14 – 2.58         | -5.6    |
| 1       | A     | 1   | ALA  | HB2  | 0.00       | 0.14 – 2.58         | -5.6    |
| 1       | A     | 1   | ALA  | HB3  | 0.00       | 0.14 – 2.58         | -5.6    |

### 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                                | 1585  |
| Intra-residue ( $ i-j =0$ )                              | 378   |
| Sequential ( $ i-j =1$ )                                 | 437   |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 443   |
| Long range ( $ i-j \geq 5$ )                             | 327   |
| Inter-chain                                              | 0     |
| Hydrogen bond restraints                                 | 0     |
| Disulfide bond restraints                                | 0     |
| Total dihedral-angle restraints                          | 0     |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 20.3  |
| Number of long range restraints per residue <sup>1</sup> | 4.2   |

<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)  | 24.5                                   | 0.2     |
| 0.2-0.5 (Medium) | 38.5                                   | 0.5     |
| >0.5 (Large)     | 113.7                                  | 4.13    |

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

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

## 9 Distance violation analysis ⓘ

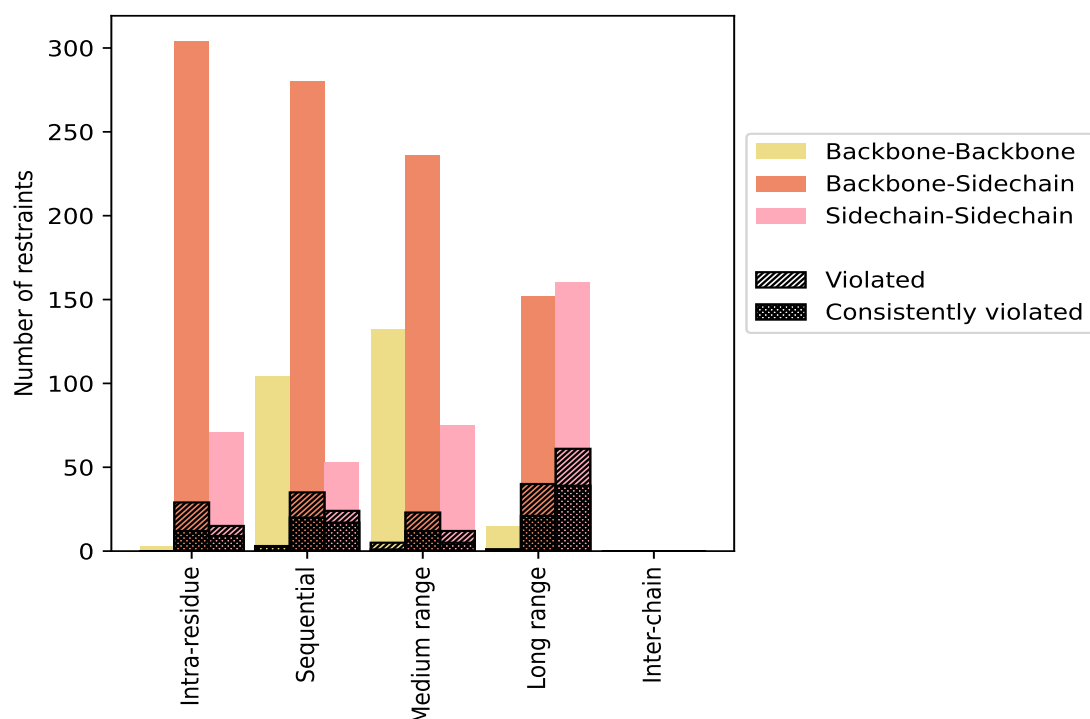
### 9.1 Summary of distance violations ⓘ

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

| Restrains type                                             | Count                | % <sup>1</sup>        | Violated <sup>3</sup> |                      |                      | Consistently Violated <sup>4</sup> |                      |                     |
|------------------------------------------------------------|----------------------|-----------------------|-----------------------|----------------------|----------------------|------------------------------------|----------------------|---------------------|
|                                                            |                      |                       | Count                 | % <sup>2</sup>       | % <sup>1</sup>       | Count                              | % <sup>2</sup>       | % <sup>1</sup>      |
| <a href="#">Intra-residue ( i-j =0)</a>                    | <a href="#">378</a>  | <a href="#">23.8</a>  | <a href="#">44</a>    | <a href="#">11.6</a> | <a href="#">2.8</a>  | <a href="#">21</a>                 | <a href="#">5.6</a>  | <a href="#">1.3</a> |
| Backbone-Backbone                                          | 3                    | 0.2                   | 0                     | 0.0                  | 0.0                  | 0                                  | 0.0                  | 0.0                 |
| Backbone-Sidechain                                         | 304                  | 19.2                  | 29                    | 9.5                  | 1.8                  | 12                                 | 3.9                  | 0.8                 |
| Sidechain-Sidechain                                        | 71                   | 4.5                   | 15                    | 21.1                 | 0.9                  | 9                                  | 12.7                 | 0.6                 |
| <a href="#">Sequential ( i-j =1)</a>                       | <a href="#">437</a>  | <a href="#">27.6</a>  | <a href="#">62</a>    | <a href="#">14.2</a> | <a href="#">3.9</a>  | <a href="#">40</a>                 | <a href="#">9.2</a>  | <a href="#">2.5</a> |
| Backbone-Backbone                                          | 104                  | 6.6                   | 3                     | 2.9                  | 0.2                  | 3                                  | 2.9                  | 0.2                 |
| Backbone-Sidechain                                         | 280                  | 17.7                  | 35                    | 12.5                 | 2.2                  | 20                                 | 7.1                  | 1.3                 |
| Sidechain-Sidechain                                        | 53                   | 3.3                   | 24                    | 45.3                 | 1.5                  | 17                                 | 32.1                 | 1.1                 |
| <a href="#">Medium range ( i-j &gt;1 &amp;  i-j &lt;5)</a> | <a href="#">443</a>  | <a href="#">27.9</a>  | <a href="#">40</a>    | <a href="#">9.0</a>  | <a href="#">2.5</a>  | <a href="#">18</a>                 | <a href="#">4.1</a>  | <a href="#">1.1</a> |
| Backbone-Backbone                                          | 132                  | 8.3                   | 5                     | 3.8                  | 0.3                  | 1                                  | 0.8                  | 0.1                 |
| Backbone-Sidechain                                         | 236                  | 14.9                  | 23                    | 9.7                  | 1.5                  | 12                                 | 5.1                  | 0.8                 |
| Sidechain-Sidechain                                        | 75                   | 4.7                   | 12                    | 16.0                 | 0.8                  | 5                                  | 6.7                  | 0.3                 |
| <a href="#">Long range ( i-j ≥5)</a>                       | <a href="#">327</a>  | <a href="#">20.6</a>  | <a href="#">102</a>   | <a href="#">31.2</a> | <a href="#">6.4</a>  | <a href="#">61</a>                 | <a href="#">18.7</a> | <a href="#">3.8</a> |
| Backbone-Backbone                                          | 15                   | 0.9                   | 1                     | 6.7                  | 0.1                  | 1                                  | 6.7                  | 0.1                 |
| Backbone-Sidechain                                         | 152                  | 9.6                   | 40                    | 26.3                 | 2.5                  | 21                                 | 13.8                 | 1.3                 |
| Sidechain-Sidechain                                        | 160                  | 10.1                  | 61                    | 38.1                 | 3.8                  | 39                                 | 24.4                 | 2.5                 |
| <a href="#">Inter-chain</a>                                | <a href="#">0</a>    | <a href="#">0.0</a>   | <a href="#">0</a>     | <a href="#">0.0</a>  | <a href="#">0.0</a>  | <a href="#">0</a>                  | <a href="#">0.0</a>  | <a href="#">0.0</a> |
| Backbone-Backbone                                          | 0                    | 0.0                   | 0                     | 0.0                  | 0.0                  | 0                                  | 0.0                  | 0.0                 |
| Backbone-Sidechain                                         | 0                    | 0.0                   | 0                     | 0.0                  | 0.0                  | 0                                  | 0.0                  | 0.0                 |
| Sidechain-Sidechain                                        | 0                    | 0.0                   | 0                     | 0.0                  | 0.0                  | 0                                  | 0.0                  | 0.0                 |
| <a href="#">Hydrogen bond</a>                              | <a href="#">0</a>    | <a href="#">0.0</a>   | <a href="#">0</a>     | <a href="#">0.0</a>  | <a href="#">0.0</a>  | <a href="#">0</a>                  | <a href="#">0.0</a>  | <a href="#">0.0</a> |
| <a href="#">Disulfide bond</a>                             | <a href="#">0</a>    | <a href="#">0.0</a>   | <a href="#">0</a>     | <a href="#">0.0</a>  | <a href="#">0.0</a>  | <a href="#">0</a>                  | <a href="#">0.0</a>  | <a href="#">0.0</a> |
| <a href="#">Total</a>                                      | <a href="#">1585</a> | <a href="#">100.0</a> | <a href="#">248</a>   | <a href="#">15.6</a> | <a href="#">15.6</a> | <a href="#">140</a>                | <a href="#">8.8</a>  | <a href="#">8.8</a> |
| Backbone-Backbone                                          | 254                  | 16.0                  | 9                     | 3.5                  | 0.6                  | 5                                  | 2.0                  | 0.3                 |
| Backbone-Sidechain                                         | 972                  | 61.3                  | 127                   | 13.1                 | 8.0                  | 65                                 | 6.7                  | 4.1                 |
| Sidechain-Sidechain                                        | 359                  | 22.6                  | 112                   | 31.2                 | 7.1                  | 70                                 | 19.5                 | 4.4                 |

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

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



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

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

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

| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 1        | 30                   | 51              | 24              | 71              | 0               | 176   | 0.91     | 3.9     | 0.75                | 0.72       |
| 2        | 30                   | 48              | 30              | 69              | 0               | 177   | 0.91     | 3.88    | 0.73                | 0.75       |
| 3        | 31                   | 52              | 27              | 70              | 0               | 180   | 0.9      | 4.0     | 0.74                | 0.73       |
| 4        | 33                   | 55              | 31              | 86              | 0               | 205   | 1.0      | 3.99    | 0.81                | 0.82       |
| 5        | 32                   | 47              | 23              | 71              | 0               | 173   | 0.94     | 3.93    | 0.74                | 0.77       |
| 6        | 33                   | 55              | 29              | 87              | 0               | 204   | 0.98     | 3.9     | 0.8                 | 0.8        |
| 7        | 30                   | 48              | 25              | 71              | 0               | 174   | 0.91     | 4.13    | 0.73                | 0.76       |
| 8        | 28                   | 49              | 28              | 70              | 0               | 175   | 0.92     | 3.86    | 0.74                | 0.76       |
| 9        | 30                   | 51              | 26              | 66              | 0               | 173   | 0.93     | 3.94    | 0.76                | 0.73       |
| 10       | 28                   | 47              | 27              | 71              | 0               | 173   | 0.94     | 4.05    | 0.74                | 0.78       |

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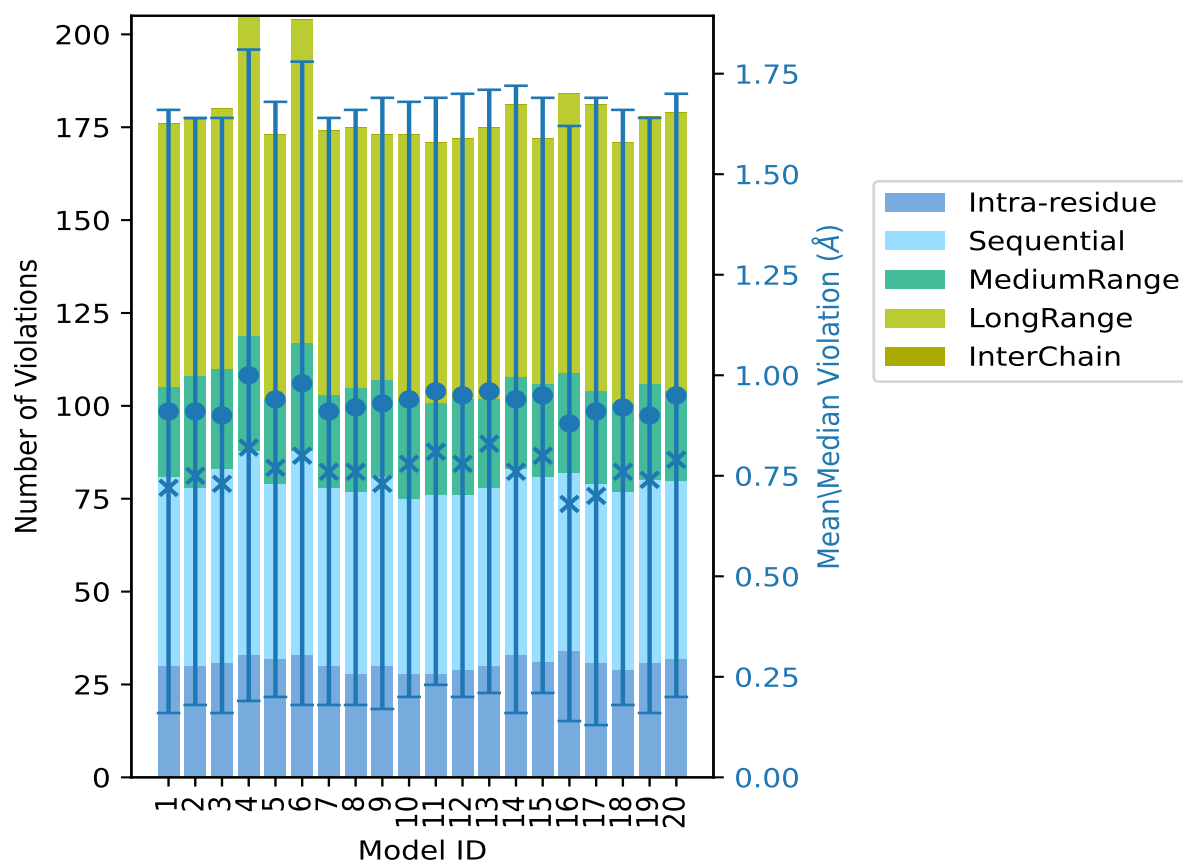
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| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 11       | 28                   | 48              | 25              | 70              | 0               | 171   | 0.96     | 3.87    | 0.73                | 0.81       |
| 12       | 29                   | 47              | 26              | 70              | 0               | 172   | 0.95     | 3.78    | 0.75                | 0.78       |
| 13       | 30                   | 48              | 24              | 73              | 0               | 175   | 0.96     | 3.82    | 0.75                | 0.83       |
| 14       | 33                   | 50              | 25              | 73              | 0               | 181   | 0.94     | 3.89    | 0.78                | 0.76       |
| 15       | 31                   | 50              | 25              | 66              | 0               | 172   | 0.95     | 4.02    | 0.74                | 0.8        |
| 16       | 34                   | 48              | 27              | 75              | 0               | 184   | 0.88     | 3.87    | 0.74                | 0.68       |
| 17       | 31                   | 48              | 25              | 77              | 0               | 181   | 0.91     | 3.94    | 0.78                | 0.7        |
| 18       | 29                   | 48              | 24              | 70              | 0               | 171   | 0.92     | 3.82    | 0.74                | 0.76       |
| 19       | 31                   | 49              | 26              | 72              | 0               | 178   | 0.9      | 4.04    | 0.74                | 0.74       |
| 20       | 32                   | 48              | 24              | 75              | 0               | 179   | 0.95     | 3.95    | 0.75                | 0.79       |

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

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

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



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

### 9.3 Distance violation statistics for the ensemble

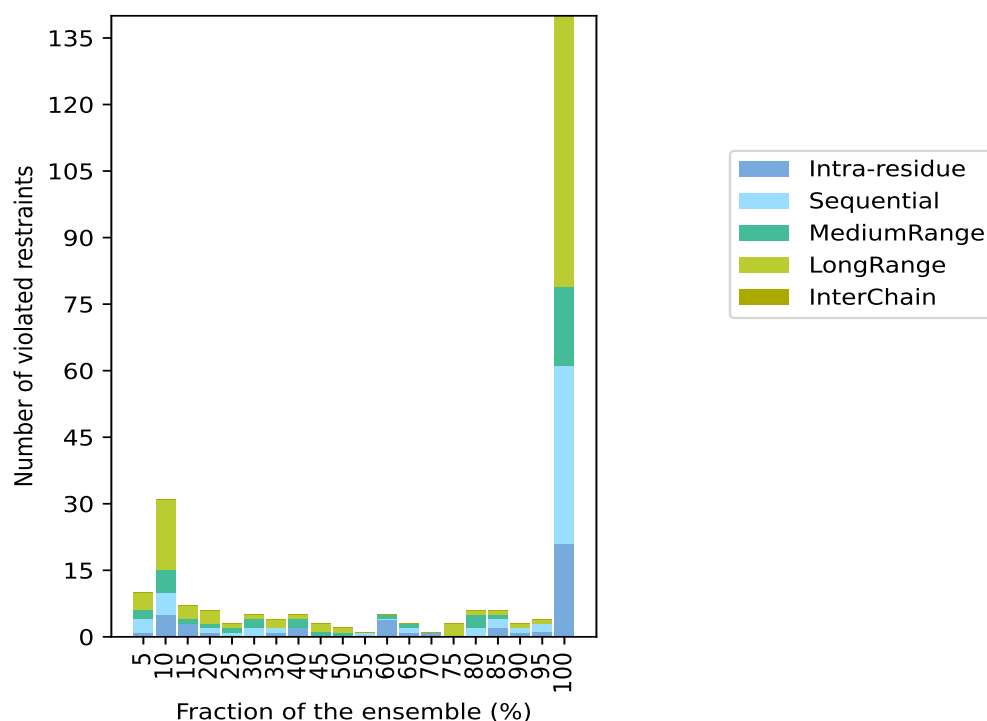
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1337(IR:334, SQ:375, MR:403, LR:225, IC:0) restraints are 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>       | %     |
| 1                             | 3               | 2               | 4               | 0               | 10    | 1                        | 5.0   |
| 5                             | 5               | 5               | 16              | 0               | 31    | 2                        | 10.0  |
| 3                             | 0               | 1               | 3               | 0               | 7     | 3                        | 15.0  |
| 1                             | 1               | 1               | 3               | 0               | 6     | 4                        | 20.0  |
| 0                             | 1               | 1               | 1               | 0               | 3     | 5                        | 25.0  |
| 0                             | 2               | 2               | 1               | 0               | 5     | 6                        | 30.0  |
| 1                             | 1               | 0               | 2               | 0               | 4     | 7                        | 35.0  |
| 2                             | 0               | 2               | 1               | 0               | 5     | 8                        | 40.0  |
| 0                             | 0               | 1               | 2               | 0               | 3     | 9                        | 45.0  |
| 0                             | 0               | 1               | 1               | 0               | 2     | 10                       | 50.0  |
| 0                             | 1               | 0               | 0               | 0               | 1     | 11                       | 55.0  |
| 4                             | 0               | 1               | 0               | 0               | 5     | 12                       | 60.0  |
| 1                             | 1               | 1               | 0               | 0               | 3     | 13                       | 65.0  |
| 1                             | 0               | 0               | 0               | 0               | 1     | 14                       | 70.0  |
| 0                             | 0               | 0               | 3               | 0               | 3     | 15                       | 75.0  |
| 0                             | 2               | 3               | 1               | 0               | 6     | 16                       | 80.0  |
| 2                             | 2               | 1               | 1               | 0               | 6     | 17                       | 85.0  |
| 1                             | 1               | 0               | 1               | 0               | 3     | 18                       | 90.0  |
| 1                             | 2               | 0               | 1               | 0               | 4     | 19                       | 95.0  |
| 21                            | 40              | 18              | 61              | 0               | 140   | 20                       | 100.0 |

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

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

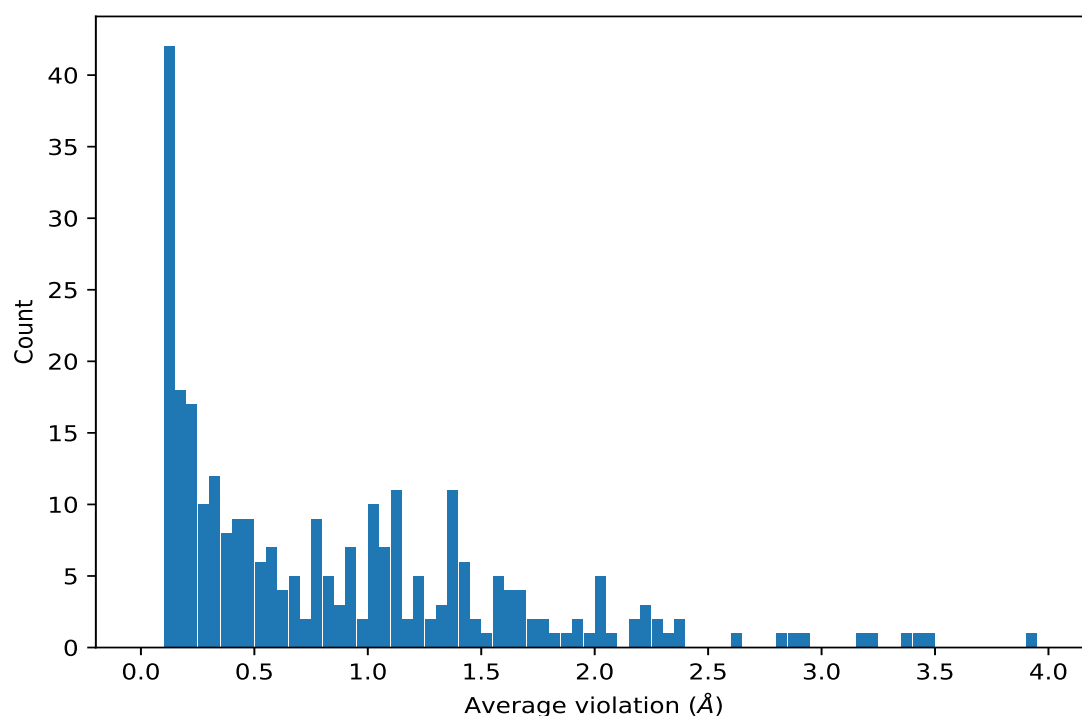
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

| Key      | Atom-1         | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,267)  | 1:11:A:PHE:HD1 | 1:19:A:ILE:HD12 | 20                  | 3.93     | 0.09                | 3.92       |
| (1,780)  | 1:62:A:PHE:HD2 | 1:67:A:PRO:HD2  | 20                  | 3.48     | 0.03                | 3.48       |
| (1,546)  | 1:43:A:MET:HG2 | 1:62:A:PHE:HD1  | 20                  | 3.41     | 0.1                 | 3.4        |
| (1,544)  | 1:43:A:MET:HG3 | 1:62:A:PHE:HD1  | 20                  | 3.24     | 0.18                | 3.24       |
| (1,747)  | 1:62:A:PHE:HD2 | 1:63:A:CYS:HA   | 20                  | 3.18     | 0.01                | 3.18       |
| (1,919)  | 1:62:A:PHE:HE2 | 1:69:A:LEU:H    | 20                  | 2.91     | 0.03                | 2.91       |
| (1,131)  | 1:10:A:ARG:HG3 | 1:11:A:PHE:HE2  | 20                  | 2.37     | 0.12                | 2.38       |
| (1,538)  | 1:43:A:MET:HB2 | 1:62:A:PHE:HE1  | 20                  | 2.32     | 0.05                | 2.33       |
| (1,754)  | 1:62:A:PHE:HD2 | 1:63:A:CYS:HB2  | 20                  | 2.3      | 0.04                | 2.3        |
| (1,545)  | 1:43:A:MET:HG3 | 1:62:A:PHE:HE1  | 20                  | 2.3      | 0.26                | 2.3        |
| (1,509)  | 1:43:A:MET:HA  | 1:62:A:PHE:HE1  | 20                  | 2.15     | 0.07                | 2.14       |
| (1,779)  | 1:62:A:PHE:HE2 | 1:67:A:PRO:HD2  | 20                  | 2.15     | 0.03                | 2.15       |
| (1,137)  | 1:10:A:ARG:HD2 | 1:11:A:PHE:HD2  | 20                  | 2.06     | 0.21                | 2.0        |
| (1,1406) | 1:10:A:ARG:HG2 | 1:11:A:PHE:HE2  | 20                  | 2.04     | 0.18                | 2.04       |
| (1,1406) | 1:10:A:ARG:HG3 | 1:11:A:PHE:HE2  | 20                  | 2.04     | 0.18                | 2.04       |
| (1,473)  | 1:62:A:PHE:HD2 | 1:69:A:LEU:HD21 | 20                  | 2.02     | 0.39                | 2.2        |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,129)  | 1:10:A:ARG:HG2  | 1:11:A:PHE:HE2  | 20                  | 1.86     | 0.38                | 1.81       |
| (1,181)  | 1:25:A:THR:HG22 | 1:40:A:GLN:HE22 | 20                  | 1.84     | 0.01                | 1.85       |
| (1,1001) | 1:11:A:PHE:HE1  | 1:24:A:LEU:H    | 20                  | 1.78     | 0.12                | 1.82       |
| (1,43)   | 1:62:A:PHE:HD2  | 1:67:A:PRO:HG3  | 20                  | 1.76     | 0.06                | 1.78       |
| (1,1206) | 1:42:A:MET:H    | 1:62:A:PHE:HE1  | 20                  | 1.72     | 0.11                | 1.68       |
| (1,1115) | 1:11:A:PHE:HD1  | 1:20:A:SER:H    | 20                  | 1.71     | 0.17                | 1.74       |
| (1,256)  | 1:11:A:PHE:HD1  | 1:19:A:ILE:HG21 | 20                  | 1.68     | 0.16                | 1.74       |
| (1,1291) | 1:62:A:PHE:HD2  | 1:63:A:CYS:H    | 20                  | 1.65     | 0.04                | 1.65       |
| (1,858)  | 1:70:A:MET:HE2  | 1:74:A:ALA:HA   | 20                  | 1.65     | 0.11                | 1.69       |
| (1,73)   | 1:7:A:ILE:HD13  | 1:8:A:PHE:HB3   | 20                  | 1.6      | 0.04                | 1.6        |
| (1,154)  | 1:19:A:ILE:HD11 | 1:59:A:PHE:HB2  | 20                  | 1.59     | 0.09                | 1.64       |
| (1,1517) | 1:47:A:ASP:HB2  | 1:54:A:ILE:HD13 | 20                  | 1.58     | 0.04                | 1.6        |
| (1,1517) | 1:47:A:ASP:HB3  | 1:54:A:ILE:HD13 | 20                  | 1.58     | 0.04                | 1.6        |
| (1,480)  | 1:39:A:VAL:HG21 | 1:40:A:GLN:HA   | 20                  | 1.47     | 0.05                | 1.49       |
| (1,144)  | 1:11:A:PHE:HA   | 1:11:A:PHE:HE2  | 20                  | 1.45     | 0.01                | 1.45       |
| (1,1196) | 1:42:A:MET:H    | 1:69:A:LEU:HD23 | 20                  | 1.45     | 0.12                | 1.52       |
| (1,1116) | 1:20:A:SER:H    | 1:53:A:PHE:HD2  | 20                  | 1.44     | 0.28                | 1.32       |
| (1,842)  | 1:75:A:LYS:HA   | 1:76:A:VAL:HG21 | 20                  | 1.43     | 0.12                | 1.48       |
| (1,21)   | 1:5:A:GLU:HA    | 1:60:A:ILE:HD13 | 20                  | 1.41     | 0.28                | 1.34       |
| (1,1408) | 1:10:A:ARG:HD2  | 1:11:A:PHE:HE2  | 20                  | 1.39     | 0.13                | 1.4        |
| (1,1408) | 1:10:A:ARG:HD3  | 1:11:A:PHE:HE2  | 20                  | 1.39     | 0.13                | 1.4        |
| (1,1170) | 1:31:A:LEU:HD21 | 1:33:A:SER:H    | 20                  | 1.38     | 0.02                | 1.38       |
| (1,398)  | 1:30:A:THR:HA   | 1:31:A:LEU:HD21 | 20                  | 1.38     | 0.04                | 1.38       |
| (1,333)  | 1:11:A:PHE:HE1  | 1:24:A:LEU:HD21 | 20                  | 1.37     | 0.34                | 1.17       |
| (1,1328) | 1:62:A:PHE:HD2  | 1:70:A:MET:H    | 20                  | 1.36     | 0.06                | 1.36       |
| (1,1431) | 1:20:A:SER:HB2  | 1:53:A:PHE:HE2  | 20                  | 1.36     | 0.34                | 1.36       |
| (1,1431) | 1:20:A:SER:HB3  | 1:53:A:PHE:HE2  | 20                  | 1.36     | 0.34                | 1.36       |
| (1,37)   | 1:46:A:ILE:HD11 | 1:58:A:GLU:HB2  | 20                  | 1.35     | 0.14                | 1.34       |
| (1,1409) | 1:10:A:ARG:HD2  | 1:11:A:PHE:HD2  | 20                  | 1.35     | 0.11                | 1.32       |
| (1,1409) | 1:10:A:ARG:HD3  | 1:11:A:PHE:HD2  | 20                  | 1.35     | 0.11                | 1.32       |
| (1,275)  | 1:20:A:SER:HA   | 1:53:A:PHE:HD2  | 20                  | 1.33     | 0.11                | 1.3        |
| (1,552)  | 1:39:A:VAL:HG21 | 1:43:A:MET:HG2  | 20                  | 1.32     | 0.21                | 1.4        |
| (1,552)  | 1:39:A:VAL:HG21 | 1:43:A:MET:HG3  | 20                  | 1.32     | 0.21                | 1.4        |
| (1,274)  | 1:20:A:SER:HA   | 1:53:A:PHE:HE2  | 20                  | 1.27     | 0.12                | 1.24       |
| (1,493)  | 1:39:A:VAL:HG21 | 1:40:A:GLN:HB2  | 20                  | 1.24     | 0.09                | 1.28       |
| (1,1109) | 1:19:A:ILE:H    | 1:53:A:PHE:HD2  | 20                  | 1.24     | 0.13                | 1.19       |
| (1,143)  | 1:11:A:PHE:HA   | 1:11:A:PHE:HD2  | 20                  | 1.24     | 0.01                | 1.24       |
| (1,75)   | 1:5:A:GLU:HA    | 1:7:A:ILE:HD13  | 20                  | 1.23     | 0.1                 | 1.25       |
| (1,1349) | 1:75:A:LYS:H    | 1:76:A:VAL:HG21 | 20                  | 1.22     | 0.1                 | 1.23       |
| (1,865)  | 1:4:A:MET:HE3   | 1:74:A:ALA:HB2  | 20                  | 1.2      | 0.41                | 1.48       |
| (1,542)  | 1:39:A:VAL:HG21 | 1:43:A:MET:HB3  | 20                  | 1.16     | 0.06                | 1.15       |
| (1,1467) | 1:33:A:SER:HB2  | 1:34:A:THR:HG23 | 20                  | 1.15     | 0.12                | 1.13       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1467) | 1:33:A:SER:HB3  | 1:34:A:THR:HG23 | 20                  | 1.15     | 0.12                | 1.13       |
| (1,205)  | 1:18:A:LYS:HB3  | 1:53:A:PHE:HD2  | 20                  | 1.13     | 0.25                | 1.1        |
| (1,205)  | 1:18:A:LYS:HB2  | 1:53:A:PHE:HD2  | 20                  | 1.13     | 0.25                | 1.1        |
| (1,809)  | 1:69:A:LEU:HD21 | 1:70:A:MET:HG2  | 20                  | 1.13     | 0.17                | 1.24       |
| (1,809)  | 1:69:A:LEU:HD21 | 1:70:A:MET:HG3  | 20                  | 1.13     | 0.17                | 1.24       |
| (1,846)  | 1:72:A:ASP:HA   | 1:76:A:VAL:HG21 | 20                  | 1.12     | 0.26                | 1.18       |
| (1,264)  | 1:19:A:ILE:HG21 | 1:19:A:ILE:HD13 | 20                  | 1.12     | 0.04                | 1.12       |
| (1,68)   | 1:7:A:ILE:HD11  | 1:74:A:ALA:H    | 20                  | 1.12     | 0.05                | 1.11       |
| (1,1357) | 1:76:A:VAL:H    | 1:76:A:VAL:HG21 | 20                  | 1.11     | 0.03                | 1.12       |
| (1,416)  | 1:33:A:SER:HA   | 1:34:A:THR:HG23 | 20                  | 1.1      | 0.08                | 1.12       |
| (1,578)  | 1:46:A:ILE:HD12 | 1:62:A:PHE:HD1  | 20                  | 1.09     | 0.03                | 1.1        |
| (1,578)  | 1:46:A:ILE:HD13 | 1:62:A:PHE:HD1  | 20                  | 1.09     | 0.03                | 1.1        |
| (1,182)  | 1:13:A:THR:HG21 | 1:14:A:ASN:HA   | 20                  | 1.08     | 0.28                | 1.02       |
| (1,1533) | 1:52:A:GLY:HA2  | 1:53:A:PHE:HE1  | 20                  | 1.07     | 0.19                | 1.14       |
| (1,1533) | 1:52:A:GLY:HA3  | 1:53:A:PHE:HE1  | 20                  | 1.07     | 0.19                | 1.14       |
| (1,576)  | 1:46:A:ILE:HD12 | 1:63:A:CYS:H    | 20                  | 1.06     | 0.05                | 1.06       |
| (1,776)  | 1:62:A:PHE:HD2  | 1:67:A:PRO:HG2  | 20                  | 1.06     | 0.01                | 1.06       |
| (1,467)  | 1:39:A:VAL:HA   | 1:69:A:LEU:HD23 | 20                  | 1.03     | 0.1                 | 1.04       |
| (1,345)  | 1:25:A:THR:HG23 | 1:26:A:ASP:HA   | 20                  | 1.03     | 0.04                | 1.04       |
| (1,325)  | 1:24:A:LEU:HG   | 1:25:A:THR:HA   | 20                  | 1.03     | 0.01                | 1.03       |
| (1,765)  | 1:60:A:ILE:HD12 | 1:63:A:CYS:HB3  | 20                  | 1.02     | 0.07                | 1.03       |
| (1,765)  | 1:60:A:ILE:HD12 | 1:63:A:CYS:HB2  | 20                  | 1.02     | 0.07                | 1.03       |
| (1,1532) | 1:52:A:GLY:HA2  | 1:53:A:PHE:HD1  | 20                  | 1.02     | 0.08                | 1.03       |
| (1,1532) | 1:52:A:GLY:HA3  | 1:53:A:PHE:HD1  | 20                  | 1.02     | 0.08                | 1.03       |
| (1,363)  | 1:27:A:ALA:HB1  | 1:28:A:LEU:HD21 | 20                  | 1.01     | 0.18                | 0.96       |
| (1,142)  | 1:10:A:ARG:HD3  | 1:11:A:PHE:HD2  | 20                  | 1.0      | 0.21                | 0.96       |
| (1,163)  | 1:12:A:ASP:HB2  | 1:19:A:ILE:HD13 | 20                  | 1.0      | 0.31                | 0.93       |
| (1,476)  | 1:39:A:VAL:HG21 | 1:40:A:GLN:H    | 20                  | 0.98     | 0.03                | 0.99       |
| (1,305)  | 1:11:A:PHE:HE1  | 1:24:A:LEU:HA   | 20                  | 0.95     | 0.1                 | 0.98       |
| (1,862)  | 1:4:A:MET:HE3   | 1:7:A:ILE:H     | 20                  | 0.95     | 0.3                 | 0.89       |
| (1,390)  | 1:10:A:ARG:HB2  | 1:11:A:PHE:HE2  | 20                  | 0.95     | 0.08                | 0.94       |
| (1,390)  | 1:10:A:ARG:HB3  | 1:11:A:PHE:HE2  | 20                  | 0.95     | 0.08                | 0.94       |
| (1,1432) | 1:20:A:SER:HB2  | 1:53:A:PHE:HD2  | 20                  | 0.91     | 0.32                | 0.96       |
| (1,1432) | 1:20:A:SER:HB3  | 1:53:A:PHE:HD2  | 20                  | 0.91     | 0.32                | 0.96       |
| (1,1161) | 1:31:A:LEU:HD21 | 1:32:A:GLY:H    | 20                  | 0.88     | 0.02                | 0.88       |
| (1,138)  | 1:10:A:ARG:HD2  | 1:11:A:PHE:HE2  | 20                  | 0.87     | 0.13                | 0.88       |
| (1,138)  | 1:10:A:ARG:HD3  | 1:11:A:PHE:HE2  | 20                  | 0.87     | 0.13                | 0.88       |
| (1,848)  | 1:31:A:LEU:HB2  | 1:76:A:VAL:HG23 | 20                  | 0.84     | 0.3                 | 0.84       |
| (1,324)  | 1:11:A:PHE:HE1  | 1:24:A:LEU:HG   | 20                  | 0.83     | 0.09                | 0.84       |
| (1,42)   | 1:62:A:PHE:HE2  | 1:67:A:PRO:HG3  | 20                  | 0.8      | 0.06                | 0.81       |
| (1,1295) | 1:60:A:ILE:HD12 | 1:63:A:CYS:H    | 20                  | 0.8      | 0.1                 | 0.77       |
| (1,1259) | 1:53:A:PHE:HD2  | 1:54:A:ILE:H    | 20                  | 0.8      | 0.03                | 0.8        |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,266)  | 1:12:A:ASP:H    | 1:19:A:ILE:HD13 | 20                  | 0.79     | 0.29                | 0.71       |
| (1,727)  | 1:5:A:GLU:H     | 1:60:A:ILE:HD13 | 20                  | 0.78     | 0.19                | 0.8        |
| (1,834)  | 1:31:A:LEU:HD13 | 1:31:A:LEU:HD22 | 20                  | 0.78     | 0.02                | 0.77       |
| (1,508)  | 1:42:A:MET:HB2  | 1:62:A:PHE:HE1  | 20                  | 0.77     | 0.1                 | 0.73       |
| (1,888)  | 1:46:A:ILE:HD12 | 1:62:A:PHE:H    | 20                  | 0.76     | 0.08                | 0.73       |
| (1,590)  | 1:11:A:PHE:HB2  | 1:11:A:PHE:HE1  | 20                  | 0.75     | 0.01                | 0.75       |
| (1,271)  | 1:19:A:ILE:HD11 | 1:54:A:ILE:HG13 | 20                  | 0.75     | 0.05                | 0.73       |
| (1,803)  | 1:62:A:PHE:HD2  | 1:70:A:MET:HG2  | 20                  | 0.73     | 0.08                | 0.72       |
| (1,184)  | 1:25:A:THR:HG22 | 1:40:A:GLN:HB2  | 20                  | 0.68     | 0.05                | 0.67       |
| (1,1333) | 1:69:A:LEU:HD21 | 1:70:A:MET:H    | 20                  | 0.67     | 0.14                | 0.68       |
| (1,74)   | 1:7:A:ILE:HD11  | 1:74:A:ALA:HB1  | 20                  | 0.64     | 0.04                | 0.64       |
| (1,74)   | 1:7:A:ILE:HD11  | 1:74:A:ALA:HB2  | 20                  | 0.64     | 0.04                | 0.64       |
| (1,610)  | 1:51:A:ASP:H    | 1:52:A:GLY:HA3  | 20                  | 0.64     | 0.01                | 0.64       |
| (1,853)  | 1:69:A:LEU:HB2  | 1:70:A:MET:HE3  | 20                  | 0.64     | 0.15                | 0.72       |
| (1,791)  | 1:67:A:PRO:HB2  | 1:69:A:LEU:HG   | 20                  | 0.6      | 0.1                 | 0.55       |
| (1,961)  | 1:60:A:ILE:H    | 1:60:A:ILE:HD12 | 20                  | 0.59     | 0.03                | 0.59       |
| (1,504)  | 1:25:A:THR:HG22 | 1:40:A:GLN:HG3  | 20                  | 0.59     | 0.06                | 0.58       |
| (1,319)  | 1:11:A:PHE:HD1  | 1:24:A:LEU:HB2  | 20                  | 0.59     | 0.08                | 0.6        |
| (1,700)  | 1:62:A:PHE:HA   | 1:62:A:PHE:HD2  | 20                  | 0.57     | 0.05                | 0.57       |
| (1,62)   | 1:7:A:ILE:HB    | 1:7:A:ILE:HD13  | 20                  | 0.52     | 0.02                | 0.52       |
| (1,277)  | 1:44:A:ALA:HA   | 1:50:A:GLY:H    | 20                  | 0.52     | 0.04                | 0.52       |
| (1,800)  | 1:62:A:PHE:HE2  | 1:70:A:MET:HG3  | 20                  | 0.52     | 0.08                | 0.53       |
| (1,652)  | 1:46:A:ILE:HB   | 1:54:A:ILE:HD13 | 20                  | 0.52     | 0.08                | 0.53       |
| (1,856)  | 1:70:A:MET:HG3  | 1:70:A:MET:HE3  | 20                  | 0.5      | 0.03                | 0.51       |
| (1,384)  | 1:28:A:LEU:H    | 1:28:A:LEU:HD21 | 20                  | 0.49     | 0.07                | 0.46       |
| (1,898)  | 1:25:A:THR:HG23 | 1:27:A:ALA:H    | 20                  | 0.48     | 0.02                | 0.48       |
| (1,1173) | 1:34:A:THR:HG23 | 1:35:A:SER:H    | 20                  | 0.46     | 0.17                | 0.4        |
| (1,801)  | 1:62:A:PHE:HD2  | 1:70:A:MET:HG3  | 20                  | 0.45     | 0.09                | 0.46       |
| (1,728)  | 1:60:A:ILE:HD12 | 1:61:A:SER:H    | 20                  | 0.44     | 0.1                 | 0.42       |
| (1,802)  | 1:62:A:PHE:HE2  | 1:70:A:MET:HG2  | 20                  | 0.44     | 0.08                | 0.42       |
| (1,235)  | 1:53:A:PHE:HB3  | 1:53:A:PHE:HD2  | 20                  | 0.43     | 0.04                | 0.4        |
| (1,235)  | 1:53:A:PHE:HB2  | 1:53:A:PHE:HD1  | 20                  | 0.43     | 0.04                | 0.4        |
| (1,313)  | 1:69:A:LEU:HB2  | 1:69:A:LEU:HD21 | 20                  | 0.42     | 0.11                | 0.48       |
| (1,370)  | 1:62:A:PHE:HD2  | 1:69:A:LEU:HB2  | 20                  | 0.42     | 0.06                | 0.4        |
| (1,370)  | 1:62:A:PHE:HD2  | 1:69:A:LEU:HB3  | 20                  | 0.42     | 0.06                | 0.4        |
| (1,411)  | 1:30:A:THR:HG22 | 1:31:A:LEU:HG   | 20                  | 0.42     | 0.3                 | 0.36       |
| (1,382)  | 1:24:A:LEU:HG   | 1:28:A:LEU:HG   | 20                  | 0.4      | 0.02                | 0.4        |
| (1,1293) | 1:60:A:ILE:HG21 | 1:63:A:CYS:H    | 20                  | 0.39     | 0.03                | 0.4        |
| (1,989)  | 1:46:A:ILE:HD11 | 1:59:A:PHE:H    | 20                  | 0.38     | 0.11                | 0.4        |
| (1,1253) | 1:53:A:PHE:H    | 1:53:A:PHE:HD1  | 20                  | 0.37     | 0.04                | 0.35       |
| (1,695)  | 1:46:A:ILE:HD11 | 1:58:A:GLU:HB3  | 20                  | 0.37     | 0.15                | 0.34       |
| (1,146)  | 1:11:A:PHE:HB2  | 1:11:A:PHE:HD1  | 20                  | 0.35     | 0.01                | 0.35       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,437)  | 1:36:A:ALA:HA   | 1:39:A:VAL:HB   | 20                  | 0.34     | 0.01                | 0.34       |
| (1,365)  | 1:28:A:LEU:HA   | 1:28:A:LEU:HD21 | 20                  | 0.31     | 0.07                | 0.29       |
| (1,433)  | 1:34:A:THR:HA   | 1:34:A:THR:HG23 | 20                  | 0.31     | 0.06                | 0.3        |
| (1,1528) | 1:51:A:ASP:H    | 1:52:A:GLY:HA2  | 20                  | 0.27     | 0.02                | 0.27       |
| (1,1528) | 1:51:A:ASP:H    | 1:52:A:GLY:HA3  | 20                  | 0.27     | 0.02                | 0.27       |
| (1,1530) | 1:52:A:GLY:HA2  | 1:53:A:PHE:H    | 20                  | 0.26     | 0.03                | 0.24       |
| (1,1530) | 1:52:A:GLY:HA3  | 1:53:A:PHE:H    | 20                  | 0.26     | 0.03                | 0.24       |
| (1,1125) | 1:21:A:LEU:HG   | 1:22:A:SER:H    | 20                  | 0.26     | 0.04                | 0.27       |
| (1,731)  | 1:60:A:ILE:HA   | 1:60:A:ILE:HD12 | 20                  | 0.24     | 0.06                | 0.22       |
| (1,1190) | 1:25:A:THR:HG22 | 1:40:A:GLN:H    | 20                  | 0.24     | 0.06                | 0.23       |
| (1,693)  | 1:46:A:ILE:HG21 | 1:58:A:GLU:HB3  | 20                  | 0.23     | 0.02                | 0.24       |
| (1,1010) | 1:42:A:MET:HG2  | 1:44:A:ALA:H    | 20                  | 0.22     | 0.02                | 0.22       |
| (1,787)  | 1:69:A:LEU:HA   | 1:69:A:LEU:HG   | 20                  | 0.21     | 0.03                | 0.22       |
| (1,479)  | 1:36:A:ALA:HA   | 1:39:A:VAL:HG23 | 20                  | 0.19     | 0.01                | 0.2        |
| (1,739)  | 1:62:A:PHE:HB3  | 1:62:A:PHE:HD2  | 20                  | 0.19     | 0.03                | 0.19       |
| (1,739)  | 1:62:A:PHE:HB2  | 1:62:A:PHE:HD1  | 20                  | 0.19     | 0.03                | 0.19       |
| (1,1192) | 1:40:A:GLN:HE22 | 1:41:A:ARG:H    | 20                  | 0.19     | 0.02                | 0.2        |
| (1,326)  | 1:24:A:LEU:HA   | 1:24:A:LEU:HG   | 20                  | 0.17     | 0.01                | 0.17       |
| (1,483)  | 1:37:A:ASP:HA   | 1:40:A:GLN:HA   | 20                  | 0.16     | 0.01                | 0.16       |
| (1,1453) | 1:23:A:GLU:HB2  | 1:27:A:ALA:HA   | 20                  | 0.15     | 0.02                | 0.15       |
| (1,1453) | 1:23:A:GLU:HB3  | 1:27:A:ALA:HA   | 20                  | 0.15     | 0.02                | 0.15       |
| (1,357)  | 1:30:A:THR:HG22 | 1:31:A:LEU:HA   | 19                  | 1.46     | 0.11                | 1.48       |
| (1,268)  | 1:19:A:ILE:HD11 | 1:59:A:PHE:HD2  | 19                  | 0.45     | 0.2                 | 0.32       |
| (1,72)   | 1:7:A:ILE:HA    | 1:7:A:ILE:HD13  | 19                  | 0.33     | 0.02                | 0.33       |
| (1,1262) | 1:53:A:PHE:HB2  | 1:54:A:ILE:H    | 19                  | 0.18     | 0.03                | 0.18       |
| (1,401)  | 1:30:A:THR:HB   | 1:31:A:LEU:HD21 | 18                  | 0.49     | 0.1                 | 0.5        |
| (1,417)  | 1:28:A:LEU:HD22 | 1:33:A:SER:HA   | 18                  | 0.35     | 0.18                | 0.29       |
| (1,1238) | 1:48:A:THR:H    | 1:48:A:THR:HG22 | 18                  | 0.33     | 0.04                | 0.34       |
| (1,70)   | 1:7:A:ILE:HD12  | 1:77:A:PHE:HD2  | 17                  | 1.6      | 1.26                | 1.31       |
| (1,611)  | 1:52:A:GLY:HA3  | 1:53:A:PHE:HD1  | 17                  | 0.2      | 0.04                | 0.19       |
| (1,611)  | 1:52:A:GLY:HA2  | 1:53:A:PHE:HD1  | 17                  | 0.2      | 0.04                | 0.19       |
| (1,1052) | 1:7:A:ILE:HD13  | 1:8:A:PHE:H     | 17                  | 0.17     | 0.03                | 0.18       |
| (1,1519) | 1:49:A:ASP:H    | 1:49:A:ASP:HB2  | 17                  | 0.13     | 0.02                | 0.12       |
| (1,1519) | 1:49:A:ASP:H    | 1:49:A:ASP:HB3  | 17                  | 0.13     | 0.02                | 0.12       |
| (1,329)  | 1:21:A:LEU:HA   | 1:24:A:LEU:HD12 | 17                  | 0.12     | 0.02                | 0.12       |
| (1,285)  | 1:31:A:LEU:HB2  | 1:31:A:LEU:HD21 | 17                  | 0.12     | 0.01                | 0.12       |
| (1,850)  | 1:31:A:LEU:HB3  | 1:76:A:VAL:HG23 | 16                  | 0.65     | 0.34                | 0.6        |
| (1,1472) | 1:34:A:THR:HG23 | 1:35:A:SER:HB2  | 16                  | 0.37     | 0.17                | 0.26       |
| (1,1472) | 1:34:A:THR:HG23 | 1:35:A:SER:HB3  | 16                  | 0.37     | 0.17                | 0.26       |
| (1,866)  | 1:4:A:MET:HE3   | 1:7:A:ILE:HD11  | 16                  | 0.31     | 0.19                | 0.26       |
| (1,866)  | 1:4:A:MET:HE3   | 1:7:A:ILE:HD13  | 16                  | 0.31     | 0.19                | 0.26       |
| (1,762)  | 1:60:A:ILE:HG12 | 1:63:A:CYS:HB3  | 16                  | 0.13     | 0.02                | 0.12       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,170)  | 1:48:A:THR:HB   | 1:49:A:ASP:H    | 16                  | 0.13     | 0.04                | 0.11       |
| (1,1193) | 1:37:A:ASP:H    | 1:40:A:GLN:HE21 | 16                  | 0.11     | 0.01                | 0.11       |
| (1,472)  | 1:62:A:PHE:HE2  | 1:69:A:LEU:HD21 | 15                  | 0.65     | 0.2                 | 0.75       |
| (1,1168) | 1:28:A:LEU:HD21 | 1:33:A:SER:H    | 15                  | 0.35     | 0.15                | 0.3        |
| (1,1510) | 1:46:A:ILE:HG21 | 1:58:A:GLU:HG2  | 15                  | 0.13     | 0.02                | 0.13       |
| (1,1510) | 1:46:A:ILE:HG21 | 1:58:A:GLU:HG3  | 15                  | 0.13     | 0.02                | 0.13       |
| (1,988)  | 1:34:A:THR:H    | 1:34:A:THR:HG23 | 14                  | 0.2      | 0.06                | 0.2        |
| (1,1575) | 1:72:A:ASP:HB2  | 1:73:A:VAL:HG22 | 13                  | 0.79     | 0.32                | 0.62       |
| (1,1575) | 1:72:A:ASP:HB3  | 1:73:A:VAL:HG22 | 13                  | 0.79     | 0.32                | 0.62       |
| (1,847)  | 1:76:A:VAL:HA   | 1:76:A:VAL:HG21 | 13                  | 0.15     | 0.0                 | 0.15       |
| (1,1114) | 1:20:A:SER:H    | 1:22:A:SER:H    | 13                  | 0.12     | 0.01                | 0.12       |
| (1,387)  | 1:24:A:LEU:HD22 | 1:28:A:LEU:HD23 | 12                  | 0.45     | 0.05                | 0.46       |
| (1,998)  | 1:24:A:LEU:H    | 1:24:A:LEU:HD21 | 12                  | 0.31     | 0.0                 | 0.31       |
| (1,307)  | 1:24:A:LEU:HA   | 1:24:A:LEU:HD21 | 12                  | 0.21     | 0.0                 | 0.21       |
| (1,338)  | 1:24:A:LEU:HB3  | 1:24:A:LEU:HD21 | 12                  | 0.19     | 0.0                 | 0.19       |
| (1,734)  | 1:60:A:ILE:HB   | 1:60:A:ILE:HD12 | 12                  | 0.17     | 0.05                | 0.17       |
| (1,952)  | 1:54:A:ILE:HG21 | 1:55:A:ASP:H    | 11                  | 0.15     | 0.03                | 0.16       |
| (1,16)   | 1:42:A:MET:HG2  | 1:62:A:PHE:HE1  | 10                  | 0.3      | 0.18                | 0.22       |
| (1,539)  | 1:43:A:MET:HB3  | 1:45:A:GLU:H    | 10                  | 0.11     | 0.01                | 0.11       |
| (1,501)  | 1:42:A:MET:HB3  | 1:62:A:PHE:HD1  | 9                   | 0.21     | 0.11                | 0.16       |
| (1,320)  | 1:11:A:PHE:HE1  | 1:24:A:LEU:HB2  | 9                   | 0.18     | 0.03                | 0.17       |
| (1,125)  | 1:21:A:LEU:HA   | 1:24:A:LEU:HB2  | 9                   | 0.11     | 0.01                | 0.11       |
| (1,1135) | 1:25:A:THR:H    | 1:43:A:MET:HE3  | 8                   | 0.5      | 0.37                | 0.29       |
| (1,332)  | 1:24:A:LEU:HD22 | 1:27:A:ALA:H    | 8                   | 0.29     | 0.01                | 0.29       |
| (1,337)  | 1:24:A:LEU:HD22 | 1:27:A:ALA:HB1  | 8                   | 0.26     | 0.01                | 0.26       |
| (1,999)  | 1:24:A:LEU:H    | 1:24:A:LEU:HD22 | 8                   | 0.24     | 0.01                | 0.24       |
| (1,321)  | 1:24:A:LEU:HB2  | 1:24:A:LEU:HD21 | 8                   | 0.18     | 0.01                | 0.18       |
| (1,861)  | 1:4:A:MET:H     | 1:4:A:MET:HE3   | 7                   | 0.73     | 0.33                | 0.54       |
| (1,572)  | 1:46:A:ILE:HG22 | 1:62:A:PHE:HD1  | 7                   | 0.18     | 0.05                | 0.17       |
| (1,572)  | 1:46:A:ILE:HG23 | 1:62:A:PHE:HD1  | 7                   | 0.18     | 0.05                | 0.17       |
| (1,1280) | 1:57:A:ASN:HD21 | 1:58:A:GLU:H    | 7                   | 0.12     | 0.01                | 0.12       |
| (1,377)  | 1:28:A:LEU:HB3  | 1:36:A:ALA:H    | 7                   | 0.12     | 0.03                | 0.11       |
| (1,7)    | 1:3:A:ASP:HB2   | 1:4:A:MET:HE3   | 6                   | 0.38     | 0.21                | 0.29       |
| (1,7)    | 1:3:A:ASP:HB3   | 1:4:A:MET:HE3   | 6                   | 0.38     | 0.21                | 0.29       |
| (1,875)  | 1:7:A:ILE:HD12  | 1:77:A:PHE:H    | 6                   | 0.26     | 0.11                | 0.28       |
| (1,548)  | 1:43:A:MET:HG2  | 1:44:A:ALA:HA   | 6                   | 0.13     | 0.01                | 0.12       |
| (1,841)  | 1:72:A:ASP:H    | 1:74:A:ALA:HB3  | 6                   | 0.12     | 0.02                | 0.11       |
| (1,904)  | 1:25:A:THR:HA   | 1:27:A:ALA:H    | 6                   | 0.11     | 0.01                | 0.11       |
| (1,376)  | 1:68:A:GLY:H    | 1:69:A:LEU:HB2  | 5                   | 0.12     | 0.02                | 0.11       |
| (1,833)  | 1:71:A:LYS:HA   | 1:73:A:VAL:HB   | 5                   | 0.12     | 0.01                | 0.13       |
| (1,575)  | 1:46:A:ILE:HD11 | 1:62:A:PHE:H    | 5                   | 0.12     | 0.01                | 0.12       |
| (1,61)   | 1:7:A:ILE:HB    | 1:77:A:PHE:HD2  | 4                   | 2.21     | 0.01                | 2.2        |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1395) | 1:7:A:ILE:HG12  | 1:77:A:PHE:HD2  | 4                   | 0.47     | 0.03                | 0.47       |
| (1,1395) | 1:7:A:ILE:HG13  | 1:77:A:PHE:HD2  | 4                   | 0.47     | 0.03                | 0.47       |
| (1,1537) | 1:55:A:ASP:HA   | 1:55:A:ASP:HB2  | 4                   | 0.23     | 0.0                 | 0.23       |
| (1,1537) | 1:55:A:ASP:HA   | 1:55:A:ASP:HB3  | 4                   | 0.23     | 0.0                 | 0.23       |
| (1,665)  | 1:55:A:ASP:HB2  | 1:56:A:PHE:H    | 4                   | 0.16     | 0.01                | 0.16       |
| (1,1490) | 1:39:A:VAL:H    | 1:41:A:ARG:HD2  | 4                   | 0.12     | 0.01                | 0.12       |
| (1,1490) | 1:39:A:VAL:H    | 1:41:A:ARG:HD3  | 4                   | 0.12     | 0.01                | 0.12       |
| (1,1417) | 1:18:A:LYS:HA   | 1:55:A:ASP:HB2  | 4                   | 0.12     | 0.02                | 0.11       |
| (1,1417) | 1:18:A:LYS:HA   | 1:55:A:ASP:HB3  | 4                   | 0.12     | 0.02                | 0.11       |
| (1,1022) | 1:31:A:LEU:H    | 1:31:A:LEU:HD21 | 3                   | 0.2      | 0.04                | 0.22       |
| (1,880)  | 1:77:A:PHE:H    | 1:77:A:PHE:HB3  | 3                   | 0.16     | 0.01                | 0.16       |
| (1,1239) | 1:21:A:LEU:HD22 | 1:48:A:THR:H    | 3                   | 0.15     | 0.05                | 0.12       |
| (1,1239) | 1:21:A:LEU:HD23 | 1:48:A:THR:H    | 3                   | 0.15     | 0.05                | 0.12       |
| (1,654)  | 1:19:A:ILE:HD11 | 1:54:A:ILE:HD12 | 3                   | 0.14     | 0.02                | 0.13       |
| (1,1285) | 1:46:A:ILE:HD12 | 1:61:A:SER:H    | 3                   | 0.13     | 0.02                | 0.14       |
| (1,1385) | 1:6:A:ARG:HB3   | 1:6:A:ARG:HD2   | 3                   | 0.12     | 0.0                 | 0.12       |
| (1,1385) | 1:6:A:ARG:HB3   | 1:6:A:ARG:HD3   | 3                   | 0.12     | 0.0                 | 0.12       |
| (1,487)  | 1:40:A:GLN:HA   | 1:44:A:ALA:HB2  | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,629)  | 1:8:A:PHE:HE1   | 1:54:A:ILE:HB   | 2                   | 3.38     | 0.05                | 3.38       |
| (1,107)  | 1:8:A:PHE:HE1   | 1:54:A:ILE:HG13 | 2                   | 2.88     | 0.09                | 2.88       |
| (1,251)  | 1:8:A:PHE:HE1   | 1:19:A:ILE:HG13 | 2                   | 2.84     | 0.06                | 2.84       |
| (1,981)  | 1:8:A:PHE:HE1   | 1:59:A:PHE:H    | 2                   | 2.64     | 0.04                | 2.64       |
| (1,159)  | 1:8:A:PHE:HD2   | 1:12:A:ASP:HB3  | 2                   | 2.4      | 0.31                | 2.4        |
| (1,93)   | 1:8:A:PHE:HE2   | 1:9:A:LYS:HA    | 2                   | 2.22     | 0.01                | 2.22       |
| (1,95)   | 1:8:A:PHE:HD2   | 1:9:A:LYS:HA    | 2                   | 2.22     | 0.01                | 2.22       |
| (1,112)  | 1:8:A:PHE:HD2   | 1:9:A:LYS:HD2   | 2                   | 2.05     | 0.51                | 2.05       |
| (1,112)  | 1:8:A:PHE:HD2   | 1:9:A:LYS:HD3   | 2                   | 2.05     | 0.51                | 2.05       |
| (1,669)  | 1:8:A:PHE:HE1   | 1:56:A:PHE:HA   | 2                   | 1.96     | 0.01                | 1.96       |
| (1,647)  | 1:8:A:PHE:HD1   | 1:54:A:ILE:HD12 | 2                   | 1.92     | 0.03                | 1.92       |
| (1,647)  | 1:8:A:PHE:HD1   | 1:54:A:ILE:HD13 | 2                   | 1.92     | 0.03                | 1.92       |
| (1,269)  | 1:8:A:PHE:HD1   | 1:19:A:ILE:HD11 | 2                   | 1.66     | 0.04                | 1.66       |
| (1,269)  | 1:8:A:PHE:HD1   | 1:19:A:ILE:HD13 | 2                   | 1.66     | 0.04                | 1.66       |
| (1,1056) | 1:8:A:PHE:HD2   | 1:9:A:LYS:H     | 2                   | 1.66     | 0.01                | 1.66       |
| (1,222)  | 1:8:A:PHE:HE1   | 1:19:A:ILE:HG12 | 2                   | 1.56     | 0.06                | 1.56       |
| (1,670)  | 1:8:A:PHE:HD1   | 1:56:A:PHE:HA   | 2                   | 1.55     | 0.01                | 1.55       |
| (1,658)  | 1:8:A:PHE:HE1   | 1:55:A:ASP:HA   | 2                   | 1.5      | 0.05                | 1.5        |
| (1,1064) | 1:8:A:PHE:HD2   | 1:10:A:ARG:H    | 2                   | 1.42     | 0.03                | 1.42       |
| (1,161)  | 1:8:A:PHE:HE2   | 1:12:A:ASP:HB2  | 2                   | 1.27     | 0.29                | 1.27       |
| (1,412)  | 1:30:A:THR:HG22 | 1:31:A:LEU:HD22 | 2                   | 0.96     | 0.56                | 0.96       |
| (1,1108) | 1:8:A:PHE:HE1   | 1:19:A:ILE:H    | 2                   | 0.91     | 0.08                | 0.91       |
| (1,78)   | 1:8:A:PHE:HA    | 1:8:A:PHE:HD1   | 2                   | 0.68     | 0.0                 | 0.68       |
| (1,759)  | 1:4:A:MET:HE2   | 1:63:A:CYS:HB3  | 2                   | 0.6      | 0.03                | 0.6        |

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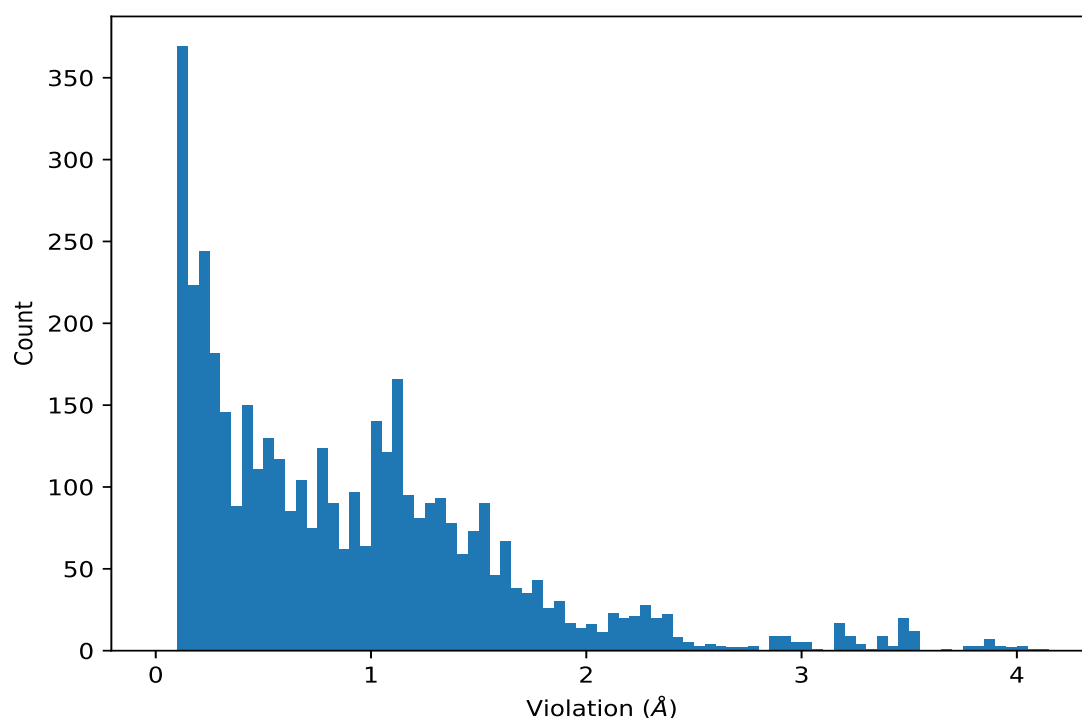
| Key      | Atom-1         | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,676)  | 1:8:A:PHE:HE1  | 1:56:A:PHE:HB2  | 2                   | 0.56     | 0.01                | 0.56       |
| (1,199)  | 1:8:A:PHE:HE1  | 1:18:A:LYS:HA   | 2                   | 0.34     | 0.11                | 0.34       |
| (1,82)   | 1:8:A:PHE:HA   | 1:19:A:ILE:HD13 | 2                   | 0.29     | 0.12                | 0.29       |
| (1,257)  | 1:8:A:PHE:HE1  | 1:19:A:ILE:HG23 | 2                   | 0.2      | 0.08                | 0.2        |
| (1,1365) | 1:4:A:MET:H    | 1:4:A:MET:HG2   | 2                   | 0.2      | 0.01                | 0.2        |
| (1,1365) | 1:4:A:MET:H    | 1:4:A:MET:HG3   | 2                   | 0.2      | 0.01                | 0.2        |
| (1,89)   | 1:8:A:PHE:HB2  | 1:8:A:PHE:HD1   | 2                   | 0.16     | 0.0                 | 0.16       |
| (1,89)   | 1:8:A:PHE:HB3  | 1:8:A:PHE:HD2   | 2                   | 0.16     | 0.0                 | 0.16       |
| (1,113)  | 1:29:A:ARG:H   | 1:29:A:ARG:HG3  | 2                   | 0.14     | 0.02                | 0.14       |
| (1,244)  | 1:35:A:SER:HA  | 1:39:A:VAL:HG13 | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,1240) | 1:49:A:ASP:H   | 1:49:A:ASP:HB3  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1445) | 1:22:A:SER:HB2 | 1:26:A:ASP:HB2  | 2                   | 0.1      | 0.0                 | 0.1        |
| (1,1445) | 1:22:A:SER:HB2 | 1:26:A:ASP:HB3  | 2                   | 0.1      | 0.0                 | 0.1        |
| (1,1445) | 1:22:A:SER:HB3 | 1:26:A:ASP:HB2  | 2                   | 0.1      | 0.0                 | 0.1        |
| (1,1445) | 1:22:A:SER:HB3 | 1:26:A:ASP:HB3  | 2                   | 0.1      | 0.0                 | 0.1        |

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

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

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

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



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

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

| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,267) | 1:11:A:PHE:HD1 | 1:19:A:ILE:HD12 | 7        | 4.13          |
| (1,267) | 1:11:A:PHE:HD1 | 1:19:A:ILE:HD12 | 10       | 4.05          |
| (1,267) | 1:11:A:PHE:HD1 | 1:19:A:ILE:HD12 | 19       | 4.04          |
| (1,267) | 1:11:A:PHE:HD1 | 1:19:A:ILE:HD12 | 15       | 4.02          |
| (1,267) | 1:11:A:PHE:HD1 | 1:19:A:ILE:HD12 | 3        | 4.0           |
| (1,267) | 1:11:A:PHE:HD1 | 1:19:A:ILE:HD12 | 4        | 3.99          |
| (1,267) | 1:11:A:PHE:HD1 | 1:19:A:ILE:HD12 | 20       | 3.95          |
| (1,267) | 1:11:A:PHE:HD1 | 1:19:A:ILE:HD12 | 9        | 3.94          |
| (1,267) | 1:11:A:PHE:HD1 | 1:19:A:ILE:HD12 | 17       | 3.94          |
| (1,267) | 1:11:A:PHE:HD1 | 1:19:A:ILE:HD12 | 5        | 3.93          |
| (1,267) | 1:11:A:PHE:HD1 | 1:19:A:ILE:HD12 | 1        | 3.9           |
| (1,267) | 1:11:A:PHE:HD1 | 1:19:A:ILE:HD12 | 6        | 3.9           |
| (1,267) | 1:11:A:PHE:HD1 | 1:19:A:ILE:HD12 | 14       | 3.89          |
| (1,267) | 1:11:A:PHE:HD1 | 1:19:A:ILE:HD12 | 2        | 3.88          |
| (1,267) | 1:11:A:PHE:HD1 | 1:19:A:ILE:HD12 | 11       | 3.87          |
| (1,267) | 1:11:A:PHE:HD1 | 1:19:A:ILE:HD12 | 16       | 3.87          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,267) | 1:11:A:PHE:HD1 | 1:19:A:ILE:HD12 | 8        | 3.86          |
| (1,267) | 1:11:A:PHE:HD1 | 1:19:A:ILE:HD12 | 13       | 3.82          |
| (1,267) | 1:11:A:PHE:HD1 | 1:19:A:ILE:HD12 | 18       | 3.82          |
| (1,70)  | 1:7:A:ILE:HD12 | 1:77:A:PHE:HD2  | 4        | 3.82          |
| (1,70)  | 1:7:A:ILE:HD12 | 1:77:A:PHE:HD2  | 20       | 3.8           |
| (1,267) | 1:11:A:PHE:HD1 | 1:19:A:ILE:HD12 | 12       | 3.78          |
| (1,70)  | 1:7:A:ILE:HD12 | 1:77:A:PHE:HD2  | 14       | 3.76          |
| (1,70)  | 1:7:A:ILE:HD12 | 1:77:A:PHE:HD2  | 17       | 3.67          |
| (1,544) | 1:43:A:MET:HG3 | 1:62:A:PHE:HD1  | 13       | 3.55          |
| (1,544) | 1:43:A:MET:HG3 | 1:62:A:PHE:HD1  | 14       | 3.54          |
| (1,780) | 1:62:A:PHE:HD2 | 1:67:A:PRO:HD2  | 8        | 3.52          |
| (1,780) | 1:62:A:PHE:HD2 | 1:67:A:PRO:HD2  | 14       | 3.52          |
| (1,780) | 1:62:A:PHE:HD2 | 1:67:A:PRO:HD2  | 16       | 3.52          |
| (1,780) | 1:62:A:PHE:HD2 | 1:67:A:PRO:HD2  | 18       | 3.52          |
| (1,546) | 1:43:A:MET:HG2 | 1:62:A:PHE:HD1  | 3        | 3.52          |
| (1,546) | 1:43:A:MET:HG2 | 1:62:A:PHE:HD1  | 19       | 3.52          |
| (1,546) | 1:43:A:MET:HG2 | 1:62:A:PHE:HD1  | 4        | 3.51          |
| (1,546) | 1:43:A:MET:HG2 | 1:62:A:PHE:HD1  | 7        | 3.51          |
| (1,780) | 1:62:A:PHE:HD2 | 1:67:A:PRO:HD2  | 1        | 3.5           |
| (1,544) | 1:43:A:MET:HG3 | 1:62:A:PHE:HD1  | 12       | 3.5           |
| (1,780) | 1:62:A:PHE:HD2 | 1:67:A:PRO:HD2  | 5        | 3.49          |
| (1,780) | 1:62:A:PHE:HD2 | 1:67:A:PRO:HD2  | 11       | 3.49          |
| (1,780) | 1:62:A:PHE:HD2 | 1:67:A:PRO:HD2  | 12       | 3.49          |
| (1,780) | 1:62:A:PHE:HD2 | 1:67:A:PRO:HD2  | 17       | 3.49          |
| (1,780) | 1:62:A:PHE:HD2 | 1:67:A:PRO:HD2  | 20       | 3.49          |
| (1,546) | 1:43:A:MET:HG2 | 1:62:A:PHE:HD1  | 2        | 3.49          |
| (1,546) | 1:43:A:MET:HG2 | 1:62:A:PHE:HD1  | 8        | 3.48          |
| (1,780) | 1:62:A:PHE:HD2 | 1:67:A:PRO:HD2  | 3        | 3.47          |
| (1,780) | 1:62:A:PHE:HD2 | 1:67:A:PRO:HD2  | 4        | 3.47          |
| (1,780) | 1:62:A:PHE:HD2 | 1:67:A:PRO:HD2  | 6        | 3.47          |
| (1,780) | 1:62:A:PHE:HD2 | 1:67:A:PRO:HD2  | 13       | 3.47          |
| (1,546) | 1:43:A:MET:HG2 | 1:62:A:PHE:HD1  | 6        | 3.47          |
| (1,546) | 1:43:A:MET:HG2 | 1:62:A:PHE:HD1  | 20       | 3.46          |
| (1,544) | 1:43:A:MET:HG3 | 1:62:A:PHE:HD1  | 18       | 3.46          |
| (1,780) | 1:62:A:PHE:HD2 | 1:67:A:PRO:HD2  | 7        | 3.45          |
| (1,780) | 1:62:A:PHE:HD2 | 1:67:A:PRO:HD2  | 9        | 3.45          |
| (1,780) | 1:62:A:PHE:HD2 | 1:67:A:PRO:HD2  | 10       | 3.45          |
| (1,780) | 1:62:A:PHE:HD2 | 1:67:A:PRO:HD2  | 15       | 3.45          |
| (1,780) | 1:62:A:PHE:HD2 | 1:67:A:PRO:HD2  | 19       | 3.45          |
| (1,546) | 1:43:A:MET:HG2 | 1:62:A:PHE:HD1  | 18       | 3.45          |
| (1,780) | 1:62:A:PHE:HD2 | 1:67:A:PRO:HD2  | 2        | 3.44          |
| (1,544) | 1:43:A:MET:HG3 | 1:62:A:PHE:HD1  | 5        | 3.44          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,629) | 1:8:A:PHE:HE1  | 1:54:A:ILE:HB  | 6        | 3.43          |
| (1,546) | 1:43:A:MET:HG2 | 1:62:A:PHE:HD1 | 11       | 3.4           |
| (1,546) | 1:43:A:MET:HG2 | 1:62:A:PHE:HD1 | 14       | 3.4           |
| (1,546) | 1:43:A:MET:HG2 | 1:62:A:PHE:HD1 | 10       | 3.39          |
| (1,546) | 1:43:A:MET:HG2 | 1:62:A:PHE:HD1 | 16       | 3.39          |
| (1,546) | 1:43:A:MET:HG2 | 1:62:A:PHE:HD1 | 1        | 3.38          |
| (1,546) | 1:43:A:MET:HG2 | 1:62:A:PHE:HD1 | 9        | 3.37          |
| (1,544) | 1:43:A:MET:HG3 | 1:62:A:PHE:HD1 | 1        | 3.37          |
| (1,546) | 1:43:A:MET:HG2 | 1:62:A:PHE:HD1 | 15       | 3.36          |
| (1,546) | 1:43:A:MET:HG2 | 1:62:A:PHE:HD1 | 17       | 3.36          |
| (1,629) | 1:8:A:PHE:HE1  | 1:54:A:ILE:HB  | 4        | 3.33          |
| (1,544) | 1:43:A:MET:HG3 | 1:62:A:PHE:HD1 | 15       | 3.28          |
| (1,544) | 1:43:A:MET:HG3 | 1:62:A:PHE:HD1 | 17       | 3.27          |
| (1,544) | 1:43:A:MET:HG3 | 1:62:A:PHE:HD1 | 9        | 3.26          |
| (1,544) | 1:43:A:MET:HG3 | 1:62:A:PHE:HD1 | 16       | 3.26          |
| (1,546) | 1:43:A:MET:HG2 | 1:62:A:PHE:HD1 | 12       | 3.23          |
| (1,544) | 1:43:A:MET:HG3 | 1:62:A:PHE:HD1 | 10       | 3.23          |
| (1,546) | 1:43:A:MET:HG2 | 1:62:A:PHE:HD1 | 5        | 3.22          |
| (1,747) | 1:62:A:PHE:HD2 | 1:63:A:CYS:HA  | 1        | 3.21          |
| (1,747) | 1:62:A:PHE:HD2 | 1:63:A:CYS:HA  | 6        | 3.2           |
| (1,747) | 1:62:A:PHE:HD2 | 1:63:A:CYS:HA  | 12       | 3.2           |
| (1,747) | 1:62:A:PHE:HD2 | 1:63:A:CYS:HA  | 14       | 3.2           |
| (1,546) | 1:43:A:MET:HG2 | 1:62:A:PHE:HD1 | 13       | 3.2           |
| (1,544) | 1:43:A:MET:HG3 | 1:62:A:PHE:HD1 | 11       | 3.2           |
| (1,747) | 1:62:A:PHE:HD2 | 1:63:A:CYS:HA  | 4        | 3.19          |
| (1,747) | 1:62:A:PHE:HD2 | 1:63:A:CYS:HA  | 16       | 3.19          |
| (1,747) | 1:62:A:PHE:HD2 | 1:63:A:CYS:HA  | 17       | 3.19          |
| (1,747) | 1:62:A:PHE:HD2 | 1:63:A:CYS:HA  | 18       | 3.19          |
| (1,747) | 1:62:A:PHE:HD2 | 1:63:A:CYS:HA  | 20       | 3.19          |
| (1,747) | 1:62:A:PHE:HD2 | 1:63:A:CYS:HA  | 2        | 3.18          |
| (1,747) | 1:62:A:PHE:HD2 | 1:63:A:CYS:HA  | 5        | 3.18          |
| (1,747) | 1:62:A:PHE:HD2 | 1:63:A:CYS:HA  | 7        | 3.18          |
| (1,747) | 1:62:A:PHE:HD2 | 1:63:A:CYS:HA  | 9        | 3.18          |
| (1,747) | 1:62:A:PHE:HD2 | 1:63:A:CYS:HA  | 11       | 3.18          |
| (1,747) | 1:62:A:PHE:HD2 | 1:63:A:CYS:HA  | 13       | 3.18          |
| (1,747) | 1:62:A:PHE:HD2 | 1:63:A:CYS:HA  | 3        | 3.17          |
| (1,747) | 1:62:A:PHE:HD2 | 1:63:A:CYS:HA  | 8        | 3.17          |
| (1,747) | 1:62:A:PHE:HD2 | 1:63:A:CYS:HA  | 10       | 3.17          |
| (1,747) | 1:62:A:PHE:HD2 | 1:63:A:CYS:HA  | 15       | 3.17          |
| (1,747) | 1:62:A:PHE:HD2 | 1:63:A:CYS:HA  | 19       | 3.17          |
| (1,544) | 1:43:A:MET:HG3 | 1:62:A:PHE:HD1 | 6        | 3.17          |
| (1,544) | 1:43:A:MET:HG3 | 1:62:A:PHE:HD1 | 4        | 3.09          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,544) | 1:43:A:MET:HG3 | 1:62:A:PHE:HD1  | 8        | 3.05          |
| (1,544) | 1:43:A:MET:HG3 | 1:62:A:PHE:HD1  | 2        | 3.04          |
| (1,544) | 1:43:A:MET:HG3 | 1:62:A:PHE:HD1  | 3        | 3.04          |
| (1,544) | 1:43:A:MET:HG3 | 1:62:A:PHE:HD1  | 20       | 3.03          |
| (1,544) | 1:43:A:MET:HG3 | 1:62:A:PHE:HD1  | 19       | 3.02          |
| (1,544) | 1:43:A:MET:HG3 | 1:62:A:PHE:HD1  | 7        | 2.99          |
| (1,919) | 1:62:A:PHE:HE2 | 1:69:A:LEU:H    | 5        | 2.97          |
| (1,919) | 1:62:A:PHE:HE2 | 1:69:A:LEU:H    | 20       | 2.97          |
| (1,107) | 1:8:A:PHE:HE1  | 1:54:A:ILE:HG13 | 6        | 2.97          |
| (1,919) | 1:62:A:PHE:HE2 | 1:69:A:LEU:H    | 10       | 2.95          |
| (1,919) | 1:62:A:PHE:HE2 | 1:69:A:LEU:H    | 7        | 2.94          |
| (1,919) | 1:62:A:PHE:HE2 | 1:69:A:LEU:H    | 19       | 2.94          |
| (1,919) | 1:62:A:PHE:HE2 | 1:69:A:LEU:H    | 15       | 2.93          |
| (1,919) | 1:62:A:PHE:HE2 | 1:69:A:LEU:H    | 4        | 2.92          |
| (1,919) | 1:62:A:PHE:HE2 | 1:69:A:LEU:H    | 11       | 2.92          |
| (1,919) | 1:62:A:PHE:HE2 | 1:69:A:LEU:H    | 1        | 2.91          |
| (1,919) | 1:62:A:PHE:HE2 | 1:69:A:LEU:H    | 6        | 2.91          |
| (1,919) | 1:62:A:PHE:HE2 | 1:69:A:LEU:H    | 14       | 2.91          |
| (1,919) | 1:62:A:PHE:HE2 | 1:69:A:LEU:H    | 17       | 2.91          |
| (1,251) | 1:8:A:PHE:HE1  | 1:19:A:ILE:HG13 | 6        | 2.9           |
| (1,919) | 1:62:A:PHE:HE2 | 1:69:A:LEU:H    | 2        | 2.89          |
| (1,919) | 1:62:A:PHE:HE2 | 1:69:A:LEU:H    | 3        | 2.89          |
| (1,919) | 1:62:A:PHE:HE2 | 1:69:A:LEU:H    | 12       | 2.89          |
| (1,919) | 1:62:A:PHE:HE2 | 1:69:A:LEU:H    | 18       | 2.89          |
| (1,919) | 1:62:A:PHE:HE2 | 1:69:A:LEU:H    | 9        | 2.88          |
| (1,919) | 1:62:A:PHE:HE2 | 1:69:A:LEU:H    | 13       | 2.87          |
| (1,919) | 1:62:A:PHE:HE2 | 1:69:A:LEU:H    | 8        | 2.86          |
| (1,919) | 1:62:A:PHE:HE2 | 1:69:A:LEU:H    | 16       | 2.86          |
| (1,107) | 1:8:A:PHE:HE1  | 1:54:A:ILE:HG13 | 4        | 2.79          |
| (1,251) | 1:8:A:PHE:HE1  | 1:19:A:ILE:HG13 | 4        | 2.78          |
| (1,545) | 1:43:A:MET:HG3 | 1:62:A:PHE:HE1  | 13       | 2.75          |
| (1,545) | 1:43:A:MET:HG3 | 1:62:A:PHE:HE1  | 14       | 2.73          |
| (1,159) | 1:8:A:PHE:HD2  | 1:12:A:ASP:HB3  | 6        | 2.7           |
| (1,981) | 1:8:A:PHE:HE1  | 1:59:A:PHE:H    | 6        | 2.69          |
| (1,545) | 1:43:A:MET:HG3 | 1:62:A:PHE:HE1  | 12       | 2.66          |
| (1,131) | 1:10:A:ARG:HG3 | 1:11:A:PHE:HE2  | 13       | 2.65          |
| (1,545) | 1:43:A:MET:HG3 | 1:62:A:PHE:HE1  | 18       | 2.61          |
| (1,981) | 1:8:A:PHE:HE1  | 1:59:A:PHE:H    | 4        | 2.6           |
| (1,545) | 1:43:A:MET:HG3 | 1:62:A:PHE:HE1  | 5        | 2.58          |
| (1,112) | 1:8:A:PHE:HD2  | 1:9:A:LYS:HD2   | 4        | 2.57          |
| (1,112) | 1:8:A:PHE:HD2  | 1:9:A:LYS:HD3   | 4        | 2.57          |
| (1,129) | 1:10:A:ARG:HG2 | 1:11:A:PHE:HE2  | 9        | 2.56          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,137)  | 1:10:A:ARG:HD2 | 1:11:A:PHE:HD2  | 6        | 2.52          |
| (1,131)  | 1:10:A:ARG:HG3 | 1:11:A:PHE:HE2  | 11       | 2.51          |
| (1,129)  | 1:10:A:ARG:HG2 | 1:11:A:PHE:HE2  | 19       | 2.5           |
| (1,131)  | 1:10:A:ARG:HG3 | 1:11:A:PHE:HE2  | 18       | 2.49          |
| (1,545)  | 1:43:A:MET:HG3 | 1:62:A:PHE:HE1  | 1        | 2.47          |
| (1,131)  | 1:10:A:ARG:HG3 | 1:11:A:PHE:HE2  | 1        | 2.46          |
| (1,131)  | 1:10:A:ARG:HG3 | 1:11:A:PHE:HE2  | 5        | 2.46          |
| (1,137)  | 1:10:A:ARG:HD2 | 1:11:A:PHE:HD2  | 17       | 2.45          |
| (1,131)  | 1:10:A:ARG:HG3 | 1:11:A:PHE:HE2  | 7        | 2.44          |
| (1,129)  | 1:10:A:ARG:HG2 | 1:11:A:PHE:HE2  | 12       | 2.43          |
| (1,538)  | 1:43:A:MET:HB2 | 1:62:A:PHE:HE1  | 14       | 2.42          |
| (1,131)  | 1:10:A:ARG:HG3 | 1:11:A:PHE:HE2  | 2        | 2.42          |
| (1,131)  | 1:10:A:ARG:HG3 | 1:11:A:PHE:HE2  | 3        | 2.42          |
| (1,538)  | 1:43:A:MET:HB2 | 1:62:A:PHE:HE1  | 18       | 2.41          |
| (1,137)  | 1:10:A:ARG:HD2 | 1:11:A:PHE:HD2  | 8        | 2.41          |
| (1,131)  | 1:10:A:ARG:HG3 | 1:11:A:PHE:HE2  | 12       | 2.41          |
| (1,473)  | 1:62:A:PHE:HD2 | 1:69:A:LEU:HD21 | 7        | 2.39          |
| (1,131)  | 1:10:A:ARG:HG3 | 1:11:A:PHE:HE2  | 16       | 2.39          |
| (1,129)  | 1:10:A:ARG:HG2 | 1:11:A:PHE:HE2  | 10       | 2.39          |
| (1,131)  | 1:10:A:ARG:HG3 | 1:11:A:PHE:HE2  | 4        | 2.38          |
| (1,473)  | 1:62:A:PHE:HD2 | 1:69:A:LEU:HD21 | 3        | 2.37          |
| (1,473)  | 1:62:A:PHE:HD2 | 1:69:A:LEU:HD21 | 19       | 2.37          |
| (1,754)  | 1:62:A:PHE:HD2 | 1:63:A:CYS:HB2  | 13       | 2.36          |
| (1,754)  | 1:62:A:PHE:HD2 | 1:63:A:CYS:HB2  | 14       | 2.36          |
| (1,473)  | 1:62:A:PHE:HD2 | 1:69:A:LEU:HD21 | 10       | 2.36          |
| (1,473)  | 1:62:A:PHE:HD2 | 1:69:A:LEU:HD21 | 11       | 2.36          |
| (1,131)  | 1:10:A:ARG:HG3 | 1:11:A:PHE:HE2  | 20       | 2.36          |
| (1,1406) | 1:10:A:ARG:HG2 | 1:11:A:PHE:HE2  | 12       | 2.35          |
| (1,1406) | 1:10:A:ARG:HG3 | 1:11:A:PHE:HE2  | 12       | 2.35          |
| (1,754)  | 1:62:A:PHE:HD2 | 1:63:A:CYS:HB2  | 17       | 2.35          |
| (1,545)  | 1:43:A:MET:HG3 | 1:62:A:PHE:HE1  | 15       | 2.35          |
| (1,538)  | 1:43:A:MET:HB2 | 1:62:A:PHE:HE1  | 1        | 2.35          |
| (1,538)  | 1:43:A:MET:HB2 | 1:62:A:PHE:HE1  | 9        | 2.35          |
| (1,538)  | 1:43:A:MET:HB2 | 1:62:A:PHE:HE1  | 15       | 2.35          |
| (1,538)  | 1:43:A:MET:HB2 | 1:62:A:PHE:HE1  | 16       | 2.35          |
| (1,538)  | 1:43:A:MET:HB2 | 1:62:A:PHE:HE1  | 17       | 2.35          |
| (1,473)  | 1:62:A:PHE:HD2 | 1:69:A:LEU:HD21 | 5        | 2.35          |
| (1,131)  | 1:10:A:ARG:HG3 | 1:11:A:PHE:HE2  | 8        | 2.35          |
| (1,538)  | 1:43:A:MET:HB2 | 1:62:A:PHE:HE1  | 10       | 2.34          |
| (1,509)  | 1:43:A:MET:HA  | 1:62:A:PHE:HE1  | 14       | 2.34          |
| (1,473)  | 1:62:A:PHE:HD2 | 1:69:A:LEU:HD21 | 15       | 2.34          |
| (1,131)  | 1:10:A:ARG:HG3 | 1:11:A:PHE:HE2  | 14       | 2.34          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,754)  | 1:62:A:PHE:HD2 | 1:63:A:CYS:HB2  | 1        | 2.33          |
| (1,754)  | 1:62:A:PHE:HD2 | 1:63:A:CYS:HB2  | 6        | 2.33          |
| (1,754)  | 1:62:A:PHE:HD2 | 1:63:A:CYS:HB2  | 12       | 2.33          |
| (1,754)  | 1:62:A:PHE:HD2 | 1:63:A:CYS:HB2  | 16       | 2.33          |
| (1,754)  | 1:62:A:PHE:HD2 | 1:63:A:CYS:HB2  | 18       | 2.33          |
| (1,754)  | 1:62:A:PHE:HD2 | 1:63:A:CYS:HB2  | 20       | 2.33          |
| (1,545)  | 1:43:A:MET:HG3 | 1:62:A:PHE:HE1  | 17       | 2.33          |
| (1,538)  | 1:43:A:MET:HB2 | 1:62:A:PHE:HE1  | 12       | 2.33          |
| (1,538)  | 1:43:A:MET:HB2 | 1:62:A:PHE:HE1  | 13       | 2.33          |
| (1,754)  | 1:62:A:PHE:HD2 | 1:63:A:CYS:HB2  | 9        | 2.32          |
| (1,545)  | 1:43:A:MET:HG3 | 1:62:A:PHE:HE1  | 9        | 2.32          |
| (1,538)  | 1:43:A:MET:HB2 | 1:62:A:PHE:HE1  | 6        | 2.32          |
| (1,509)  | 1:43:A:MET:HA  | 1:62:A:PHE:HE1  | 18       | 2.32          |
| (1,473)  | 1:62:A:PHE:HD2 | 1:69:A:LEU:HD21 | 20       | 2.32          |
| (1,131)  | 1:10:A:ARG:HG3 | 1:11:A:PHE:HE2  | 10       | 2.32          |
| (1,545)  | 1:43:A:MET:HG3 | 1:62:A:PHE:HE1  | 16       | 2.31          |
| (1,538)  | 1:43:A:MET:HB2 | 1:62:A:PHE:HE1  | 5        | 2.3           |
| (1,538)  | 1:43:A:MET:HB2 | 1:62:A:PHE:HE1  | 11       | 2.3           |
| (1,473)  | 1:62:A:PHE:HD2 | 1:69:A:LEU:HD21 | 8        | 2.3           |
| (1,1406) | 1:10:A:ARG:HG2 | 1:11:A:PHE:HE2  | 10       | 2.29          |
| (1,1406) | 1:10:A:ARG:HG3 | 1:11:A:PHE:HE2  | 10       | 2.29          |
| (1,1406) | 1:10:A:ARG:HG2 | 1:11:A:PHE:HE2  | 19       | 2.29          |
| (1,1406) | 1:10:A:ARG:HG3 | 1:11:A:PHE:HE2  | 19       | 2.29          |
| (1,754)  | 1:62:A:PHE:HD2 | 1:63:A:CYS:HB2  | 4        | 2.29          |
| (1,754)  | 1:62:A:PHE:HD2 | 1:63:A:CYS:HB2  | 5        | 2.29          |
| (1,754)  | 1:62:A:PHE:HD2 | 1:63:A:CYS:HB2  | 11       | 2.29          |
| (1,754)  | 1:62:A:PHE:HD2 | 1:63:A:CYS:HB2  | 15       | 2.29          |
| (1,538)  | 1:43:A:MET:HB2 | 1:62:A:PHE:HE1  | 4        | 2.29          |
| (1,545)  | 1:43:A:MET:HG3 | 1:62:A:PHE:HE1  | 10       | 2.28          |
| (1,754)  | 1:62:A:PHE:HD2 | 1:63:A:CYS:HB2  | 2        | 2.27          |
| (1,754)  | 1:62:A:PHE:HD2 | 1:63:A:CYS:HB2  | 10       | 2.27          |
| (1,538)  | 1:43:A:MET:HB2 | 1:62:A:PHE:HE1  | 3        | 2.27          |
| (1,1406) | 1:10:A:ARG:HG2 | 1:11:A:PHE:HE2  | 9        | 2.26          |
| (1,1406) | 1:10:A:ARG:HG3 | 1:11:A:PHE:HE2  | 9        | 2.26          |
| (1,754)  | 1:62:A:PHE:HD2 | 1:63:A:CYS:HB2  | 7        | 2.26          |
| (1,754)  | 1:62:A:PHE:HD2 | 1:63:A:CYS:HB2  | 8        | 2.26          |
| (1,754)  | 1:62:A:PHE:HD2 | 1:63:A:CYS:HB2  | 19       | 2.26          |
| (1,538)  | 1:43:A:MET:HB2 | 1:62:A:PHE:HE1  | 2        | 2.26          |
| (1,538)  | 1:43:A:MET:HB2 | 1:62:A:PHE:HE1  | 8        | 2.26          |
| (1,538)  | 1:43:A:MET:HB2 | 1:62:A:PHE:HE1  | 20       | 2.26          |
| (1,131)  | 1:10:A:ARG:HG3 | 1:11:A:PHE:HE2  | 17       | 2.26          |
| (1,754)  | 1:62:A:PHE:HD2 | 1:63:A:CYS:HB2  | 3        | 2.25          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,545)  | 1:43:A:MET:HG3 | 1:62:A:PHE:HE1  | 11       | 2.25          |
| (1,137)  | 1:10:A:ARG:HD2 | 1:11:A:PHE:HD2  | 9        | 2.25          |
| (1,538)  | 1:43:A:MET:HB2 | 1:62:A:PHE:HE1  | 19       | 2.24          |
| (1,129)  | 1:10:A:ARG:HG2 | 1:11:A:PHE:HE2  | 15       | 2.24          |
| (1,1116) | 1:20:A:SER:H   | 1:53:A:PHE:HD2  | 13       | 2.23          |
| (1,538)  | 1:43:A:MET:HB2 | 1:62:A:PHE:HE1  | 7        | 2.23          |
| (1,473)  | 1:62:A:PHE:HD2 | 1:69:A:LEU:HD21 | 2        | 2.23          |
| (1,131)  | 1:10:A:ARG:HG3 | 1:11:A:PHE:HE2  | 6        | 2.23          |
| (1,131)  | 1:10:A:ARG:HG3 | 1:11:A:PHE:HE2  | 15       | 2.23          |
| (1,93)   | 1:8:A:PHE:HE2  | 1:9:A:LYS:HA    | 4        | 2.23          |
| (1,61)   | 1:7:A:ILE:HB   | 1:77:A:PHE:HD2  | 20       | 2.23          |
| (1,779)  | 1:62:A:PHE:HE2 | 1:67:A:PRO:HD2  | 8        | 2.22          |
| (1,131)  | 1:10:A:ARG:HG3 | 1:11:A:PHE:HE2  | 19       | 2.22          |
| (1,95)   | 1:8:A:PHE:HD2  | 1:9:A:LYS:HA    | 4        | 2.22          |
| (1,779)  | 1:62:A:PHE:HE2 | 1:67:A:PRO:HD2  | 16       | 2.21          |
| (1,509)  | 1:43:A:MET:HA  | 1:62:A:PHE:HE1  | 1        | 2.21          |
| (1,95)   | 1:8:A:PHE:HD2  | 1:9:A:LYS:HA    | 6        | 2.21          |
| (1,93)   | 1:8:A:PHE:HE2  | 1:9:A:LYS:HA    | 6        | 2.21          |
| (1,61)   | 1:7:A:ILE:HB   | 1:77:A:PHE:HD2  | 4        | 2.21          |
| (1,545)  | 1:43:A:MET:HG3 | 1:62:A:PHE:HE1  | 6        | 2.2           |
| (1,509)  | 1:43:A:MET:HA  | 1:62:A:PHE:HE1  | 13       | 2.2           |
| (1,137)  | 1:10:A:ARG:HD2 | 1:11:A:PHE:HD2  | 12       | 2.2           |
| (1,61)   | 1:7:A:ILE:HB   | 1:77:A:PHE:HD2  | 17       | 2.2           |
| (1,1406) | 1:10:A:ARG:HG2 | 1:11:A:PHE:HE2  | 15       | 2.19          |
| (1,1406) | 1:10:A:ARG:HG3 | 1:11:A:PHE:HE2  | 15       | 2.19          |
| (1,61)   | 1:7:A:ILE:HB   | 1:77:A:PHE:HD2  | 14       | 2.19          |
| (1,779)  | 1:62:A:PHE:HE2 | 1:67:A:PRO:HD2  | 1        | 2.18          |
| (1,779)  | 1:62:A:PHE:HE2 | 1:67:A:PRO:HD2  | 14       | 2.18          |
| (1,779)  | 1:62:A:PHE:HE2 | 1:67:A:PRO:HD2  | 18       | 2.18          |
| (1,473)  | 1:62:A:PHE:HD2 | 1:69:A:LEU:HD21 | 9        | 2.18          |
| (1,1406) | 1:10:A:ARG:HG2 | 1:11:A:PHE:HE2  | 13       | 2.17          |
| (1,1406) | 1:10:A:ARG:HG3 | 1:11:A:PHE:HE2  | 13       | 2.17          |
| (1,779)  | 1:62:A:PHE:HE2 | 1:67:A:PRO:HD2  | 12       | 2.17          |
| (1,779)  | 1:62:A:PHE:HE2 | 1:67:A:PRO:HD2  | 5        | 2.16          |
| (1,779)  | 1:62:A:PHE:HE2 | 1:67:A:PRO:HD2  | 11       | 2.16          |
| (1,779)  | 1:62:A:PHE:HE2 | 1:67:A:PRO:HD2  | 17       | 2.16          |
| (1,509)  | 1:43:A:MET:HA  | 1:62:A:PHE:HE1  | 6        | 2.16          |
| (1,509)  | 1:43:A:MET:HA  | 1:62:A:PHE:HE1  | 12       | 2.16          |
| (1,779)  | 1:62:A:PHE:HE2 | 1:67:A:PRO:HD2  | 4        | 2.15          |
| (1,779)  | 1:62:A:PHE:HE2 | 1:67:A:PRO:HD2  | 6        | 2.15          |
| (1,779)  | 1:62:A:PHE:HE2 | 1:67:A:PRO:HD2  | 20       | 2.15          |
| (1,509)  | 1:43:A:MET:HA  | 1:62:A:PHE:HE1  | 16       | 2.15          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,509)  | 1:43:A:MET:HA  | 1:62:A:PHE:HE1 | 17       | 2.15          |
| (1,1431) | 1:20:A:SER:HB2 | 1:53:A:PHE:HE2 | 13       | 2.14          |
| (1,1431) | 1:20:A:SER:HB3 | 1:53:A:PHE:HE2 | 13       | 2.14          |
| (1,779)  | 1:62:A:PHE:HE2 | 1:67:A:PRO:HD2 | 3        | 2.14          |
| (1,509)  | 1:43:A:MET:HA  | 1:62:A:PHE:HE1 | 4        | 2.14          |
| (1,509)  | 1:43:A:MET:HA  | 1:62:A:PHE:HE1 | 9        | 2.14          |
| (1,509)  | 1:43:A:MET:HA  | 1:62:A:PHE:HE1 | 10       | 2.14          |
| (1,509)  | 1:43:A:MET:HA  | 1:62:A:PHE:HE1 | 15       | 2.14          |
| (1,509)  | 1:43:A:MET:HA  | 1:62:A:PHE:HE1 | 5        | 2.13          |
| (1,137)  | 1:10:A:ARG:HD2 | 1:11:A:PHE:HD2 | 3        | 2.13          |
| (1,137)  | 1:10:A:ARG:HD2 | 1:11:A:PHE:HD2 | 5        | 2.13          |
| (1,131)  | 1:10:A:ARG:HG3 | 1:11:A:PHE:HE2 | 9        | 2.13          |
| (1,779)  | 1:62:A:PHE:HE2 | 1:67:A:PRO:HD2 | 2        | 2.12          |
| (1,779)  | 1:62:A:PHE:HE2 | 1:67:A:PRO:HD2 | 7        | 2.12          |
| (1,779)  | 1:62:A:PHE:HE2 | 1:67:A:PRO:HD2 | 19       | 2.12          |
| (1,779)  | 1:62:A:PHE:HE2 | 1:67:A:PRO:HD2 | 9        | 2.11          |
| (1,779)  | 1:62:A:PHE:HE2 | 1:67:A:PRO:HD2 | 10       | 2.11          |
| (1,509)  | 1:43:A:MET:HA  | 1:62:A:PHE:HE1 | 2        | 2.11          |
| (1,509)  | 1:43:A:MET:HA  | 1:62:A:PHE:HE1 | 11       | 2.11          |
| (1,1116) | 1:20:A:SER:H   | 1:53:A:PHE:HD2 | 12       | 2.1           |
| (1,779)  | 1:62:A:PHE:HE2 | 1:67:A:PRO:HD2 | 13       | 2.1           |
| (1,779)  | 1:62:A:PHE:HE2 | 1:67:A:PRO:HD2 | 15       | 2.1           |
| (1,509)  | 1:43:A:MET:HA  | 1:62:A:PHE:HE1 | 3        | 2.1           |
| (1,509)  | 1:43:A:MET:HA  | 1:62:A:PHE:HE1 | 20       | 2.1           |
| (1,1406) | 1:10:A:ARG:HG2 | 1:11:A:PHE:HE2 | 8        | 2.09          |
| (1,1406) | 1:10:A:ARG:HG3 | 1:11:A:PHE:HE2 | 8        | 2.09          |
| (1,545)  | 1:43:A:MET:HG3 | 1:62:A:PHE:HE1 | 4        | 2.09          |
| (1,509)  | 1:43:A:MET:HA  | 1:62:A:PHE:HE1 | 7        | 2.09          |
| (1,509)  | 1:43:A:MET:HA  | 1:62:A:PHE:HE1 | 19       | 2.09          |
| (1,159)  | 1:8:A:PHE:HD2  | 1:12:A:ASP:HB3 | 4        | 2.09          |
| (1,1406) | 1:10:A:ARG:HG2 | 1:11:A:PHE:HE2 | 1        | 2.08          |
| (1,1406) | 1:10:A:ARG:HG3 | 1:11:A:PHE:HE2 | 1        | 2.08          |
| (1,509)  | 1:43:A:MET:HA  | 1:62:A:PHE:HE1 | 8        | 2.08          |
| (1,1406) | 1:10:A:ARG:HG2 | 1:11:A:PHE:HE2 | 6        | 2.07          |
| (1,1406) | 1:10:A:ARG:HG3 | 1:11:A:PHE:HE2 | 6        | 2.07          |
| (1,1406) | 1:10:A:ARG:HG2 | 1:11:A:PHE:HE2 | 17       | 2.05          |
| (1,1406) | 1:10:A:ARG:HG3 | 1:11:A:PHE:HE2 | 17       | 2.05          |
| (1,137)  | 1:10:A:ARG:HD2 | 1:11:A:PHE:HD2 | 18       | 2.04          |
| (1,137)  | 1:10:A:ARG:HD2 | 1:11:A:PHE:HD2 | 19       | 2.04          |
| (1,1406) | 1:10:A:ARG:HG2 | 1:11:A:PHE:HE2 | 18       | 2.03          |
| (1,1406) | 1:10:A:ARG:HG3 | 1:11:A:PHE:HE2 | 18       | 2.03          |
| (1,545)  | 1:43:A:MET:HG3 | 1:62:A:PHE:HE1 | 8        | 2.03          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,545)  | 1:43:A:MET:HG3 | 1:62:A:PHE:HE1  | 20       | 2.03          |
| (1,473)  | 1:62:A:PHE:HD2 | 1:69:A:LEU:HD21 | 4        | 2.03          |
| (1,1406) | 1:10:A:ARG:HG2 | 1:11:A:PHE:HE2  | 11       | 2.02          |
| (1,1406) | 1:10:A:ARG:HG3 | 1:11:A:PHE:HE2  | 11       | 2.02          |
| (1,545)  | 1:43:A:MET:HG3 | 1:62:A:PHE:HE1  | 2        | 2.01          |
| (1,545)  | 1:43:A:MET:HG3 | 1:62:A:PHE:HE1  | 3        | 2.01          |
| (1,137)  | 1:10:A:ARG:HD2 | 1:11:A:PHE:HD2  | 4        | 2.0           |
| (1,137)  | 1:10:A:ARG:HD2 | 1:11:A:PHE:HD2  | 10       | 2.0           |
| (1,129)  | 1:10:A:ARG:HG2 | 1:11:A:PHE:HE2  | 6        | 2.0           |
| (1,1431) | 1:20:A:SER:HB2 | 1:53:A:PHE:HE2  | 12       | 1.99          |
| (1,1431) | 1:20:A:SER:HB3 | 1:53:A:PHE:HE2  | 12       | 1.99          |
| (1,1001) | 1:11:A:PHE:HE1 | 1:24:A:LEU:H    | 4        | 1.99          |
| (1,1206) | 1:42:A:MET:H   | 1:62:A:PHE:HE1  | 13       | 1.98          |
| (1,137)  | 1:10:A:ARG:HD2 | 1:11:A:PHE:HD2  | 1        | 1.98          |
| (1,1406) | 1:10:A:ARG:HG2 | 1:11:A:PHE:HE2  | 3        | 1.97          |
| (1,1406) | 1:10:A:ARG:HG3 | 1:11:A:PHE:HE2  | 3        | 1.97          |
| (1,1206) | 1:42:A:MET:H   | 1:62:A:PHE:HE1  | 14       | 1.97          |
| (1,1115) | 1:11:A:PHE:HD1 | 1:20:A:SER:H    | 4        | 1.97          |
| (1,669)  | 1:8:A:PHE:HE1  | 1:56:A:PHE:HA   | 6        | 1.97          |
| (1,545)  | 1:43:A:MET:HG3 | 1:62:A:PHE:HE1  | 19       | 1.97          |
| (1,256)  | 1:11:A:PHE:HD1 | 1:19:A:ILE:HG21 | 3        | 1.97          |
| (1,669)  | 1:8:A:PHE:HE1  | 1:56:A:PHE:HA   | 4        | 1.96          |
| (1,137)  | 1:10:A:ARG:HD2 | 1:11:A:PHE:HD2  | 13       | 1.96          |
| (1,1406) | 1:10:A:ARG:HG2 | 1:11:A:PHE:HE2  | 2        | 1.95          |
| (1,1406) | 1:10:A:ARG:HG3 | 1:11:A:PHE:HE2  | 2        | 1.95          |
| (1,647)  | 1:8:A:PHE:HD1  | 1:54:A:ILE:HD12 | 6        | 1.95          |
| (1,647)  | 1:8:A:PHE:HD1  | 1:54:A:ILE:HD13 | 6        | 1.95          |
| (1,545)  | 1:43:A:MET:HG3 | 1:62:A:PHE:HE1  | 7        | 1.95          |
| (1,333)  | 1:11:A:PHE:HE1 | 1:24:A:LEU:HD21 | 14       | 1.95          |
| (1,137)  | 1:10:A:ARG:HD2 | 1:11:A:PHE:HD2  | 20       | 1.95          |
| (1,1406) | 1:10:A:ARG:HG2 | 1:11:A:PHE:HE2  | 5        | 1.94          |
| (1,1406) | 1:10:A:ARG:HG3 | 1:11:A:PHE:HE2  | 5        | 1.94          |
| (1,1001) | 1:11:A:PHE:HE1 | 1:24:A:LEU:H    | 6        | 1.94          |
| (1,129)  | 1:10:A:ARG:HG2 | 1:11:A:PHE:HE2  | 8        | 1.94          |
| (1,473)  | 1:62:A:PHE:HD2 | 1:69:A:LEU:HD21 | 6        | 1.93          |
| (1,129)  | 1:10:A:ARG:HG2 | 1:11:A:PHE:HE2  | 17       | 1.93          |
| (1,1206) | 1:42:A:MET:H   | 1:62:A:PHE:HE1  | 18       | 1.92          |
| (1,137)  | 1:10:A:ARG:HD2 | 1:11:A:PHE:HD2  | 11       | 1.92          |
| (1,1115) | 1:11:A:PHE:HD1 | 1:20:A:SER:H    | 6        | 1.91          |
| (1,129)  | 1:10:A:ARG:HG2 | 1:11:A:PHE:HE2  | 13       | 1.91          |
| (1,1115) | 1:11:A:PHE:HD1 | 1:20:A:SER:H    | 1        | 1.9           |
| (1,647)  | 1:8:A:PHE:HD1  | 1:54:A:ILE:HD12 | 4        | 1.9           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,647)  | 1:8:A:PHE:HD1   | 1:54:A:ILE:HD13 | 4        | 1.9           |
| (1,473)  | 1:62:A:PHE:HD2  | 1:69:A:LEU:HD21 | 17       | 1.9           |
| (1,1115) | 1:11:A:PHE:HD1  | 1:20:A:SER:H    | 7        | 1.89          |
| (1,1115) | 1:11:A:PHE:HD1  | 1:20:A:SER:H    | 16       | 1.89          |
| (1,1001) | 1:11:A:PHE:HE1  | 1:24:A:LEU:H    | 16       | 1.89          |
| (1,1116) | 1:20:A:SER:H    | 1:53:A:PHE:HD2  | 3        | 1.88          |
| (1,1001) | 1:11:A:PHE:HE1  | 1:24:A:LEU:H    | 2        | 1.88          |
| (1,333)  | 1:11:A:PHE:HE1  | 1:24:A:LEU:HD21 | 11       | 1.88          |
| (1,137)  | 1:10:A:ARG:HD2  | 1:11:A:PHE:HD2  | 2        | 1.88          |
| (1,137)  | 1:10:A:ARG:HD2  | 1:11:A:PHE:HD2  | 14       | 1.88          |
| (1,1001) | 1:11:A:PHE:HE1  | 1:24:A:LEU:H    | 7        | 1.87          |
| (1,1001) | 1:11:A:PHE:HE1  | 1:24:A:LEU:H    | 19       | 1.87          |
| (1,181)  | 1:25:A:THR:HG22 | 1:40:A:GLN:HE22 | 14       | 1.87          |
| (1,181)  | 1:25:A:THR:HG22 | 1:40:A:GLN:HE22 | 1        | 1.86          |
| (1,181)  | 1:25:A:THR:HG22 | 1:40:A:GLN:HE22 | 9        | 1.86          |
| (1,181)  | 1:25:A:THR:HG22 | 1:40:A:GLN:HE22 | 10       | 1.86          |
| (1,181)  | 1:25:A:THR:HG22 | 1:40:A:GLN:HE22 | 15       | 1.86          |
| (1,181)  | 1:25:A:THR:HG22 | 1:40:A:GLN:HE22 | 17       | 1.86          |
| (1,137)  | 1:10:A:ARG:HD2  | 1:11:A:PHE:HD2  | 7        | 1.86          |
| (1,129)  | 1:10:A:ARG:HG2  | 1:11:A:PHE:HE2  | 1        | 1.86          |
| (1,1406) | 1:10:A:ARG:HG2  | 1:11:A:PHE:HE2  | 16       | 1.85          |
| (1,1406) | 1:10:A:ARG:HG3  | 1:11:A:PHE:HE2  | 16       | 1.85          |
| (1,1115) | 1:11:A:PHE:HD1  | 1:20:A:SER:H    | 17       | 1.85          |
| (1,1001) | 1:11:A:PHE:HE1  | 1:24:A:LEU:H    | 5        | 1.85          |
| (1,181)  | 1:25:A:THR:HG22 | 1:40:A:GLN:HE22 | 5        | 1.85          |
| (1,181)  | 1:25:A:THR:HG22 | 1:40:A:GLN:HE22 | 6        | 1.85          |
| (1,181)  | 1:25:A:THR:HG22 | 1:40:A:GLN:HE22 | 13       | 1.85          |
| (1,181)  | 1:25:A:THR:HG22 | 1:40:A:GLN:HE22 | 18       | 1.85          |
| (1,1406) | 1:10:A:ARG:HG2  | 1:11:A:PHE:HE2  | 7        | 1.84          |
| (1,1406) | 1:10:A:ARG:HG3  | 1:11:A:PHE:HE2  | 7        | 1.84          |
| (1,256)  | 1:11:A:PHE:HD1  | 1:19:A:ILE:HG21 | 1        | 1.84          |
| (1,181)  | 1:25:A:THR:HG22 | 1:40:A:GLN:HE22 | 2        | 1.84          |
| (1,181)  | 1:25:A:THR:HG22 | 1:40:A:GLN:HE22 | 4        | 1.84          |
| (1,181)  | 1:25:A:THR:HG22 | 1:40:A:GLN:HE22 | 12       | 1.84          |
| (1,181)  | 1:25:A:THR:HG22 | 1:40:A:GLN:HE22 | 16       | 1.84          |
| (1,1115) | 1:11:A:PHE:HD1  | 1:20:A:SER:H    | 5        | 1.83          |
| (1,1001) | 1:11:A:PHE:HE1  | 1:24:A:LEU:H    | 3        | 1.83          |
| (1,256)  | 1:11:A:PHE:HD1  | 1:19:A:ILE:HG21 | 7        | 1.83          |
| (1,181)  | 1:25:A:THR:HG22 | 1:40:A:GLN:HE22 | 7        | 1.83          |
| (1,181)  | 1:25:A:THR:HG22 | 1:40:A:GLN:HE22 | 11       | 1.83          |
| (1,181)  | 1:25:A:THR:HG22 | 1:40:A:GLN:HE22 | 19       | 1.83          |
| (1,43)   | 1:62:A:PHE:HD2  | 1:67:A:PRO:HG3  | 19       | 1.83          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1001) | 1:11:A:PHE:HE1  | 1:24:A:LEU:H    | 8        | 1.82          |
| (1,1001) | 1:11:A:PHE:HE1  | 1:24:A:LEU:H    | 17       | 1.82          |
| (1,181)  | 1:25:A:THR:HG22 | 1:40:A:GLN:HE22 | 3        | 1.82          |
| (1,181)  | 1:25:A:THR:HG22 | 1:40:A:GLN:HE22 | 8        | 1.82          |
| (1,181)  | 1:25:A:THR:HG22 | 1:40:A:GLN:HE22 | 20       | 1.82          |
| (1,43)   | 1:62:A:PHE:HD2  | 1:67:A:PRO:HG3  | 3        | 1.82          |
| (1,43)   | 1:62:A:PHE:HD2  | 1:67:A:PRO:HG3  | 7        | 1.82          |
| (1,1001) | 1:11:A:PHE:HE1  | 1:24:A:LEU:H    | 9        | 1.81          |
| (1,43)   | 1:62:A:PHE:HD2  | 1:67:A:PRO:HG3  | 2        | 1.81          |
| (1,43)   | 1:62:A:PHE:HD2  | 1:67:A:PRO:HG3  | 8        | 1.81          |
| (1,333)  | 1:11:A:PHE:HE1  | 1:24:A:LEU:HD21 | 1        | 1.8           |
| (1,256)  | 1:11:A:PHE:HD1  | 1:19:A:ILE:HG21 | 17       | 1.8           |
| (1,1206) | 1:42:A:MET:H    | 1:62:A:PHE:HE1  | 1        | 1.79          |
| (1,333)  | 1:11:A:PHE:HE1  | 1:24:A:LEU:HD21 | 9        | 1.79          |
| (1,256)  | 1:11:A:PHE:HD1  | 1:19:A:ILE:HG21 | 6        | 1.79          |
| (1,256)  | 1:11:A:PHE:HD1  | 1:19:A:ILE:HG21 | 20       | 1.79          |
| (1,43)   | 1:62:A:PHE:HD2  | 1:67:A:PRO:HG3  | 10       | 1.79          |
| (1,43)   | 1:62:A:PHE:HD2  | 1:67:A:PRO:HG3  | 15       | 1.79          |
| (1,1406) | 1:10:A:ARG:HG2  | 1:11:A:PHE:HE2  | 20       | 1.78          |
| (1,1406) | 1:10:A:ARG:HG3  | 1:11:A:PHE:HE2  | 20       | 1.78          |
| (1,1115) | 1:11:A:PHE:HD1  | 1:20:A:SER:H    | 9        | 1.78          |
| (1,1115) | 1:11:A:PHE:HD1  | 1:20:A:SER:H    | 19       | 1.78          |
| (1,862)  | 1:4:A:MET:HE3   | 1:7:A:ILE:H     | 14       | 1.78          |
| (1,862)  | 1:4:A:MET:HE3   | 1:7:A:ILE:H     | 20       | 1.78          |
| (1,256)  | 1:11:A:PHE:HD1  | 1:19:A:ILE:HG21 | 16       | 1.78          |
| (1,43)   | 1:62:A:PHE:HD2  | 1:67:A:PRO:HG3  | 4        | 1.78          |
| (1,43)   | 1:62:A:PHE:HD2  | 1:67:A:PRO:HG3  | 9        | 1.78          |
| (1,43)   | 1:62:A:PHE:HD2  | 1:67:A:PRO:HG3  | 11       | 1.78          |
| (1,858)  | 1:70:A:MET:HE2  | 1:74:A:ALA:HA   | 17       | 1.77          |
| (1,137)  | 1:10:A:ARG:HD2  | 1:11:A:PHE:HD2  | 16       | 1.77          |
| (1,43)   | 1:62:A:PHE:HD2  | 1:67:A:PRO:HG3  | 5        | 1.77          |
| (1,1115) | 1:11:A:PHE:HD1  | 1:20:A:SER:H    | 15       | 1.76          |
| (1,1001) | 1:11:A:PHE:HE1  | 1:24:A:LEU:H    | 11       | 1.76          |
| (1,1001) | 1:11:A:PHE:HE1  | 1:24:A:LEU:H    | 12       | 1.76          |
| (1,858)  | 1:70:A:MET:HE2  | 1:74:A:ALA:HA   | 4        | 1.76          |
| (1,256)  | 1:11:A:PHE:HD1  | 1:19:A:ILE:HG21 | 4        | 1.76          |
| (1,43)   | 1:62:A:PHE:HD2  | 1:67:A:PRO:HG3  | 6        | 1.76          |
| (1,43)   | 1:62:A:PHE:HD2  | 1:67:A:PRO:HG3  | 16       | 1.76          |
| (1,43)   | 1:62:A:PHE:HD2  | 1:67:A:PRO:HG3  | 17       | 1.76          |
| (1,43)   | 1:62:A:PHE:HD2  | 1:67:A:PRO:HG3  | 20       | 1.76          |
| (1,21)   | 1:5:A:GLU:HA    | 1:60:A:ILE:HD13 | 16       | 1.76          |
| (1,1406) | 1:10:A:ARG:HG2  | 1:11:A:PHE:HE2  | 4        | 1.75          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1406) | 1:10:A:ARG:HG3 | 1:11:A:PHE:HE2  | 4        | 1.75          |
| (1,1406) | 1:10:A:ARG:HG2 | 1:11:A:PHE:HE2  | 14       | 1.75          |
| (1,1406) | 1:10:A:ARG:HG3 | 1:11:A:PHE:HE2  | 14       | 1.75          |
| (1,1206) | 1:42:A:MET:H   | 1:62:A:PHE:HE1  | 6        | 1.75          |
| (1,1001) | 1:11:A:PHE:HE1 | 1:24:A:LEU:H    | 10       | 1.75          |
| (1,858)  | 1:70:A:MET:HE2 | 1:74:A:ALA:HA   | 9        | 1.75          |
| (1,858)  | 1:70:A:MET:HE2 | 1:74:A:ALA:HA   | 20       | 1.75          |
| (1,333)  | 1:11:A:PHE:HE1 | 1:24:A:LEU:HD21 | 16       | 1.75          |
| (1,256)  | 1:11:A:PHE:HD1 | 1:19:A:ILE:HG21 | 5        | 1.75          |
| (1,256)  | 1:11:A:PHE:HD1 | 1:19:A:ILE:HG21 | 14       | 1.75          |
| (1,137)  | 1:10:A:ARG:HD2 | 1:11:A:PHE:HD2  | 15       | 1.75          |
| (1,129)  | 1:10:A:ARG:HG2 | 1:11:A:PHE:HE2  | 18       | 1.75          |
| (1,21)   | 1:5:A:GLU:HA   | 1:60:A:ILE:HD13 | 14       | 1.75          |
| (1,1206) | 1:42:A:MET:H   | 1:62:A:PHE:HE1  | 12       | 1.74          |
| (1,858)  | 1:70:A:MET:HE2 | 1:74:A:ALA:HA   | 13       | 1.74          |
| (1,858)  | 1:70:A:MET:HE2 | 1:74:A:ALA:HA   | 16       | 1.74          |
| (1,256)  | 1:11:A:PHE:HD1 | 1:19:A:ILE:HG21 | 9        | 1.74          |
| (1,256)  | 1:11:A:PHE:HD1 | 1:19:A:ILE:HG21 | 15       | 1.74          |
| (1,205)  | 1:18:A:LYS:HB3 | 1:53:A:PHE:HD2  | 13       | 1.74          |
| (1,205)  | 1:18:A:LYS:HB2 | 1:53:A:PHE:HD2  | 13       | 1.74          |
| (1,21)   | 1:5:A:GLU:HA   | 1:60:A:ILE:HD13 | 9        | 1.74          |
| (1,21)   | 1:5:A:GLU:HA   | 1:60:A:ILE:HD13 | 13       | 1.74          |
| (1,21)   | 1:5:A:GLU:HA   | 1:60:A:ILE:HD13 | 20       | 1.74          |
| (1,1115) | 1:11:A:PHE:HD1 | 1:20:A:SER:H    | 14       | 1.73          |
| (1,1001) | 1:11:A:PHE:HE1 | 1:24:A:LEU:H    | 15       | 1.73          |
| (1,858)  | 1:70:A:MET:HE2 | 1:74:A:ALA:HA   | 6        | 1.73          |
| (1,129)  | 1:10:A:ARG:HG2 | 1:11:A:PHE:HE2  | 11       | 1.73          |
| (1,43)   | 1:62:A:PHE:HD2 | 1:67:A:PRO:HG3  | 12       | 1.73          |
| (1,1431) | 1:20:A:SER:HB2 | 1:53:A:PHE:HE2  | 15       | 1.72          |
| (1,1431) | 1:20:A:SER:HB3 | 1:53:A:PHE:HE2  | 15       | 1.72          |
| (1,1408) | 1:10:A:ARG:HD2 | 1:11:A:PHE:HE2  | 9        | 1.72          |
| (1,1408) | 1:10:A:ARG:HD3 | 1:11:A:PHE:HE2  | 9        | 1.72          |
| (1,1291) | 1:62:A:PHE:HD2 | 1:63:A:CYS:H    | 13       | 1.72          |
| (1,1291) | 1:62:A:PHE:HD2 | 1:63:A:CYS:H    | 14       | 1.72          |
| (1,1206) | 1:42:A:MET:H   | 1:62:A:PHE:HE1  | 4        | 1.72          |
| (1,1206) | 1:42:A:MET:H   | 1:62:A:PHE:HE1  | 16       | 1.72          |
| (1,858)  | 1:70:A:MET:HE2 | 1:74:A:ALA:HA   | 1        | 1.72          |
| (1,333)  | 1:11:A:PHE:HE1 | 1:24:A:LEU:HD21 | 8        | 1.72          |
| (1,256)  | 1:11:A:PHE:HD1 | 1:19:A:ILE:HG21 | 19       | 1.72          |
| (1,1291) | 1:62:A:PHE:HD2 | 1:63:A:CYS:H    | 18       | 1.71          |
| (1,1115) | 1:11:A:PHE:HD1 | 1:20:A:SER:H    | 3        | 1.71          |
| (1,1001) | 1:11:A:PHE:HE1 | 1:24:A:LEU:H    | 1        | 1.71          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,858)  | 1:70:A:MET:HE2  | 1:74:A:ALA:HA   | 14       | 1.71          |
| (1,269)  | 1:8:A:PHE:HD1   | 1:19:A:ILE:HD11 | 6        | 1.71          |
| (1,269)  | 1:8:A:PHE:HD1   | 1:19:A:ILE:HD13 | 6        | 1.71          |
| (1,205)  | 1:18:A:LYS:HB3  | 1:53:A:PHE:HD2  | 3        | 1.71          |
| (1,205)  | 1:18:A:LYS:HB2  | 1:53:A:PHE:HD2  | 3        | 1.71          |
| (1,154)  | 1:19:A:ILE:HD11 | 1:59:A:PHE:HB2  | 6        | 1.71          |
| (1,1206) | 1:42:A:MET:H    | 1:62:A:PHE:HE1  | 17       | 1.7           |
| (1,858)  | 1:70:A:MET:HE2  | 1:74:A:ALA:HA   | 18       | 1.7           |
| (1,473)  | 1:62:A:PHE:HD2  | 1:69:A:LEU:HD21 | 16       | 1.7           |
| (1,333)  | 1:11:A:PHE:HE1  | 1:24:A:LEU:HD21 | 19       | 1.7           |
| (1,43)   | 1:62:A:PHE:HD2  | 1:67:A:PRO:HG3  | 1        | 1.7           |
| (1,21)   | 1:5:A:GLU:HA    | 1:60:A:ILE:HD13 | 17       | 1.7           |
| (1,1291) | 1:62:A:PHE:HD2  | 1:63:A:CYS:H    | 1        | 1.69          |
| (1,1291) | 1:62:A:PHE:HD2  | 1:63:A:CYS:H    | 12       | 1.69          |
| (1,1001) | 1:11:A:PHE:HE1  | 1:24:A:LEU:H    | 13       | 1.69          |
| (1,1431) | 1:20:A:SER:HB2  | 1:53:A:PHE:HE2  | 16       | 1.68          |
| (1,1431) | 1:20:A:SER:HB3  | 1:53:A:PHE:HE2  | 16       | 1.68          |
| (1,1206) | 1:42:A:MET:H    | 1:62:A:PHE:HE1  | 5        | 1.68          |
| (1,1206) | 1:42:A:MET:H    | 1:62:A:PHE:HE1  | 20       | 1.68          |
| (1,1115) | 1:11:A:PHE:HD1  | 1:20:A:SER:H    | 20       | 1.68          |
| (1,858)  | 1:70:A:MET:HE2  | 1:74:A:ALA:HA   | 2        | 1.68          |
| (1,411)  | 1:30:A:THR:HG22 | 1:31:A:LEU:HG   | 20       | 1.68          |
| (1,154)  | 1:19:A:ILE:HD11 | 1:59:A:PHE:HB2  | 1        | 1.68          |
| (1,154)  | 1:19:A:ILE:HD11 | 1:59:A:PHE:HB2  | 16       | 1.68          |
| (1,129)  | 1:10:A:ARG:HG2  | 1:11:A:PHE:HE2  | 3        | 1.68          |
| (1,1291) | 1:62:A:PHE:HD2  | 1:63:A:CYS:H    | 6        | 1.67          |
| (1,1206) | 1:42:A:MET:H    | 1:62:A:PHE:HE1  | 9        | 1.67          |
| (1,1206) | 1:42:A:MET:H    | 1:62:A:PHE:HE1  | 11       | 1.67          |
| (1,1206) | 1:42:A:MET:H    | 1:62:A:PHE:HE1  | 15       | 1.67          |
| (1,1056) | 1:8:A:PHE:HD2   | 1:9:A:LYS:H     | 4        | 1.67          |
| (1,73)   | 1:7:A:ILE:HD13  | 1:8:A:PHE:HB3   | 6        | 1.67          |
| (1,73)   | 1:7:A:ILE:HD13  | 1:8:A:PHE:HB3   | 7        | 1.67          |
| (1,21)   | 1:5:A:GLU:HA    | 1:60:A:ILE:HD13 | 12       | 1.67          |
| (1,1291) | 1:62:A:PHE:HD2  | 1:63:A:CYS:H    | 17       | 1.66          |
| (1,1291) | 1:62:A:PHE:HD2  | 1:63:A:CYS:H    | 20       | 1.66          |
| (1,1206) | 1:42:A:MET:H    | 1:62:A:PHE:HE1  | 10       | 1.66          |
| (1,1109) | 1:19:A:ILE:H    | 1:53:A:PHE:HD2  | 13       | 1.66          |
| (1,1056) | 1:8:A:PHE:HD2   | 1:9:A:LYS:H     | 6        | 1.66          |
| (1,473)  | 1:62:A:PHE:HD2  | 1:69:A:LEU:HD21 | 12       | 1.66          |
| (1,154)  | 1:19:A:ILE:HD11 | 1:59:A:PHE:HB2  | 5        | 1.66          |
| (1,154)  | 1:19:A:ILE:HD11 | 1:59:A:PHE:HB2  | 9        | 1.66          |
| (1,154)  | 1:19:A:ILE:HD11 | 1:59:A:PHE:HB2  | 14       | 1.66          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,154)  | 1:19:A:ILE:HD11 | 1:59:A:PHE:HB2  | 17       | 1.66          |
| (1,43)   | 1:62:A:PHE:HD2  | 1:67:A:PRO:HG3  | 14       | 1.66          |
| (1,1291) | 1:62:A:PHE:HD2  | 1:63:A:CYS:H    | 5        | 1.65          |
| (1,1291) | 1:62:A:PHE:HD2  | 1:63:A:CYS:H    | 11       | 1.65          |
| (1,1291) | 1:62:A:PHE:HD2  | 1:63:A:CYS:H    | 16       | 1.65          |
| (1,1206) | 1:42:A:MET:H    | 1:62:A:PHE:HE1  | 2        | 1.65          |
| (1,858)  | 1:70:A:MET:HE2  | 1:74:A:ALA:HA   | 3        | 1.65          |
| (1,858)  | 1:70:A:MET:HE2  | 1:74:A:ALA:HA   | 8        | 1.65          |
| (1,129)  | 1:10:A:ARG:HG2  | 1:11:A:PHE:HE2  | 2        | 1.65          |
| (1,73)   | 1:7:A:ILE:HD13  | 1:8:A:PHE:HB3   | 15       | 1.65          |
| (1,43)   | 1:62:A:PHE:HD2  | 1:67:A:PRO:HG3  | 18       | 1.65          |
| (1,1517) | 1:47:A:ASP:HB2  | 1:54:A:ILE:HD13 | 1        | 1.64          |
| (1,1517) | 1:47:A:ASP:HB3  | 1:54:A:ILE:HD13 | 1        | 1.64          |
| (1,1517) | 1:47:A:ASP:HB2  | 1:54:A:ILE:HD13 | 2        | 1.64          |
| (1,1517) | 1:47:A:ASP:HB3  | 1:54:A:ILE:HD13 | 2        | 1.64          |
| (1,1291) | 1:62:A:PHE:HD2  | 1:63:A:CYS:H    | 4        | 1.64          |
| (1,1291) | 1:62:A:PHE:HD2  | 1:63:A:CYS:H    | 9        | 1.64          |
| (1,1206) | 1:42:A:MET:H    | 1:62:A:PHE:HE1  | 3        | 1.64          |
| (1,1206) | 1:42:A:MET:H    | 1:62:A:PHE:HE1  | 8        | 1.64          |
| (1,154)  | 1:19:A:ILE:HD11 | 1:59:A:PHE:HB2  | 2        | 1.64          |
| (1,154)  | 1:19:A:ILE:HD11 | 1:59:A:PHE:HB2  | 4        | 1.64          |
| (1,154)  | 1:19:A:ILE:HD11 | 1:59:A:PHE:HB2  | 11       | 1.64          |
| (1,154)  | 1:19:A:ILE:HD11 | 1:59:A:PHE:HB2  | 12       | 1.64          |
| (1,73)   | 1:7:A:ILE:HD13  | 1:8:A:PHE:HB3   | 1        | 1.64          |
| (1,73)   | 1:7:A:ILE:HD13  | 1:8:A:PHE:HB3   | 19       | 1.64          |
| (1,1206) | 1:42:A:MET:H    | 1:62:A:PHE:HE1  | 7        | 1.63          |
| (1,274)  | 1:20:A:SER:HA   | 1:53:A:PHE:HE2  | 13       | 1.63          |
| (1,73)   | 1:7:A:ILE:HD13  | 1:8:A:PHE:HB3   | 18       | 1.63          |
| (1,1517) | 1:47:A:ASP:HB2  | 1:54:A:ILE:HD13 | 16       | 1.62          |
| (1,1517) | 1:47:A:ASP:HB3  | 1:54:A:ILE:HD13 | 16       | 1.62          |
| (1,1517) | 1:47:A:ASP:HB2  | 1:54:A:ILE:HD13 | 17       | 1.62          |
| (1,1517) | 1:47:A:ASP:HB3  | 1:54:A:ILE:HD13 | 17       | 1.62          |
| (1,1291) | 1:62:A:PHE:HD2  | 1:63:A:CYS:H    | 10       | 1.62          |
| (1,1291) | 1:62:A:PHE:HD2  | 1:63:A:CYS:H    | 15       | 1.62          |
| (1,1206) | 1:42:A:MET:H    | 1:62:A:PHE:HE1  | 19       | 1.62          |
| (1,1115) | 1:11:A:PHE:HD1  | 1:20:A:SER:H    | 2        | 1.62          |
| (1,1001) | 1:11:A:PHE:HE1  | 1:24:A:LEU:H    | 14       | 1.62          |
| (1,552)  | 1:39:A:VAL:HG21 | 1:43:A:MET:HG2  | 14       | 1.62          |
| (1,552)  | 1:39:A:VAL:HG21 | 1:43:A:MET:HG3  | 14       | 1.62          |
| (1,333)  | 1:11:A:PHE:HE1  | 1:24:A:LEU:HD21 | 15       | 1.62          |
| (1,269)  | 1:8:A:PHE:HD1   | 1:19:A:ILE:HD11 | 4        | 1.62          |
| (1,269)  | 1:8:A:PHE:HD1   | 1:19:A:ILE:HD13 | 4        | 1.62          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,163)  | 1:12:A:ASP:HB2  | 1:19:A:ILE:HD13 | 10       | 1.62          |
| (1,129)  | 1:10:A:ARG:HG2  | 1:11:A:PHE:HE2  | 5        | 1.62          |
| (1,73)   | 1:7:A:ILE:HD13  | 1:8:A:PHE:HB3   | 8        | 1.62          |
| (1,73)   | 1:7:A:ILE:HD13  | 1:8:A:PHE:HB3   | 12       | 1.62          |
| (1,43)   | 1:62:A:PHE:HD2  | 1:67:A:PRO:HG3  | 13       | 1.62          |
| (1,1517) | 1:47:A:ASP:HB2  | 1:54:A:ILE:HD13 | 5        | 1.61          |
| (1,1517) | 1:47:A:ASP:HB3  | 1:54:A:ILE:HD13 | 5        | 1.61          |
| (1,1517) | 1:47:A:ASP:HB2  | 1:54:A:ILE:HD13 | 12       | 1.61          |
| (1,1517) | 1:47:A:ASP:HB3  | 1:54:A:ILE:HD13 | 12       | 1.61          |
| (1,1291) | 1:62:A:PHE:HD2  | 1:63:A:CYS:H    | 2        | 1.61          |
| (1,1291) | 1:62:A:PHE:HD2  | 1:63:A:CYS:H    | 8        | 1.61          |
| (1,275)  | 1:20:A:SER:HA   | 1:53:A:PHE:HD2  | 13       | 1.61          |
| (1,222)  | 1:8:A:PHE:HE1   | 1:19:A:ILE:HG12 | 6        | 1.61          |
| (1,73)   | 1:7:A:ILE:HD13  | 1:8:A:PHE:HB3   | 3        | 1.61          |
| (1,1517) | 1:47:A:ASP:HB2  | 1:54:A:ILE:HD13 | 3        | 1.6           |
| (1,1517) | 1:47:A:ASP:HB3  | 1:54:A:ILE:HD13 | 3        | 1.6           |
| (1,1517) | 1:47:A:ASP:HB2  | 1:54:A:ILE:HD13 | 8        | 1.6           |
| (1,1517) | 1:47:A:ASP:HB3  | 1:54:A:ILE:HD13 | 8        | 1.6           |
| (1,1517) | 1:47:A:ASP:HB2  | 1:54:A:ILE:HD13 | 9        | 1.6           |
| (1,1517) | 1:47:A:ASP:HB3  | 1:54:A:ILE:HD13 | 9        | 1.6           |
| (1,1517) | 1:47:A:ASP:HB2  | 1:54:A:ILE:HD13 | 14       | 1.6           |
| (1,1517) | 1:47:A:ASP:HB3  | 1:54:A:ILE:HD13 | 14       | 1.6           |
| (1,1291) | 1:62:A:PHE:HD2  | 1:63:A:CYS:H    | 3        | 1.6           |
| (1,1291) | 1:62:A:PHE:HD2  | 1:63:A:CYS:H    | 7        | 1.6           |
| (1,1291) | 1:62:A:PHE:HD2  | 1:63:A:CYS:H    | 19       | 1.6           |
| (1,73)   | 1:7:A:ILE:HD13  | 1:8:A:PHE:HB3   | 5        | 1.6           |
| (1,37)   | 1:46:A:ILE:HD11 | 1:58:A:GLU:HB2  | 5        | 1.6           |
| (1,1517) | 1:47:A:ASP:HB2  | 1:54:A:ILE:HD13 | 4        | 1.59          |
| (1,1517) | 1:47:A:ASP:HB3  | 1:54:A:ILE:HD13 | 4        | 1.59          |
| (1,1408) | 1:10:A:ARG:HD2  | 1:11:A:PHE:HE2  | 13       | 1.59          |
| (1,1408) | 1:10:A:ARG:HD3  | 1:11:A:PHE:HE2  | 13       | 1.59          |
| (1,858)  | 1:70:A:MET:HE2  | 1:74:A:ALA:HA   | 12       | 1.59          |
| (1,73)   | 1:7:A:ILE:HD13  | 1:8:A:PHE:HB3   | 9        | 1.59          |
| (1,73)   | 1:7:A:ILE:HD13  | 1:8:A:PHE:HB3   | 11       | 1.59          |
| (1,1517) | 1:47:A:ASP:HB2  | 1:54:A:ILE:HD13 | 6        | 1.58          |
| (1,1517) | 1:47:A:ASP:HB3  | 1:54:A:ILE:HD13 | 6        | 1.58          |
| (1,1517) | 1:47:A:ASP:HB2  | 1:54:A:ILE:HD13 | 7        | 1.58          |
| (1,1517) | 1:47:A:ASP:HB3  | 1:54:A:ILE:HD13 | 7        | 1.58          |
| (1,256)  | 1:11:A:PHE:HD1  | 1:19:A:ILE:HG21 | 10       | 1.58          |
| (1,154)  | 1:19:A:ILE:HD11 | 1:59:A:PHE:HB2  | 8        | 1.58          |
| (1,154)  | 1:19:A:ILE:HD11 | 1:59:A:PHE:HB2  | 20       | 1.58          |
| (1,73)   | 1:7:A:ILE:HD13  | 1:8:A:PHE:HB3   | 2        | 1.58          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,73)   | 1:7:A:ILE:HD13  | 1:8:A:PHE:HB3   | 4        | 1.58          |
| (1,1517) | 1:47:A:ASP:HB2  | 1:54:A:ILE:HD13 | 11       | 1.57          |
| (1,1517) | 1:47:A:ASP:HB3  | 1:54:A:ILE:HD13 | 11       | 1.57          |
| (1,1517) | 1:47:A:ASP:HB2  | 1:54:A:ILE:HD13 | 18       | 1.57          |
| (1,1517) | 1:47:A:ASP:HB3  | 1:54:A:ILE:HD13 | 18       | 1.57          |
| (1,1115) | 1:11:A:PHE:HD1  | 1:20:A:SER:H    | 10       | 1.57          |
| (1,163)  | 1:12:A:ASP:HB2  | 1:19:A:ILE:HD13 | 6        | 1.57          |
| (1,154)  | 1:19:A:ILE:HD11 | 1:59:A:PHE:HB2  | 18       | 1.57          |
| (1,1517) | 1:47:A:ASP:HB2  | 1:54:A:ILE:HD13 | 19       | 1.56          |
| (1,1517) | 1:47:A:ASP:HB3  | 1:54:A:ILE:HD13 | 19       | 1.56          |
| (1,1115) | 1:11:A:PHE:HD1  | 1:20:A:SER:H    | 8        | 1.56          |
| (1,858)  | 1:70:A:MET:HE2  | 1:74:A:ALA:HA   | 7        | 1.56          |
| (1,670)  | 1:8:A:PHE:HD1   | 1:56:A:PHE:HA   | 4        | 1.56          |
| (1,73)   | 1:7:A:ILE:HD13  | 1:8:A:PHE:HB3   | 16       | 1.56          |
| (1,73)   | 1:7:A:ILE:HD13  | 1:8:A:PHE:HB3   | 20       | 1.56          |
| (1,1431) | 1:20:A:SER:HB2  | 1:53:A:PHE:HE2  | 2        | 1.55          |
| (1,1431) | 1:20:A:SER:HB3  | 1:53:A:PHE:HE2  | 2        | 1.55          |
| (1,1196) | 1:42:A:MET:H    | 1:69:A:LEU:HD23 | 2        | 1.55          |
| (1,1196) | 1:42:A:MET:H    | 1:69:A:LEU:HD23 | 7        | 1.55          |
| (1,858)  | 1:70:A:MET:HE2  | 1:74:A:ALA:HA   | 5        | 1.55          |
| (1,846)  | 1:72:A:ASP:HA   | 1:76:A:VAL:HG21 | 14       | 1.55          |
| (1,842)  | 1:75:A:LYS:HA   | 1:76:A:VAL:HG21 | 6        | 1.55          |
| (1,842)  | 1:75:A:LYS:HA   | 1:76:A:VAL:HG21 | 13       | 1.55          |
| (1,658)  | 1:8:A:PHE:HE1   | 1:55:A:ASP:HA   | 6        | 1.55          |
| (1,473)  | 1:62:A:PHE:HD2  | 1:69:A:LEU:HD21 | 1        | 1.55          |
| (1,275)  | 1:20:A:SER:HA   | 1:53:A:PHE:HD2  | 3        | 1.55          |
| (1,161)  | 1:8:A:PHE:HE2   | 1:12:A:ASP:HB2  | 6        | 1.55          |
| (1,73)   | 1:7:A:ILE:HD13  | 1:8:A:PHE:HB3   | 13       | 1.55          |
| (1,73)   | 1:7:A:ILE:HD13  | 1:8:A:PHE:HB3   | 14       | 1.55          |
| (1,37)   | 1:46:A:ILE:HD11 | 1:58:A:GLU:HB2  | 10       | 1.55          |
| (1,21)   | 1:5:A:GLU:HA    | 1:60:A:ILE:HD13 | 15       | 1.55          |
| (1,1517) | 1:47:A:ASP:HB2  | 1:54:A:ILE:HD13 | 13       | 1.54          |
| (1,1517) | 1:47:A:ASP:HB3  | 1:54:A:ILE:HD13 | 13       | 1.54          |
| (1,1517) | 1:47:A:ASP:HB2  | 1:54:A:ILE:HD13 | 15       | 1.54          |
| (1,1517) | 1:47:A:ASP:HB3  | 1:54:A:ILE:HD13 | 15       | 1.54          |
| (1,1409) | 1:10:A:ARG:HD2  | 1:11:A:PHE:HD2  | 13       | 1.54          |
| (1,1409) | 1:10:A:ARG:HD3  | 1:11:A:PHE:HD2  | 13       | 1.54          |
| (1,1196) | 1:42:A:MET:H    | 1:69:A:LEU:HD23 | 5        | 1.54          |
| (1,1196) | 1:42:A:MET:H    | 1:69:A:LEU:HD23 | 9        | 1.54          |
| (1,1001) | 1:11:A:PHE:HE1  | 1:24:A:LEU:H    | 18       | 1.54          |
| (1,865)  | 1:4:A:MET:HE3   | 1:74:A:ALA:HB2  | 3        | 1.54          |
| (1,842)  | 1:75:A:LYS:HA   | 1:76:A:VAL:HG21 | 5        | 1.54          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,842)  | 1:75:A:LYS:HA   | 1:76:A:VAL:HG21 | 8        | 1.54          |
| (1,670)  | 1:8:A:PHE:HD1   | 1:56:A:PHE:HA   | 6        | 1.54          |
| (1,357)  | 1:30:A:THR:HG22 | 1:31:A:LEU:HA   | 16       | 1.54          |
| (1,112)  | 1:8:A:PHE:HD2   | 1:9:A:LYS:HD2   | 6        | 1.54          |
| (1,112)  | 1:8:A:PHE:HD2   | 1:9:A:LYS:HD3   | 6        | 1.54          |
| (1,73)   | 1:7:A:ILE:HD13  | 1:8:A:PHE:HB3   | 17       | 1.54          |
| (1,1196) | 1:42:A:MET:H    | 1:69:A:LEU:HD23 | 3        | 1.53          |
| (1,1196) | 1:42:A:MET:H    | 1:69:A:LEU:HD23 | 8        | 1.53          |
| (1,1196) | 1:42:A:MET:H    | 1:69:A:LEU:HD23 | 10       | 1.53          |
| (1,1196) | 1:42:A:MET:H    | 1:69:A:LEU:HD23 | 19       | 1.53          |
| (1,1109) | 1:19:A:ILE:H    | 1:53:A:PHE:HD2  | 12       | 1.53          |
| (1,1001) | 1:11:A:PHE:HE1  | 1:24:A:LEU:H    | 20       | 1.53          |
| (1,842)  | 1:75:A:LYS:HA   | 1:76:A:VAL:HG21 | 14       | 1.53          |
| (1,842)  | 1:75:A:LYS:HA   | 1:76:A:VAL:HG21 | 20       | 1.53          |
| (1,552)  | 1:39:A:VAL:HG21 | 1:43:A:MET:HG2  | 1        | 1.53          |
| (1,552)  | 1:39:A:VAL:HG21 | 1:43:A:MET:HG3  | 1        | 1.53          |
| (1,552)  | 1:39:A:VAL:HG21 | 1:43:A:MET:HG2  | 5        | 1.53          |
| (1,552)  | 1:39:A:VAL:HG21 | 1:43:A:MET:HG3  | 5        | 1.53          |
| (1,275)  | 1:20:A:SER:HA   | 1:53:A:PHE:HD2  | 12       | 1.53          |
| (1,256)  | 1:11:A:PHE:HD1  | 1:19:A:ILE:HG21 | 18       | 1.53          |
| (1,182)  | 1:13:A:THR:HG21 | 1:14:A:ASN:HA   | 11       | 1.53          |
| (1,154)  | 1:19:A:ILE:HD11 | 1:59:A:PHE:HB2  | 13       | 1.53          |
| (1,37)   | 1:46:A:ILE:HD11 | 1:58:A:GLU:HB2  | 15       | 1.53          |
| (1,1517) | 1:47:A:ASP:HB2  | 1:54:A:ILE:HD13 | 20       | 1.52          |
| (1,1517) | 1:47:A:ASP:HB3  | 1:54:A:ILE:HD13 | 20       | 1.52          |
| (1,1409) | 1:10:A:ARG:HD2  | 1:11:A:PHE:HD2  | 11       | 1.52          |
| (1,1409) | 1:10:A:ARG:HD3  | 1:11:A:PHE:HD2  | 11       | 1.52          |
| (1,1408) | 1:10:A:ARG:HD2  | 1:11:A:PHE:HE2  | 19       | 1.52          |
| (1,1408) | 1:10:A:ARG:HD3  | 1:11:A:PHE:HE2  | 19       | 1.52          |
| (1,1196) | 1:42:A:MET:H    | 1:69:A:LEU:HD23 | 4        | 1.52          |
| (1,1196) | 1:42:A:MET:H    | 1:69:A:LEU:HD23 | 11       | 1.52          |
| (1,1196) | 1:42:A:MET:H    | 1:69:A:LEU:HD23 | 20       | 1.52          |
| (1,1115) | 1:11:A:PHE:HD1  | 1:20:A:SER:H    | 18       | 1.52          |
| (1,842)  | 1:75:A:LYS:HA   | 1:76:A:VAL:HG21 | 16       | 1.52          |
| (1,480)  | 1:39:A:VAL:HG21 | 1:40:A:GLN:HA   | 17       | 1.52          |
| (1,412)  | 1:30:A:THR:HG22 | 1:31:A:LEU:HD22 | 20       | 1.52          |
| (1,256)  | 1:11:A:PHE:HD1  | 1:19:A:ILE:HG21 | 2        | 1.52          |
| (1,37)   | 1:46:A:ILE:HD11 | 1:58:A:GLU:HB2  | 13       | 1.52          |
| (1,1408) | 1:10:A:ARG:HD2  | 1:11:A:PHE:HE2  | 12       | 1.51          |
| (1,1408) | 1:10:A:ARG:HD3  | 1:11:A:PHE:HE2  | 12       | 1.51          |
| (1,1196) | 1:42:A:MET:H    | 1:69:A:LEU:HD23 | 15       | 1.51          |
| (1,865)  | 1:4:A:MET:HE3   | 1:74:A:ALA:HB2  | 4        | 1.51          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,865)  | 1:4:A:MET:HE3   | 1:74:A:ALA:HB2  | 11       | 1.51          |
| (1,842)  | 1:75:A:LYS:HA   | 1:76:A:VAL:HG21 | 10       | 1.51          |
| (1,480)  | 1:39:A:VAL:HG21 | 1:40:A:GLN:HA   | 3        | 1.51          |
| (1,480)  | 1:39:A:VAL:HG21 | 1:40:A:GLN:HA   | 8        | 1.51          |
| (1,480)  | 1:39:A:VAL:HG21 | 1:40:A:GLN:HA   | 14       | 1.51          |
| (1,473)  | 1:62:A:PHE:HD2  | 1:69:A:LEU:HD21 | 13       | 1.51          |
| (1,357)  | 1:30:A:THR:HG22 | 1:31:A:LEU:HA   | 6        | 1.51          |
| (1,357)  | 1:30:A:THR:HG22 | 1:31:A:LEU:HA   | 15       | 1.51          |
| (1,205)  | 1:18:A:LYS:HB3  | 1:53:A:PHE:HD2  | 12       | 1.51          |
| (1,205)  | 1:18:A:LYS:HB2  | 1:53:A:PHE:HD2  | 12       | 1.51          |
| (1,182)  | 1:13:A:THR:HG21 | 1:14:A:ASN:HA   | 10       | 1.51          |
| (1,154)  | 1:19:A:ILE:HD11 | 1:59:A:PHE:HB2  | 15       | 1.51          |
| (1,129)  | 1:10:A:ARG:HG2  | 1:11:A:PHE:HE2  | 16       | 1.51          |
| (1,73)   | 1:7:A:ILE:HD13  | 1:8:A:PHE:HB3   | 10       | 1.51          |
| (1,1409) | 1:10:A:ARG:HD2  | 1:11:A:PHE:HD2  | 7        | 1.5           |
| (1,1409) | 1:10:A:ARG:HD3  | 1:11:A:PHE:HD2  | 7        | 1.5           |
| (1,1409) | 1:10:A:ARG:HD2  | 1:11:A:PHE:HD2  | 16       | 1.5           |
| (1,1409) | 1:10:A:ARG:HD3  | 1:11:A:PHE:HD2  | 16       | 1.5           |
| (1,865)  | 1:4:A:MET:HE3   | 1:74:A:ALA:HB2  | 2        | 1.5           |
| (1,865)  | 1:4:A:MET:HE3   | 1:74:A:ALA:HB2  | 5        | 1.5           |
| (1,865)  | 1:4:A:MET:HE3   | 1:74:A:ALA:HB2  | 7        | 1.5           |
| (1,865)  | 1:4:A:MET:HE3   | 1:74:A:ALA:HB2  | 19       | 1.5           |
| (1,842)  | 1:75:A:LYS:HA   | 1:76:A:VAL:HG21 | 4        | 1.5           |
| (1,552)  | 1:39:A:VAL:HG21 | 1:43:A:MET:HG2  | 11       | 1.5           |
| (1,552)  | 1:39:A:VAL:HG21 | 1:43:A:MET:HG3  | 11       | 1.5           |
| (1,552)  | 1:39:A:VAL:HG21 | 1:43:A:MET:HG2  | 12       | 1.5           |
| (1,552)  | 1:39:A:VAL:HG21 | 1:43:A:MET:HG3  | 12       | 1.5           |
| (1,480)  | 1:39:A:VAL:HG21 | 1:40:A:GLN:HA   | 4        | 1.5           |
| (1,480)  | 1:39:A:VAL:HG21 | 1:40:A:GLN:HA   | 6        | 1.5           |
| (1,480)  | 1:39:A:VAL:HG21 | 1:40:A:GLN:HA   | 7        | 1.5           |
| (1,357)  | 1:30:A:THR:HG22 | 1:31:A:LEU:HA   | 4        | 1.5           |
| (1,357)  | 1:30:A:THR:HG22 | 1:31:A:LEU:HA   | 10       | 1.5           |
| (1,357)  | 1:30:A:THR:HG22 | 1:31:A:LEU:HA   | 18       | 1.5           |
| (1,274)  | 1:20:A:SER:HA   | 1:53:A:PHE:HE2  | 3        | 1.5           |
| (1,222)  | 1:8:A:PHE:HE1   | 1:19:A:ILE:HG12 | 4        | 1.5           |
| (1,182)  | 1:13:A:THR:HG21 | 1:14:A:ASN:HA   | 5        | 1.5           |
| (1,70)   | 1:7:A:ILE:HD12  | 1:77:A:PHE:HD2  | 18       | 1.5           |
| (1,1517) | 1:47:A:ASP:HB2  | 1:54:A:ILE:HD13 | 10       | 1.49          |
| (1,1517) | 1:47:A:ASP:HB3  | 1:54:A:ILE:HD13 | 10       | 1.49          |
| (1,1409) | 1:10:A:ARG:HD2  | 1:11:A:PHE:HD2  | 2        | 1.49          |
| (1,1409) | 1:10:A:ARG:HD3  | 1:11:A:PHE:HD2  | 2        | 1.49          |
| (1,1408) | 1:10:A:ARG:HD2  | 1:11:A:PHE:HE2  | 11       | 1.49          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1408) | 1:10:A:ARG:HD3  | 1:11:A:PHE:HE2  | 11       | 1.49          |
| (1,1115) | 1:11:A:PHE:HD1  | 1:20:A:SER:H    | 13       | 1.49          |
| (1,865)  | 1:4:A:MET:HE3   | 1:74:A:ALA:HB2  | 10       | 1.49          |
| (1,865)  | 1:4:A:MET:HE3   | 1:74:A:ALA:HB2  | 18       | 1.49          |
| (1,858)  | 1:70:A:MET:HE2  | 1:74:A:ALA:HA   | 11       | 1.49          |
| (1,842)  | 1:75:A:LYS:HA   | 1:76:A:VAL:HG21 | 17       | 1.49          |
| (1,552)  | 1:39:A:VAL:HG21 | 1:43:A:MET:HG2  | 15       | 1.49          |
| (1,552)  | 1:39:A:VAL:HG21 | 1:43:A:MET:HG3  | 15       | 1.49          |
| (1,552)  | 1:39:A:VAL:HG21 | 1:43:A:MET:HG2  | 18       | 1.49          |
| (1,552)  | 1:39:A:VAL:HG21 | 1:43:A:MET:HG3  | 18       | 1.49          |
| (1,480)  | 1:39:A:VAL:HG21 | 1:40:A:GLN:HA   | 2        | 1.49          |
| (1,480)  | 1:39:A:VAL:HG21 | 1:40:A:GLN:HA   | 9        | 1.49          |
| (1,480)  | 1:39:A:VAL:HG21 | 1:40:A:GLN:HA   | 15       | 1.49          |
| (1,480)  | 1:39:A:VAL:HG21 | 1:40:A:GLN:HA   | 19       | 1.49          |
| (1,357)  | 1:30:A:THR:HG22 | 1:31:A:LEU:HA   | 1        | 1.49          |
| (1,357)  | 1:30:A:THR:HG22 | 1:31:A:LEU:HA   | 11       | 1.49          |
| (1,256)  | 1:11:A:PHE:HD1  | 1:19:A:ILE:HG21 | 8        | 1.49          |
| (1,1409) | 1:10:A:ARG:HD2  | 1:11:A:PHE:HD2  | 9        | 1.48          |
| (1,1409) | 1:10:A:ARG:HD3  | 1:11:A:PHE:HD2  | 9        | 1.48          |
| (1,1196) | 1:42:A:MET:H    | 1:69:A:LEU:HD23 | 6        | 1.48          |
| (1,1116) | 1:20:A:SER:H    | 1:53:A:PHE:HD2  | 11       | 1.48          |
| (1,865)  | 1:4:A:MET:HE3   | 1:74:A:ALA:HB2  | 6        | 1.48          |
| (1,865)  | 1:4:A:MET:HE3   | 1:74:A:ALA:HB2  | 8        | 1.48          |
| (1,480)  | 1:39:A:VAL:HG21 | 1:40:A:GLN:HA   | 11       | 1.48          |
| (1,357)  | 1:30:A:THR:HG22 | 1:31:A:LEU:HA   | 8        | 1.48          |
| (1,357)  | 1:30:A:THR:HG22 | 1:31:A:LEU:HA   | 9        | 1.48          |
| (1,357)  | 1:30:A:THR:HG22 | 1:31:A:LEU:HA   | 17       | 1.48          |
| (1,357)  | 1:30:A:THR:HG22 | 1:31:A:LEU:HA   | 19       | 1.48          |
| (1,144)  | 1:11:A:PHE:HA   | 1:11:A:PHE:HE2  | 6        | 1.48          |
| (1,37)   | 1:46:A:ILE:HD11 | 1:58:A:GLU:HB2  | 11       | 1.48          |
| (1,37)   | 1:46:A:ILE:HD11 | 1:58:A:GLU:HB2  | 18       | 1.48          |
| (1,1432) | 1:20:A:SER:HB2  | 1:53:A:PHE:HD2  | 13       | 1.47          |
| (1,1432) | 1:20:A:SER:HB3  | 1:53:A:PHE:HD2  | 13       | 1.47          |
| (1,1408) | 1:10:A:ARG:HD2  | 1:11:A:PHE:HE2  | 10       | 1.47          |
| (1,1408) | 1:10:A:ARG:HD3  | 1:11:A:PHE:HE2  | 10       | 1.47          |
| (1,1328) | 1:62:A:PHE:HD2  | 1:70:A:MET:H    | 13       | 1.47          |
| (1,1328) | 1:62:A:PHE:HD2  | 1:70:A:MET:H    | 14       | 1.47          |
| (1,1115) | 1:11:A:PHE:HD1  | 1:20:A:SER:H    | 11       | 1.47          |
| (1,842)  | 1:75:A:LYS:HA   | 1:76:A:VAL:HG21 | 1        | 1.47          |
| (1,842)  | 1:75:A:LYS:HA   | 1:76:A:VAL:HG21 | 7        | 1.47          |
| (1,480)  | 1:39:A:VAL:HG21 | 1:40:A:GLN:HA   | 1        | 1.47          |
| (1,480)  | 1:39:A:VAL:HG21 | 1:40:A:GLN:HA   | 10       | 1.47          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,480)  | 1:39:A:VAL:HG21 | 1:40:A:GLN:HA   | 16       | 1.47          |
| (1,357)  | 1:30:A:THR:HG22 | 1:31:A:LEU:HA   | 2        | 1.47          |
| (1,357)  | 1:30:A:THR:HG22 | 1:31:A:LEU:HA   | 7        | 1.47          |
| (1,357)  | 1:30:A:THR:HG22 | 1:31:A:LEU:HA   | 12       | 1.47          |
| (1,357)  | 1:30:A:THR:HG22 | 1:31:A:LEU:HA   | 13       | 1.47          |
| (1,256)  | 1:11:A:PHE:HD1  | 1:19:A:ILE:HG21 | 13       | 1.47          |
| (1,182)  | 1:13:A:THR:HG21 | 1:14:A:ASN:HA   | 1        | 1.47          |
| (1,154)  | 1:19:A:ILE:HD11 | 1:59:A:PHE:HB2  | 3        | 1.47          |
| (1,144)  | 1:11:A:PHE:HA   | 1:11:A:PHE:HE2  | 14       | 1.47          |
| (1,144)  | 1:11:A:PHE:HA   | 1:11:A:PHE:HE2  | 17       | 1.47          |
| (1,129)  | 1:10:A:ARG:HG2  | 1:11:A:PHE:HE2  | 7        | 1.47          |
| (1,1432) | 1:20:A:SER:HB2  | 1:53:A:PHE:HD2  | 12       | 1.46          |
| (1,1432) | 1:20:A:SER:HB3  | 1:53:A:PHE:HD2  | 12       | 1.46          |
| (1,858)  | 1:70:A:MET:HE2  | 1:74:A:ALA:HA   | 15       | 1.46          |
| (1,858)  | 1:70:A:MET:HE2  | 1:74:A:ALA:HA   | 19       | 1.46          |
| (1,552)  | 1:39:A:VAL:HG21 | 1:43:A:MET:HG2  | 13       | 1.46          |
| (1,552)  | 1:39:A:VAL:HG21 | 1:43:A:MET:HG3  | 13       | 1.46          |
| (1,154)  | 1:19:A:ILE:HD11 | 1:59:A:PHE:HB2  | 7        | 1.46          |
| (1,144)  | 1:11:A:PHE:HA   | 1:11:A:PHE:HE2  | 1        | 1.46          |
| (1,144)  | 1:11:A:PHE:HA   | 1:11:A:PHE:HE2  | 2        | 1.46          |
| (1,144)  | 1:11:A:PHE:HA   | 1:11:A:PHE:HE2  | 7        | 1.46          |
| (1,144)  | 1:11:A:PHE:HA   | 1:11:A:PHE:HE2  | 9        | 1.46          |
| (1,144)  | 1:11:A:PHE:HA   | 1:11:A:PHE:HE2  | 15       | 1.46          |
| (1,144)  | 1:11:A:PHE:HA   | 1:11:A:PHE:HE2  | 20       | 1.46          |
| (1,70)   | 1:7:A:ILE:HD12  | 1:77:A:PHE:HD2  | 2        | 1.46          |
| (1,21)   | 1:5:A:GLU:HA    | 1:60:A:ILE:HD13 | 10       | 1.46          |
| (1,1408) | 1:10:A:ARG:HD2  | 1:11:A:PHE:HE2  | 7        | 1.45          |
| (1,1408) | 1:10:A:ARG:HD3  | 1:11:A:PHE:HE2  | 7        | 1.45          |
| (1,1064) | 1:8:A:PHE:HD2   | 1:10:A:ARG:H    | 4        | 1.45          |
| (1,865)  | 1:4:A:MET:HE3   | 1:74:A:ALA:HB2  | 1        | 1.45          |
| (1,858)  | 1:70:A:MET:HE2  | 1:74:A:ALA:HA   | 10       | 1.45          |
| (1,842)  | 1:75:A:LYS:HA   | 1:76:A:VAL:HG21 | 19       | 1.45          |
| (1,658)  | 1:8:A:PHE:HE1   | 1:55:A:ASP:HA   | 4        | 1.45          |
| (1,552)  | 1:39:A:VAL:HG21 | 1:43:A:MET:HG2  | 17       | 1.45          |
| (1,552)  | 1:39:A:VAL:HG21 | 1:43:A:MET:HG3  | 17       | 1.45          |
| (1,480)  | 1:39:A:VAL:HG21 | 1:40:A:GLN:HA   | 5        | 1.45          |
| (1,144)  | 1:11:A:PHE:HA   | 1:11:A:PHE:HE2  | 8        | 1.45          |
| (1,144)  | 1:11:A:PHE:HA   | 1:11:A:PHE:HE2  | 10       | 1.45          |
| (1,144)  | 1:11:A:PHE:HA   | 1:11:A:PHE:HE2  | 16       | 1.45          |
| (1,70)   | 1:7:A:ILE:HD12  | 1:77:A:PHE:HD2  | 11       | 1.45          |
| (1,1575) | 1:72:A:ASP:HB2  | 1:73:A:VAL:HG22 | 4        | 1.44          |
| (1,1575) | 1:72:A:ASP:HB3  | 1:73:A:VAL:HG22 | 4        | 1.44          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1431) | 1:20:A:SER:HB2  | 1:53:A:PHE:HE2  | 17       | 1.44          |
| (1,1431) | 1:20:A:SER:HB3  | 1:53:A:PHE:HE2  | 17       | 1.44          |
| (1,1328) | 1:62:A:PHE:HD2  | 1:70:A:MET:H    | 18       | 1.44          |
| (1,1196) | 1:42:A:MET:H    | 1:69:A:LEU:HD23 | 17       | 1.44          |
| (1,398)  | 1:30:A:THR:HA   | 1:31:A:LEU:HD21 | 9        | 1.44          |
| (1,163)  | 1:12:A:ASP:HB2  | 1:19:A:ILE:HD13 | 7        | 1.44          |
| (1,144)  | 1:11:A:PHE:HA   | 1:11:A:PHE:HE2  | 3        | 1.44          |
| (1,144)  | 1:11:A:PHE:HA   | 1:11:A:PHE:HE2  | 4        | 1.44          |
| (1,144)  | 1:11:A:PHE:HA   | 1:11:A:PHE:HE2  | 5        | 1.44          |
| (1,144)  | 1:11:A:PHE:HA   | 1:11:A:PHE:HE2  | 11       | 1.44          |
| (1,144)  | 1:11:A:PHE:HA   | 1:11:A:PHE:HE2  | 18       | 1.44          |
| (1,144)  | 1:11:A:PHE:HA   | 1:11:A:PHE:HE2  | 19       | 1.44          |
| (1,37)   | 1:46:A:ILE:HD11 | 1:58:A:GLU:HB2  | 3        | 1.44          |
| (1,37)   | 1:46:A:ILE:HD11 | 1:58:A:GLU:HB2  | 7        | 1.44          |
| (1,1328) | 1:62:A:PHE:HD2  | 1:70:A:MET:H    | 20       | 1.43          |
| (1,1170) | 1:31:A:LEU:HD21 | 1:33:A:SER:H    | 16       | 1.43          |
| (1,398)  | 1:30:A:THR:HA   | 1:31:A:LEU:HD21 | 20       | 1.43          |
| (1,357)  | 1:30:A:THR:HG22 | 1:31:A:LEU:HA   | 3        | 1.43          |
| (1,144)  | 1:11:A:PHE:HA   | 1:11:A:PHE:HE2  | 12       | 1.43          |
| (1,144)  | 1:11:A:PHE:HA   | 1:11:A:PHE:HE2  | 13       | 1.43          |
| (1,1408) | 1:10:A:ARG:HD2  | 1:11:A:PHE:HE2  | 2        | 1.42          |
| (1,1408) | 1:10:A:ARG:HD3  | 1:11:A:PHE:HE2  | 2        | 1.42          |
| (1,1408) | 1:10:A:ARG:HD2  | 1:11:A:PHE:HE2  | 15       | 1.42          |
| (1,1408) | 1:10:A:ARG:HD3  | 1:11:A:PHE:HE2  | 15       | 1.42          |
| (1,846)  | 1:72:A:ASP:HA   | 1:76:A:VAL:HG21 | 16       | 1.42          |
| (1,398)  | 1:30:A:THR:HA   | 1:31:A:LEU:HD21 | 15       | 1.42          |
| (1,274)  | 1:20:A:SER:HA   | 1:53:A:PHE:HE2  | 12       | 1.42          |
| (1,154)  | 1:19:A:ILE:HD11 | 1:59:A:PHE:HB2  | 10       | 1.42          |
| (1,154)  | 1:19:A:ILE:HD11 | 1:59:A:PHE:HB2  | 19       | 1.42          |
| (1,1431) | 1:20:A:SER:HB2  | 1:53:A:PHE:HE2  | 9        | 1.41          |
| (1,1431) | 1:20:A:SER:HB3  | 1:53:A:PHE:HE2  | 9        | 1.41          |
| (1,1408) | 1:10:A:ARG:HD2  | 1:11:A:PHE:HE2  | 1        | 1.41          |
| (1,1408) | 1:10:A:ARG:HD3  | 1:11:A:PHE:HE2  | 1        | 1.41          |
| (1,1328) | 1:62:A:PHE:HD2  | 1:70:A:MET:H    | 5        | 1.41          |
| (1,1170) | 1:31:A:LEU:HD21 | 1:33:A:SER:H    | 5        | 1.41          |
| (1,1170) | 1:31:A:LEU:HD21 | 1:33:A:SER:H    | 8        | 1.41          |
| (1,552)  | 1:39:A:VAL:HG21 | 1:43:A:MET:HG2  | 9        | 1.41          |
| (1,552)  | 1:39:A:VAL:HG21 | 1:43:A:MET:HG3  | 9        | 1.41          |
| (1,480)  | 1:39:A:VAL:HG21 | 1:40:A:GLN:HA   | 18       | 1.41          |
| (1,398)  | 1:30:A:THR:HA   | 1:31:A:LEU:HD21 | 1        | 1.41          |
| (1,398)  | 1:30:A:THR:HA   | 1:31:A:LEU:HD21 | 5        | 1.41          |
| (1,398)  | 1:30:A:THR:HA   | 1:31:A:LEU:HD21 | 13       | 1.41          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,363)  | 1:27:A:ALA:HB1  | 1:28:A:LEU:HD21 | 2        | 1.41          |
| (1,1431) | 1:20:A:SER:HB2  | 1:53:A:PHE:HE2  | 5        | 1.4           |
| (1,1431) | 1:20:A:SER:HB3  | 1:53:A:PHE:HE2  | 5        | 1.4           |
| (1,1170) | 1:31:A:LEU:HD21 | 1:33:A:SER:H    | 2        | 1.4           |
| (1,1170) | 1:31:A:LEU:HD21 | 1:33:A:SER:H    | 19       | 1.4           |
| (1,1116) | 1:20:A:SER:H    | 1:53:A:PHE:HD2  | 8        | 1.4           |
| (1,1064) | 1:8:A:PHE:HD2   | 1:10:A:ARG:H    | 6        | 1.4           |
| (1,398)  | 1:30:A:THR:HA   | 1:31:A:LEU:HD21 | 19       | 1.4           |
| (1,129)  | 1:10:A:ARG:HG2  | 1:11:A:PHE:HE2  | 20       | 1.4           |
| (1,1431) | 1:20:A:SER:HB2  | 1:53:A:PHE:HE2  | 11       | 1.39          |
| (1,1431) | 1:20:A:SER:HB3  | 1:53:A:PHE:HE2  | 11       | 1.39          |
| (1,1409) | 1:10:A:ARG:HD2  | 1:11:A:PHE:HD2  | 1        | 1.39          |
| (1,1409) | 1:10:A:ARG:HD3  | 1:11:A:PHE:HD2  | 1        | 1.39          |
| (1,1408) | 1:10:A:ARG:HD2  | 1:11:A:PHE:HE2  | 16       | 1.39          |
| (1,1408) | 1:10:A:ARG:HD3  | 1:11:A:PHE:HE2  | 16       | 1.39          |
| (1,1408) | 1:10:A:ARG:HD2  | 1:11:A:PHE:HE2  | 18       | 1.39          |
| (1,1408) | 1:10:A:ARG:HD3  | 1:11:A:PHE:HE2  | 18       | 1.39          |
| (1,1328) | 1:62:A:PHE:HD2  | 1:70:A:MET:H    | 10       | 1.39          |
| (1,1170) | 1:31:A:LEU:HD21 | 1:33:A:SER:H    | 1        | 1.39          |
| (1,1170) | 1:31:A:LEU:HD21 | 1:33:A:SER:H    | 4        | 1.39          |
| (1,1170) | 1:31:A:LEU:HD21 | 1:33:A:SER:H    | 20       | 1.39          |
| (1,398)  | 1:30:A:THR:HA   | 1:31:A:LEU:HD21 | 11       | 1.39          |
| (1,398)  | 1:30:A:THR:HA   | 1:31:A:LEU:HD21 | 17       | 1.39          |
| (1,182)  | 1:13:A:THR:HG21 | 1:14:A:ASN:HA   | 14       | 1.39          |
| (1,1431) | 1:20:A:SER:HB2  | 1:53:A:PHE:HE2  | 8        | 1.38          |
| (1,1431) | 1:20:A:SER:HB3  | 1:53:A:PHE:HE2  | 8        | 1.38          |
| (1,1328) | 1:62:A:PHE:HD2  | 1:70:A:MET:H    | 1        | 1.38          |
| (1,1328) | 1:62:A:PHE:HD2  | 1:70:A:MET:H    | 15       | 1.38          |
| (1,1170) | 1:31:A:LEU:HD21 | 1:33:A:SER:H    | 14       | 1.38          |
| (1,1170) | 1:31:A:LEU:HD21 | 1:33:A:SER:H    | 18       | 1.38          |
| (1,552)  | 1:39:A:VAL:HG21 | 1:43:A:MET:HG2  | 16       | 1.38          |
| (1,552)  | 1:39:A:VAL:HG21 | 1:43:A:MET:HG3  | 16       | 1.38          |
| (1,398)  | 1:30:A:THR:HA   | 1:31:A:LEU:HD21 | 4        | 1.38          |
| (1,256)  | 1:11:A:PHE:HD1  | 1:19:A:ILE:HG21 | 11       | 1.38          |
| (1,256)  | 1:11:A:PHE:HD1  | 1:19:A:ILE:HG21 | 12       | 1.38          |
| (1,21)   | 1:5:A:GLU:HA    | 1:60:A:ILE:HD13 | 11       | 1.38          |
| (1,1467) | 1:33:A:SER:HB2  | 1:34:A:THR:HG23 | 5        | 1.37          |
| (1,1467) | 1:33:A:SER:HB3  | 1:34:A:THR:HG23 | 5        | 1.37          |
| (1,1328) | 1:62:A:PHE:HD2  | 1:70:A:MET:H    | 6        | 1.37          |
| (1,1328) | 1:62:A:PHE:HD2  | 1:70:A:MET:H    | 11       | 1.37          |
| (1,1170) | 1:31:A:LEU:HD21 | 1:33:A:SER:H    | 6        | 1.37          |
| (1,1170) | 1:31:A:LEU:HD21 | 1:33:A:SER:H    | 7        | 1.37          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1170) | 1:31:A:LEU:HD21 | 1:33:A:SER:H    | 10       | 1.37          |
| (1,1170) | 1:31:A:LEU:HD21 | 1:33:A:SER:H    | 13       | 1.37          |
| (1,1170) | 1:31:A:LEU:HD21 | 1:33:A:SER:H    | 17       | 1.37          |
| (1,1116) | 1:20:A:SER:H    | 1:53:A:PHE:HD2  | 17       | 1.37          |
| (1,1115) | 1:11:A:PHE:HD1  | 1:20:A:SER:H    | 12       | 1.37          |
| (1,1109) | 1:19:A:ILE:H    | 1:53:A:PHE:HD2  | 3        | 1.37          |
| (1,846)  | 1:72:A:ASP:HA   | 1:76:A:VAL:HG21 | 20       | 1.37          |
| (1,398)  | 1:30:A:THR:HA   | 1:31:A:LEU:HD21 | 8        | 1.37          |
| (1,398)  | 1:30:A:THR:HA   | 1:31:A:LEU:HD21 | 10       | 1.37          |
| (1,163)  | 1:12:A:ASP:HB2  | 1:19:A:ILE:HD13 | 17       | 1.37          |
| (1,129)  | 1:10:A:ARG:HG2  | 1:11:A:PHE:HE2  | 14       | 1.37          |
| (1,1196) | 1:42:A:MET:H    | 1:69:A:LEU:HD23 | 12       | 1.36          |
| (1,1196) | 1:42:A:MET:H    | 1:69:A:LEU:HD23 | 16       | 1.36          |
| (1,1170) | 1:31:A:LEU:HD21 | 1:33:A:SER:H    | 3        | 1.36          |
| (1,1170) | 1:31:A:LEU:HD21 | 1:33:A:SER:H    | 12       | 1.36          |
| (1,552)  | 1:39:A:VAL:HG21 | 1:43:A:MET:HG2  | 10       | 1.36          |
| (1,552)  | 1:39:A:VAL:HG21 | 1:43:A:MET:HG3  | 10       | 1.36          |
| (1,480)  | 1:39:A:VAL:HG21 | 1:40:A:GLN:HA   | 12       | 1.36          |
| (1,480)  | 1:39:A:VAL:HG21 | 1:40:A:GLN:HA   | 20       | 1.36          |
| (1,398)  | 1:30:A:THR:HA   | 1:31:A:LEU:HD21 | 6        | 1.36          |
| (1,398)  | 1:30:A:THR:HA   | 1:31:A:LEU:HD21 | 12       | 1.36          |
| (1,398)  | 1:30:A:THR:HA   | 1:31:A:LEU:HD21 | 18       | 1.36          |
| (1,129)  | 1:10:A:ARG:HG2  | 1:11:A:PHE:HE2  | 4        | 1.36          |
| (1,75)   | 1:5:A:GLU:HA    | 1:7:A:ILE:HD13  | 9        | 1.36          |
| (1,70)   | 1:7:A:ILE:HD12  | 1:77:A:PHE:HD2  | 3        | 1.36          |
| (1,1328) | 1:62:A:PHE:HD2  | 1:70:A:MET:H    | 4        | 1.35          |
| (1,1328) | 1:62:A:PHE:HD2  | 1:70:A:MET:H    | 12       | 1.35          |
| (1,1328) | 1:62:A:PHE:HD2  | 1:70:A:MET:H    | 17       | 1.35          |
| (1,1170) | 1:31:A:LEU:HD21 | 1:33:A:SER:H    | 11       | 1.35          |
| (1,1116) | 1:20:A:SER:H    | 1:53:A:PHE:HD2  | 9        | 1.35          |
| (1,865)  | 1:4:A:MET:HE3   | 1:74:A:ALA:HB2  | 12       | 1.35          |
| (1,398)  | 1:30:A:THR:HA   | 1:31:A:LEU:HD21 | 2        | 1.35          |
| (1,398)  | 1:30:A:THR:HA   | 1:31:A:LEU:HD21 | 7        | 1.35          |
| (1,182)  | 1:13:A:THR:HG21 | 1:14:A:ASN:HA   | 4        | 1.35          |
| (1,142)  | 1:10:A:ARG:HD3  | 1:11:A:PHE:HD2  | 16       | 1.35          |
| (1,75)   | 1:5:A:GLU:HA    | 1:7:A:ILE:HD13  | 12       | 1.35          |
| (1,37)   | 1:46:A:ILE:HD11 | 1:58:A:GLU:HB2  | 19       | 1.35          |
| (1,1467) | 1:33:A:SER:HB2  | 1:34:A:THR:HG23 | 10       | 1.34          |
| (1,1467) | 1:33:A:SER:HB3  | 1:34:A:THR:HG23 | 10       | 1.34          |
| (1,1431) | 1:20:A:SER:HB2  | 1:53:A:PHE:HE2  | 3        | 1.34          |
| (1,1431) | 1:20:A:SER:HB3  | 1:53:A:PHE:HE2  | 3        | 1.34          |
| (1,1409) | 1:10:A:ARG:HD2  | 1:11:A:PHE:HD2  | 4        | 1.34          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1409) | 1:10:A:ARG:HD3  | 1:11:A:PHE:HD2  | 4        | 1.34          |
| (1,1328) | 1:62:A:PHE:HD2  | 1:70:A:MET:H    | 7        | 1.34          |
| (1,1170) | 1:31:A:LEU:HD21 | 1:33:A:SER:H    | 15       | 1.34          |
| (1,1116) | 1:20:A:SER:H    | 1:53:A:PHE:HD2  | 2        | 1.34          |
| (1,809)  | 1:69:A:LEU:HD21 | 1:70:A:MET:HG2  | 9        | 1.34          |
| (1,809)  | 1:69:A:LEU:HD21 | 1:70:A:MET:HG3  | 9        | 1.34          |
| (1,398)  | 1:30:A:THR:HA   | 1:31:A:LEU:HD21 | 14       | 1.34          |
| (1,357)  | 1:30:A:THR:HG22 | 1:31:A:LEU:HA   | 14       | 1.34          |
| (1,275)  | 1:20:A:SER:HA   | 1:53:A:PHE:HD2  | 2        | 1.34          |
| (1,275)  | 1:20:A:SER:HA   | 1:53:A:PHE:HD2  | 8        | 1.34          |
| (1,275)  | 1:20:A:SER:HA   | 1:53:A:PHE:HD2  | 17       | 1.34          |
| (1,275)  | 1:20:A:SER:HA   | 1:53:A:PHE:HD2  | 20       | 1.34          |
| (1,37)   | 1:46:A:ILE:HD11 | 1:58:A:GLU:HB2  | 20       | 1.34          |
| (1,1575) | 1:72:A:ASP:HB2  | 1:73:A:VAL:HG22 | 13       | 1.33          |
| (1,1575) | 1:72:A:ASP:HB3  | 1:73:A:VAL:HG22 | 13       | 1.33          |
| (1,1349) | 1:75:A:LYS:H    | 1:76:A:VAL:HG21 | 5        | 1.33          |
| (1,1170) | 1:31:A:LEU:HD21 | 1:33:A:SER:H    | 9        | 1.33          |
| (1,1116) | 1:20:A:SER:H    | 1:53:A:PHE:HD2  | 15       | 1.33          |
| (1,493)  | 1:39:A:VAL:HG21 | 1:40:A:GLN:HB2  | 8        | 1.33          |
| (1,480)  | 1:39:A:VAL:HG21 | 1:40:A:GLN:HA   | 13       | 1.33          |
| (1,275)  | 1:20:A:SER:HA   | 1:53:A:PHE:HD2  | 9        | 1.33          |
| (1,75)   | 1:5:A:GLU:HA    | 1:7:A:ILE:HD13  | 20       | 1.33          |
| (1,37)   | 1:46:A:ILE:HD11 | 1:58:A:GLU:HB2  | 9        | 1.33          |
| (1,1467) | 1:33:A:SER:HB2  | 1:34:A:THR:HG23 | 11       | 1.32          |
| (1,1467) | 1:33:A:SER:HB3  | 1:34:A:THR:HG23 | 11       | 1.32          |
| (1,1409) | 1:10:A:ARG:HD2  | 1:11:A:PHE:HD2  | 3        | 1.32          |
| (1,1409) | 1:10:A:ARG:HD3  | 1:11:A:PHE:HD2  | 3        | 1.32          |
| (1,1409) | 1:10:A:ARG:HD2  | 1:11:A:PHE:HD2  | 18       | 1.32          |
| (1,1409) | 1:10:A:ARG:HD3  | 1:11:A:PHE:HD2  | 18       | 1.32          |
| (1,1349) | 1:75:A:LYS:H    | 1:76:A:VAL:HG21 | 10       | 1.32          |
| (1,1349) | 1:75:A:LYS:H    | 1:76:A:VAL:HG21 | 15       | 1.32          |
| (1,1328) | 1:62:A:PHE:HD2  | 1:70:A:MET:H    | 19       | 1.32          |
| (1,1196) | 1:42:A:MET:H    | 1:69:A:LEU:HD23 | 1        | 1.32          |
| (1,1116) | 1:20:A:SER:H    | 1:53:A:PHE:HD2  | 5        | 1.32          |
| (1,1116) | 1:20:A:SER:H    | 1:53:A:PHE:HD2  | 14       | 1.32          |
| (1,1116) | 1:20:A:SER:H    | 1:53:A:PHE:HD2  | 16       | 1.32          |
| (1,846)  | 1:72:A:ASP:HA   | 1:76:A:VAL:HG21 | 5        | 1.32          |
| (1,493)  | 1:39:A:VAL:HG21 | 1:40:A:GLN:HB2  | 3        | 1.32          |
| (1,493)  | 1:39:A:VAL:HG21 | 1:40:A:GLN:HB2  | 4        | 1.32          |
| (1,493)  | 1:39:A:VAL:HG21 | 1:40:A:GLN:HB2  | 19       | 1.32          |
| (1,275)  | 1:20:A:SER:HA   | 1:53:A:PHE:HD2  | 14       | 1.32          |
| (1,182)  | 1:13:A:THR:HG21 | 1:14:A:ASN:HA   | 19       | 1.32          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,142)  | 1:10:A:ARG:HD3  | 1:11:A:PHE:HD2  | 13       | 1.32          |
| (1,1467) | 1:33:A:SER:HB2  | 1:34:A:THR:HG23 | 3        | 1.31          |
| (1,1467) | 1:33:A:SER:HB3  | 1:34:A:THR:HG23 | 3        | 1.31          |
| (1,1431) | 1:20:A:SER:HB2  | 1:53:A:PHE:HE2  | 6        | 1.31          |
| (1,1431) | 1:20:A:SER:HB3  | 1:53:A:PHE:HE2  | 6        | 1.31          |
| (1,1409) | 1:10:A:ARG:HD2  | 1:11:A:PHE:HD2  | 12       | 1.31          |
| (1,1409) | 1:10:A:ARG:HD3  | 1:11:A:PHE:HD2  | 12       | 1.31          |
| (1,1349) | 1:75:A:LYS:H    | 1:76:A:VAL:HG21 | 2        | 1.31          |
| (1,1349) | 1:75:A:LYS:H    | 1:76:A:VAL:HG21 | 18       | 1.31          |
| (1,1116) | 1:20:A:SER:H    | 1:53:A:PHE:HD2  | 10       | 1.31          |
| (1,542)  | 1:39:A:VAL:HG21 | 1:43:A:MET:HB3  | 11       | 1.31          |
| (1,493)  | 1:39:A:VAL:HG21 | 1:40:A:GLN:HB2  | 7        | 1.31          |
| (1,493)  | 1:39:A:VAL:HG21 | 1:40:A:GLN:HB2  | 17       | 1.31          |
| (1,398)  | 1:30:A:THR:HA   | 1:31:A:LEU:HD21 | 3        | 1.31          |
| (1,363)  | 1:27:A:ALA:HB1  | 1:28:A:LEU:HD21 | 12       | 1.31          |
| (1,275)  | 1:20:A:SER:HA   | 1:53:A:PHE:HD2  | 16       | 1.31          |
| (1,142)  | 1:10:A:ARG:HD3  | 1:11:A:PHE:HD2  | 11       | 1.31          |
| (1,75)   | 1:5:A:GLU:HA    | 1:7:A:ILE:HD13  | 15       | 1.31          |
| (1,70)   | 1:7:A:ILE:HD12  | 1:77:A:PHE:HD2  | 10       | 1.31          |
| (1,21)   | 1:5:A:GLU:HA    | 1:60:A:ILE:HD13 | 8        | 1.31          |
| (1,1575) | 1:72:A:ASP:HB2  | 1:73:A:VAL:HG22 | 12       | 1.3           |
| (1,1575) | 1:72:A:ASP:HB3  | 1:73:A:VAL:HG22 | 12       | 1.3           |
| (1,1467) | 1:33:A:SER:HB2  | 1:34:A:THR:HG23 | 1        | 1.3           |
| (1,1467) | 1:33:A:SER:HB3  | 1:34:A:THR:HG23 | 1        | 1.3           |
| (1,1409) | 1:10:A:ARG:HD2  | 1:11:A:PHE:HD2  | 14       | 1.3           |
| (1,1409) | 1:10:A:ARG:HD3  | 1:11:A:PHE:HD2  | 14       | 1.3           |
| (1,1409) | 1:10:A:ARG:HD2  | 1:11:A:PHE:HD2  | 20       | 1.3           |
| (1,1409) | 1:10:A:ARG:HD3  | 1:11:A:PHE:HD2  | 20       | 1.3           |
| (1,1408) | 1:10:A:ARG:HD2  | 1:11:A:PHE:HE2  | 3        | 1.3           |
| (1,1408) | 1:10:A:ARG:HD3  | 1:11:A:PHE:HE2  | 3        | 1.3           |
| (1,1349) | 1:75:A:LYS:H    | 1:76:A:VAL:HG21 | 7        | 1.3           |
| (1,1349) | 1:75:A:LYS:H    | 1:76:A:VAL:HG21 | 9        | 1.3           |
| (1,1328) | 1:62:A:PHE:HD2  | 1:70:A:MET:H    | 3        | 1.3           |
| (1,1196) | 1:42:A:MET:H    | 1:69:A:LEU:HD23 | 13       | 1.3           |
| (1,846)  | 1:72:A:ASP:HA   | 1:76:A:VAL:HG21 | 6        | 1.3           |
| (1,846)  | 1:72:A:ASP:HA   | 1:76:A:VAL:HG21 | 8        | 1.3           |
| (1,842)  | 1:75:A:LYS:HA   | 1:76:A:VAL:HG21 | 2        | 1.3           |
| (1,842)  | 1:75:A:LYS:HA   | 1:76:A:VAL:HG21 | 3        | 1.3           |
| (1,842)  | 1:75:A:LYS:HA   | 1:76:A:VAL:HG21 | 9        | 1.3           |
| (1,809)  | 1:69:A:LEU:HD21 | 1:70:A:MET:HG2  | 3        | 1.3           |
| (1,809)  | 1:69:A:LEU:HD21 | 1:70:A:MET:HG3  | 3        | 1.3           |
| (1,493)  | 1:39:A:VAL:HG21 | 1:40:A:GLN:HB2  | 2        | 1.3           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,493)  | 1:39:A:VAL:HG21 | 1:40:A:GLN:HB2  | 6        | 1.3           |
| (1,493)  | 1:39:A:VAL:HG21 | 1:40:A:GLN:HB2  | 15       | 1.3           |
| (1,363)  | 1:27:A:ALA:HB1  | 1:28:A:LEU:HD21 | 4        | 1.3           |
| (1,274)  | 1:20:A:SER:HA   | 1:53:A:PHE:HE2  | 20       | 1.3           |
| (1,1408) | 1:10:A:ARG:HD2  | 1:11:A:PHE:HE2  | 4        | 1.29          |
| (1,1408) | 1:10:A:ARG:HD3  | 1:11:A:PHE:HE2  | 4        | 1.29          |
| (1,1408) | 1:10:A:ARG:HD2  | 1:11:A:PHE:HE2  | 5        | 1.29          |
| (1,1408) | 1:10:A:ARG:HD3  | 1:11:A:PHE:HE2  | 5        | 1.29          |
| (1,1328) | 1:62:A:PHE:HD2  | 1:70:A:MET:H    | 16       | 1.29          |
| (1,1116) | 1:20:A:SER:H    | 1:53:A:PHE:HD2  | 18       | 1.29          |
| (1,1116) | 1:20:A:SER:H    | 1:53:A:PHE:HD2  | 19       | 1.29          |
| (1,842)  | 1:75:A:LYS:HA   | 1:76:A:VAL:HG21 | 11       | 1.29          |
| (1,842)  | 1:75:A:LYS:HA   | 1:76:A:VAL:HG21 | 18       | 1.29          |
| (1,809)  | 1:69:A:LEU:HD21 | 1:70:A:MET:HG2  | 11       | 1.29          |
| (1,809)  | 1:69:A:LEU:HD21 | 1:70:A:MET:HG3  | 11       | 1.29          |
| (1,493)  | 1:39:A:VAL:HG21 | 1:40:A:GLN:HB2  | 9        | 1.29          |
| (1,275)  | 1:20:A:SER:HA   | 1:53:A:PHE:HD2  | 15       | 1.29          |
| (1,142)  | 1:10:A:ARG:HD3  | 1:11:A:PHE:HD2  | 7        | 1.29          |
| (1,75)   | 1:5:A:GLU:HA    | 1:7:A:ILE:HD13  | 13       | 1.29          |
| (1,75)   | 1:5:A:GLU:HA    | 1:7:A:ILE:HD13  | 16       | 1.29          |
| (1,37)   | 1:46:A:ILE:HD11 | 1:58:A:GLU:HB2  | 12       | 1.29          |
| (1,1409) | 1:10:A:ARG:HD2  | 1:11:A:PHE:HD2  | 15       | 1.28          |
| (1,1409) | 1:10:A:ARG:HD3  | 1:11:A:PHE:HD2  | 15       | 1.28          |
| (1,1408) | 1:10:A:ARG:HD2  | 1:11:A:PHE:HE2  | 14       | 1.28          |
| (1,1408) | 1:10:A:ARG:HD3  | 1:11:A:PHE:HE2  | 14       | 1.28          |
| (1,1349) | 1:75:A:LYS:H    | 1:76:A:VAL:HG21 | 19       | 1.28          |
| (1,1328) | 1:62:A:PHE:HD2  | 1:70:A:MET:H    | 2        | 1.28          |
| (1,1116) | 1:20:A:SER:H    | 1:53:A:PHE:HD2  | 4        | 1.28          |
| (1,1116) | 1:20:A:SER:H    | 1:53:A:PHE:HD2  | 7        | 1.28          |
| (1,1116) | 1:20:A:SER:H    | 1:53:A:PHE:HD2  | 20       | 1.28          |
| (1,850)  | 1:31:A:LEU:HB3  | 1:76:A:VAL:HG23 | 20       | 1.28          |
| (1,846)  | 1:72:A:ASP:HA   | 1:76:A:VAL:HG21 | 1        | 1.28          |
| (1,842)  | 1:75:A:LYS:HA   | 1:76:A:VAL:HG21 | 15       | 1.28          |
| (1,809)  | 1:69:A:LEU:HD21 | 1:70:A:MET:HG2  | 5        | 1.28          |
| (1,809)  | 1:69:A:LEU:HD21 | 1:70:A:MET:HG3  | 5        | 1.28          |
| (1,493)  | 1:39:A:VAL:HG21 | 1:40:A:GLN:HB2  | 10       | 1.28          |
| (1,493)  | 1:39:A:VAL:HG21 | 1:40:A:GLN:HB2  | 16       | 1.28          |
| (1,275)  | 1:20:A:SER:HA   | 1:53:A:PHE:HD2  | 1        | 1.28          |
| (1,275)  | 1:20:A:SER:HA   | 1:53:A:PHE:HD2  | 6        | 1.28          |
| (1,274)  | 1:20:A:SER:HA   | 1:53:A:PHE:HE2  | 2        | 1.28          |
| (1,163)  | 1:12:A:ASP:HB2  | 1:19:A:ILE:HD13 | 15       | 1.28          |
| (1,142)  | 1:10:A:ARG:HD3  | 1:11:A:PHE:HD2  | 2        | 1.28          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,75)   | 1:5:A:GLU:HA    | 1:7:A:ILE:HD13  | 5        | 1.28          |
| (1,37)   | 1:46:A:ILE:HD11 | 1:58:A:GLU:HB2  | 8        | 1.28          |
| (1,21)   | 1:5:A:GLU:HA    | 1:60:A:ILE:HD13 | 2        | 1.28          |
| (1,1431) | 1:20:A:SER:HB2  | 1:53:A:PHE:HE2  | 4        | 1.27          |
| (1,1431) | 1:20:A:SER:HB3  | 1:53:A:PHE:HE2  | 4        | 1.27          |
| (1,1409) | 1:10:A:ARG:HD2  | 1:11:A:PHE:HD2  | 6        | 1.27          |
| (1,1409) | 1:10:A:ARG:HD3  | 1:11:A:PHE:HD2  | 6        | 1.27          |
| (1,1408) | 1:10:A:ARG:HD2  | 1:11:A:PHE:HE2  | 20       | 1.27          |
| (1,1408) | 1:10:A:ARG:HD3  | 1:11:A:PHE:HE2  | 20       | 1.27          |
| (1,1349) | 1:75:A:LYS:H    | 1:76:A:VAL:HG21 | 11       | 1.27          |
| (1,1328) | 1:62:A:PHE:HD2  | 1:70:A:MET:H    | 8        | 1.27          |
| (1,1328) | 1:62:A:PHE:HD2  | 1:70:A:MET:H    | 9        | 1.27          |
| (1,1116) | 1:20:A:SER:H    | 1:53:A:PHE:HD2  | 1        | 1.27          |
| (1,1116) | 1:20:A:SER:H    | 1:53:A:PHE:HD2  | 6        | 1.27          |
| (1,861)  | 1:4:A:MET:H     | 1:4:A:MET:HE3   | 15       | 1.27          |
| (1,846)  | 1:72:A:ASP:HA   | 1:76:A:VAL:HG21 | 13       | 1.27          |
| (1,809)  | 1:69:A:LEU:HD21 | 1:70:A:MET:HG2  | 2        | 1.27          |
| (1,809)  | 1:69:A:LEU:HD21 | 1:70:A:MET:HG3  | 2        | 1.27          |
| (1,275)  | 1:20:A:SER:HA   | 1:53:A:PHE:HD2  | 4        | 1.27          |
| (1,275)  | 1:20:A:SER:HA   | 1:53:A:PHE:HD2  | 11       | 1.27          |
| (1,274)  | 1:20:A:SER:HA   | 1:53:A:PHE:HE2  | 14       | 1.27          |
| (1,75)   | 1:5:A:GLU:HA    | 1:7:A:ILE:HD13  | 1        | 1.27          |
| (1,21)   | 1:5:A:GLU:HA    | 1:60:A:ILE:HD13 | 1        | 1.27          |
| (1,1467) | 1:33:A:SER:HB2  | 1:34:A:THR:HG23 | 12       | 1.26          |
| (1,1467) | 1:33:A:SER:HB3  | 1:34:A:THR:HG23 | 12       | 1.26          |
| (1,1431) | 1:20:A:SER:HB2  | 1:53:A:PHE:HE2  | 20       | 1.26          |
| (1,1431) | 1:20:A:SER:HB3  | 1:53:A:PHE:HE2  | 20       | 1.26          |
| (1,1409) | 1:10:A:ARG:HD2  | 1:11:A:PHE:HD2  | 5        | 1.26          |
| (1,1409) | 1:10:A:ARG:HD3  | 1:11:A:PHE:HD2  | 5        | 1.26          |
| (1,848)  | 1:31:A:LEU:HB2  | 1:76:A:VAL:HG23 | 20       | 1.26          |
| (1,552)  | 1:39:A:VAL:HG21 | 1:43:A:MET:HG2  | 6        | 1.26          |
| (1,552)  | 1:39:A:VAL:HG21 | 1:43:A:MET:HG3  | 6        | 1.26          |
| (1,275)  | 1:20:A:SER:HA   | 1:53:A:PHE:HD2  | 18       | 1.26          |
| (1,274)  | 1:20:A:SER:HA   | 1:53:A:PHE:HE2  | 9        | 1.26          |
| (1,274)  | 1:20:A:SER:HA   | 1:53:A:PHE:HE2  | 17       | 1.26          |
| (1,266)  | 1:12:A:ASP:H    | 1:19:A:ILE:HD13 | 10       | 1.26          |
| (1,21)   | 1:5:A:GLU:HA    | 1:60:A:ILE:HD13 | 5        | 1.26          |
| (1,809)  | 1:69:A:LEU:HD21 | 1:70:A:MET:HG2  | 8        | 1.25          |
| (1,809)  | 1:69:A:LEU:HD21 | 1:70:A:MET:HG3  | 8        | 1.25          |
| (1,809)  | 1:69:A:LEU:HD21 | 1:70:A:MET:HG2  | 10       | 1.25          |
| (1,809)  | 1:69:A:LEU:HD21 | 1:70:A:MET:HG3  | 10       | 1.25          |
| (1,809)  | 1:69:A:LEU:HD21 | 1:70:A:MET:HG2  | 15       | 1.25          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,809)  | 1:69:A:LEU:HD21 | 1:70:A:MET:HG3  | 15       | 1.25          |
| (1,398)  | 1:30:A:THR:HA   | 1:31:A:LEU:HD21 | 16       | 1.25          |
| (1,275)  | 1:20:A:SER:HA   | 1:53:A:PHE:HD2  | 10       | 1.25          |
| (1,274)  | 1:20:A:SER:HA   | 1:53:A:PHE:HE2  | 8        | 1.25          |
| (1,266)  | 1:12:A:ASP:H    | 1:19:A:ILE:HD13 | 6        | 1.25          |
| (1,143)  | 1:11:A:PHE:HA   | 1:11:A:PHE:HD2  | 6        | 1.25          |
| (1,143)  | 1:11:A:PHE:HA   | 1:11:A:PHE:HD2  | 14       | 1.25          |
| (1,143)  | 1:11:A:PHE:HA   | 1:11:A:PHE:HD2  | 17       | 1.25          |
| (1,75)   | 1:5:A:GLU:HA    | 1:7:A:ILE:HD13  | 14       | 1.25          |
| (1,75)   | 1:5:A:GLU:HA    | 1:7:A:ILE:HD13  | 17       | 1.25          |
| (1,1349) | 1:75:A:LYS:H    | 1:76:A:VAL:HG21 | 8        | 1.24          |
| (1,1109) | 1:19:A:ILE:H    | 1:53:A:PHE:HD2  | 18       | 1.24          |
| (1,846)  | 1:72:A:ASP:HA   | 1:76:A:VAL:HG21 | 17       | 1.24          |
| (1,809)  | 1:69:A:LEU:HD21 | 1:70:A:MET:HG2  | 7        | 1.24          |
| (1,809)  | 1:69:A:LEU:HD21 | 1:70:A:MET:HG3  | 7        | 1.24          |
| (1,809)  | 1:69:A:LEU:HD21 | 1:70:A:MET:HG2  | 19       | 1.24          |
| (1,809)  | 1:69:A:LEU:HD21 | 1:70:A:MET:HG3  | 19       | 1.24          |
| (1,809)  | 1:69:A:LEU:HD21 | 1:70:A:MET:HG2  | 20       | 1.24          |
| (1,809)  | 1:69:A:LEU:HD21 | 1:70:A:MET:HG3  | 20       | 1.24          |
| (1,493)  | 1:39:A:VAL:HG21 | 1:40:A:GLN:HB2  | 1        | 1.24          |
| (1,363)  | 1:27:A:ALA:HB1  | 1:28:A:LEU:HD21 | 13       | 1.24          |
| (1,333)  | 1:11:A:PHE:HE1  | 1:24:A:LEU:HD21 | 18       | 1.24          |
| (1,275)  | 1:20:A:SER:HA   | 1:53:A:PHE:HD2  | 19       | 1.24          |
| (1,274)  | 1:20:A:SER:HA   | 1:53:A:PHE:HE2  | 1        | 1.24          |
| (1,274)  | 1:20:A:SER:HA   | 1:53:A:PHE:HE2  | 15       | 1.24          |
| (1,143)  | 1:11:A:PHE:HA   | 1:11:A:PHE:HD2  | 1        | 1.24          |
| (1,143)  | 1:11:A:PHE:HA   | 1:11:A:PHE:HD2  | 2        | 1.24          |
| (1,143)  | 1:11:A:PHE:HA   | 1:11:A:PHE:HD2  | 3        | 1.24          |
| (1,143)  | 1:11:A:PHE:HA   | 1:11:A:PHE:HD2  | 4        | 1.24          |
| (1,143)  | 1:11:A:PHE:HA   | 1:11:A:PHE:HD2  | 7        | 1.24          |
| (1,143)  | 1:11:A:PHE:HA   | 1:11:A:PHE:HD2  | 8        | 1.24          |
| (1,143)  | 1:11:A:PHE:HA   | 1:11:A:PHE:HD2  | 9        | 1.24          |
| (1,143)  | 1:11:A:PHE:HA   | 1:11:A:PHE:HD2  | 10       | 1.24          |
| (1,143)  | 1:11:A:PHE:HA   | 1:11:A:PHE:HD2  | 11       | 1.24          |
| (1,143)  | 1:11:A:PHE:HA   | 1:11:A:PHE:HD2  | 15       | 1.24          |
| (1,143)  | 1:11:A:PHE:HA   | 1:11:A:PHE:HD2  | 16       | 1.24          |
| (1,143)  | 1:11:A:PHE:HA   | 1:11:A:PHE:HD2  | 19       | 1.24          |
| (1,143)  | 1:11:A:PHE:HA   | 1:11:A:PHE:HD2  | 20       | 1.24          |
| (1,75)   | 1:5:A:GLU:HA    | 1:7:A:ILE:HD13  | 7        | 1.24          |
| (1,1432) | 1:20:A:SER:HB2  | 1:53:A:PHE:HD2  | 15       | 1.23          |
| (1,1432) | 1:20:A:SER:HB3  | 1:53:A:PHE:HD2  | 15       | 1.23          |
| (1,1432) | 1:20:A:SER:HB2  | 1:53:A:PHE:HD2  | 16       | 1.23          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1432) | 1:20:A:SER:HB3  | 1:53:A:PHE:HD2  | 16       | 1.23          |
| (1,1409) | 1:10:A:ARG:HD2  | 1:11:A:PHE:HD2  | 17       | 1.23          |
| (1,1409) | 1:10:A:ARG:HD3  | 1:11:A:PHE:HD2  | 17       | 1.23          |
| (1,1408) | 1:10:A:ARG:HD2  | 1:11:A:PHE:HE2  | 6        | 1.23          |
| (1,1408) | 1:10:A:ARG:HD3  | 1:11:A:PHE:HE2  | 6        | 1.23          |
| (1,1349) | 1:75:A:LYS:H    | 1:76:A:VAL:HG21 | 3        | 1.23          |
| (1,1349) | 1:75:A:LYS:H    | 1:76:A:VAL:HG21 | 20       | 1.23          |
| (1,1109) | 1:19:A:ILE:H    | 1:53:A:PHE:HD2  | 10       | 1.23          |
| (1,542)  | 1:39:A:VAL:HG21 | 1:43:A:MET:HB3  | 13       | 1.23          |
| (1,473)  | 1:62:A:PHE:HD2  | 1:69:A:LEU:HD21 | 14       | 1.23          |
| (1,473)  | 1:62:A:PHE:HD2  | 1:69:A:LEU:HD21 | 18       | 1.23          |
| (1,275)  | 1:20:A:SER:HA   | 1:53:A:PHE:HD2  | 5        | 1.23          |
| (1,275)  | 1:20:A:SER:HA   | 1:53:A:PHE:HD2  | 7        | 1.23          |
| (1,274)  | 1:20:A:SER:HA   | 1:53:A:PHE:HE2  | 16       | 1.23          |
| (1,274)  | 1:20:A:SER:HA   | 1:53:A:PHE:HE2  | 18       | 1.23          |
| (1,205)  | 1:18:A:LYS:HB3  | 1:53:A:PHE:HD2  | 4        | 1.23          |
| (1,205)  | 1:18:A:LYS:HB2  | 1:53:A:PHE:HD2  | 4        | 1.23          |
| (1,143)  | 1:11:A:PHE:HA   | 1:11:A:PHE:HD2  | 5        | 1.23          |
| (1,143)  | 1:11:A:PHE:HA   | 1:11:A:PHE:HD2  | 12       | 1.23          |
| (1,143)  | 1:11:A:PHE:HA   | 1:11:A:PHE:HD2  | 13       | 1.23          |
| (1,143)  | 1:11:A:PHE:HA   | 1:11:A:PHE:HD2  | 18       | 1.23          |
| (1,75)   | 1:5:A:GLU:HA    | 1:7:A:ILE:HD13  | 6        | 1.23          |
| (1,75)   | 1:5:A:GLU:HA    | 1:7:A:ILE:HD13  | 11       | 1.23          |
| (1,37)   | 1:46:A:ILE:HD11 | 1:58:A:GLU:HB2  | 6        | 1.23          |
| (1,37)   | 1:46:A:ILE:HD11 | 1:58:A:GLU:HB2  | 17       | 1.23          |
| (1,21)   | 1:5:A:GLU:HA    | 1:60:A:ILE:HD13 | 18       | 1.23          |
| (1,1409) | 1:10:A:ARG:HD2  | 1:11:A:PHE:HD2  | 19       | 1.22          |
| (1,1409) | 1:10:A:ARG:HD3  | 1:11:A:PHE:HD2  | 19       | 1.22          |
| (1,1408) | 1:10:A:ARG:HD2  | 1:11:A:PHE:HE2  | 8        | 1.22          |
| (1,1408) | 1:10:A:ARG:HD3  | 1:11:A:PHE:HE2  | 8        | 1.22          |
| (1,1109) | 1:19:A:ILE:H    | 1:53:A:PHE:HD2  | 1        | 1.22          |
| (1,1109) | 1:19:A:ILE:H    | 1:53:A:PHE:HD2  | 5        | 1.22          |
| (1,1109) | 1:19:A:ILE:H    | 1:53:A:PHE:HD2  | 7        | 1.22          |
| (1,848)  | 1:31:A:LEU:HB2  | 1:76:A:VAL:HG23 | 14       | 1.22          |
| (1,727)  | 1:5:A:GLU:H     | 1:60:A:ILE:HD13 | 12       | 1.22          |
| (1,493)  | 1:39:A:VAL:HG21 | 1:40:A:GLN:HB2  | 14       | 1.22          |
| (1,416)  | 1:33:A:SER:HA   | 1:34:A:THR:HG23 | 10       | 1.22          |
| (1,68)   | 1:7:A:ILE:HD11  | 1:74:A:ALA:H    | 14       | 1.22          |
| (1,68)   | 1:7:A:ILE:HD11  | 1:74:A:ALA:H    | 19       | 1.22          |
| (1,1533) | 1:52:A:GLY:HA2  | 1:53:A:PHE:HE1  | 11       | 1.21          |
| (1,1533) | 1:52:A:GLY:HA3  | 1:53:A:PHE:HE1  | 11       | 1.21          |
| (1,1109) | 1:19:A:ILE:H    | 1:53:A:PHE:HD2  | 19       | 1.21          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,861)  | 1:4:A:MET:H     | 1:4:A:MET:HE3   | 13       | 1.21          |
| (1,846)  | 1:72:A:ASP:HA   | 1:76:A:VAL:HG21 | 19       | 1.21          |
| (1,493)  | 1:39:A:VAL:HG21 | 1:40:A:GLN:HB2  | 5        | 1.21          |
| (1,416)  | 1:33:A:SER:HA   | 1:34:A:THR:HG23 | 5        | 1.21          |
| (1,274)  | 1:20:A:SER:HA   | 1:53:A:PHE:HE2  | 6        | 1.21          |
| (1,264)  | 1:19:A:ILE:HG21 | 1:19:A:ILE:HD13 | 11       | 1.21          |
| (1,37)   | 1:46:A:ILE:HD11 | 1:58:A:GLU:HB2  | 1        | 1.21          |
| (1,1533) | 1:52:A:GLY:HA2  | 1:53:A:PHE:HE1  | 5        | 1.2           |
| (1,1533) | 1:52:A:GLY:HA3  | 1:53:A:PHE:HE1  | 5        | 1.2           |
| (1,1409) | 1:10:A:ARG:HD2  | 1:11:A:PHE:HD2  | 10       | 1.2           |
| (1,1409) | 1:10:A:ARG:HD3  | 1:11:A:PHE:HD2  | 10       | 1.2           |
| (1,1408) | 1:10:A:ARG:HD2  | 1:11:A:PHE:HE2  | 17       | 1.2           |
| (1,1408) | 1:10:A:ARG:HD3  | 1:11:A:PHE:HE2  | 17       | 1.2           |
| (1,1109) | 1:19:A:ILE:H    | 1:53:A:PHE:HD2  | 6        | 1.2           |
| (1,542)  | 1:39:A:VAL:HG21 | 1:43:A:MET:HB3  | 2        | 1.2           |
| (1,542)  | 1:39:A:VAL:HG21 | 1:43:A:MET:HB3  | 4        | 1.2           |
| (1,542)  | 1:39:A:VAL:HG21 | 1:43:A:MET:HB3  | 6        | 1.2           |
| (1,542)  | 1:39:A:VAL:HG21 | 1:43:A:MET:HB3  | 8        | 1.2           |
| (1,493)  | 1:39:A:VAL:HG21 | 1:40:A:GLN:HB2  | 11       | 1.2           |
| (1,467)  | 1:39:A:VAL:HA   | 1:69:A:LEU:HD23 | 20       | 1.2           |
| (1,274)  | 1:20:A:SER:HA   | 1:53:A:PHE:HE2  | 4        | 1.2           |
| (1,205)  | 1:18:A:LYS:HB3  | 1:53:A:PHE:HD2  | 17       | 1.2           |
| (1,205)  | 1:18:A:LYS:HB2  | 1:53:A:PHE:HD2  | 17       | 1.2           |
| (1,138)  | 1:10:A:ARG:HD2  | 1:11:A:PHE:HE2  | 9        | 1.2           |
| (1,138)  | 1:10:A:ARG:HD3  | 1:11:A:PHE:HE2  | 9        | 1.2           |
| (1,75)   | 1:5:A:GLU:HA    | 1:7:A:ILE:HD13  | 3        | 1.2           |
| (1,75)   | 1:5:A:GLU:HA    | 1:7:A:ILE:HD13  | 8        | 1.2           |
| (1,68)   | 1:7:A:ILE:HD11  | 1:74:A:ALA:H    | 18       | 1.2           |
| (1,37)   | 1:46:A:ILE:HD11 | 1:58:A:GLU:HB2  | 14       | 1.2           |
| (1,21)   | 1:5:A:GLU:HA    | 1:60:A:ILE:HD13 | 4        | 1.2           |
| (1,1409) | 1:10:A:ARG:HD2  | 1:11:A:PHE:HD2  | 8        | 1.19          |
| (1,1409) | 1:10:A:ARG:HD3  | 1:11:A:PHE:HD2  | 8        | 1.19          |
| (1,1196) | 1:42:A:MET:H    | 1:69:A:LEU:HD23 | 14       | 1.19          |
| (1,1109) | 1:19:A:ILE:H    | 1:53:A:PHE:HD2  | 15       | 1.19          |
| (1,1109) | 1:19:A:ILE:H    | 1:53:A:PHE:HD2  | 20       | 1.19          |
| (1,850)  | 1:31:A:LEU:HB3  | 1:76:A:VAL:HG23 | 14       | 1.19          |
| (1,842)  | 1:75:A:LYS:HA   | 1:76:A:VAL:HG21 | 12       | 1.19          |
| (1,542)  | 1:39:A:VAL:HG21 | 1:43:A:MET:HB3  | 5        | 1.19          |
| (1,542)  | 1:39:A:VAL:HG21 | 1:43:A:MET:HB3  | 20       | 1.19          |
| (1,416)  | 1:33:A:SER:HA   | 1:34:A:THR:HG23 | 1        | 1.19          |
| (1,416)  | 1:33:A:SER:HA   | 1:34:A:THR:HG23 | 11       | 1.19          |
| (1,274)  | 1:20:A:SER:HA   | 1:53:A:PHE:HE2  | 7        | 1.19          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,266)  | 1:12:A:ASP:H    | 1:19:A:ILE:HD13 | 8        | 1.19          |
| (1,205)  | 1:18:A:LYS:HB3  | 1:53:A:PHE:HD2  | 6        | 1.19          |
| (1,205)  | 1:18:A:LYS:HB2  | 1:53:A:PHE:HD2  | 6        | 1.19          |
| (1,37)   | 1:46:A:ILE:HD11 | 1:58:A:GLU:HB2  | 4        | 1.19          |
| (1,37)   | 1:46:A:ILE:HD11 | 1:58:A:GLU:HB2  | 16       | 1.19          |
| (1,1533) | 1:52:A:GLY:HA2  | 1:53:A:PHE:HE1  | 10       | 1.18          |
| (1,1533) | 1:52:A:GLY:HA3  | 1:53:A:PHE:HE1  | 10       | 1.18          |
| (1,1533) | 1:52:A:GLY:HA2  | 1:53:A:PHE:HE1  | 19       | 1.18          |
| (1,1533) | 1:52:A:GLY:HA3  | 1:53:A:PHE:HE1  | 19       | 1.18          |
| (1,1349) | 1:75:A:LYS:H    | 1:76:A:VAL:HG21 | 1        | 1.18          |
| (1,1109) | 1:19:A:ILE:H    | 1:53:A:PHE:HD2  | 4        | 1.18          |
| (1,1109) | 1:19:A:ILE:H    | 1:53:A:PHE:HD2  | 9        | 1.18          |
| (1,1109) | 1:19:A:ILE:H    | 1:53:A:PHE:HD2  | 14       | 1.18          |
| (1,1109) | 1:19:A:ILE:H    | 1:53:A:PHE:HD2  | 16       | 1.18          |
| (1,848)  | 1:31:A:LEU:HB2  | 1:76:A:VAL:HG23 | 6        | 1.18          |
| (1,416)  | 1:33:A:SER:HA   | 1:34:A:THR:HG23 | 12       | 1.18          |
| (1,416)  | 1:33:A:SER:HA   | 1:34:A:THR:HG23 | 16       | 1.18          |
| (1,274)  | 1:20:A:SER:HA   | 1:53:A:PHE:HE2  | 10       | 1.18          |
| (1,274)  | 1:20:A:SER:HA   | 1:53:A:PHE:HE2  | 19       | 1.18          |
| (1,266)  | 1:12:A:ASP:H    | 1:19:A:ILE:HD13 | 7        | 1.18          |
| (1,264)  | 1:19:A:ILE:HG21 | 1:19:A:ILE:HD13 | 12       | 1.18          |
| (1,1533) | 1:52:A:GLY:HA2  | 1:53:A:PHE:HE1  | 7        | 1.17          |
| (1,1533) | 1:52:A:GLY:HA3  | 1:53:A:PHE:HE1  | 7        | 1.17          |
| (1,1533) | 1:52:A:GLY:HA2  | 1:53:A:PHE:HE1  | 15       | 1.17          |
| (1,1533) | 1:52:A:GLY:HA3  | 1:53:A:PHE:HE1  | 15       | 1.17          |
| (1,1467) | 1:33:A:SER:HB2  | 1:34:A:THR:HG23 | 6        | 1.17          |
| (1,1467) | 1:33:A:SER:HB3  | 1:34:A:THR:HG23 | 6        | 1.17          |
| (1,1431) | 1:20:A:SER:HB2  | 1:53:A:PHE:HE2  | 10       | 1.17          |
| (1,1431) | 1:20:A:SER:HB3  | 1:53:A:PHE:HE2  | 10       | 1.17          |
| (1,1431) | 1:20:A:SER:HB2  | 1:53:A:PHE:HE2  | 19       | 1.17          |
| (1,1431) | 1:20:A:SER:HB3  | 1:53:A:PHE:HE2  | 19       | 1.17          |
| (1,1357) | 1:76:A:VAL:H    | 1:76:A:VAL:HG21 | 12       | 1.17          |
| (1,1349) | 1:75:A:LYS:H    | 1:76:A:VAL:HG21 | 17       | 1.17          |
| (1,1196) | 1:42:A:MET:H    | 1:69:A:LEU:HD23 | 18       | 1.17          |
| (1,1109) | 1:19:A:ILE:H    | 1:53:A:PHE:HD2  | 2        | 1.17          |
| (1,1109) | 1:19:A:ILE:H    | 1:53:A:PHE:HD2  | 8        | 1.17          |
| (1,576)  | 1:46:A:ILE:HD12 | 1:63:A:CYS:H    | 5        | 1.17          |
| (1,333)  | 1:11:A:PHE:HE1  | 1:24:A:LEU:HD21 | 2        | 1.17          |
| (1,333)  | 1:11:A:PHE:HE1  | 1:24:A:LEU:HD21 | 20       | 1.17          |
| (1,264)  | 1:19:A:ILE:HG21 | 1:19:A:ILE:HD13 | 4        | 1.17          |
| (1,75)   | 1:5:A:GLU:HA    | 1:7:A:ILE:HD13  | 2        | 1.17          |
| (1,75)   | 1:5:A:GLU:HA    | 1:7:A:ILE:HD13  | 19       | 1.17          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,37)   | 1:46:A:ILE:HD11 | 1:58:A:GLU:HB2  | 2        | 1.17          |
| (1,21)   | 1:5:A:GLU:HA    | 1:60:A:ILE:HD13 | 6        | 1.17          |
| (1,1533) | 1:52:A:GLY:HA2  | 1:53:A:PHE:HE1  | 1        | 1.16          |
| (1,1533) | 1:52:A:GLY:HA3  | 1:53:A:PHE:HE1  | 1        | 1.16          |
| (1,1349) | 1:75:A:LYS:H    | 1:76:A:VAL:HG21 | 14       | 1.16          |
| (1,1135) | 1:25:A:THR:H    | 1:43:A:MET:HE3  | 13       | 1.16          |
| (1,846)  | 1:72:A:ASP:HA   | 1:76:A:VAL:HG21 | 4        | 1.16          |
| (1,578)  | 1:46:A:ILE:HD12 | 1:62:A:PHE:HD1  | 14       | 1.16          |
| (1,578)  | 1:46:A:ILE:HD13 | 1:62:A:PHE:HD1  | 14       | 1.16          |
| (1,576)  | 1:46:A:ILE:HD12 | 1:63:A:CYS:H    | 13       | 1.16          |
| (1,542)  | 1:39:A:VAL:HG21 | 1:43:A:MET:HB3  | 3        | 1.16          |
| (1,542)  | 1:39:A:VAL:HG21 | 1:43:A:MET:HB3  | 12       | 1.16          |
| (1,264)  | 1:19:A:ILE:HG21 | 1:19:A:ILE:HD13 | 15       | 1.16          |
| (1,163)  | 1:12:A:ASP:HB2  | 1:19:A:ILE:HD13 | 3        | 1.16          |
| (1,163)  | 1:12:A:ASP:HB2  | 1:19:A:ILE:HD13 | 8        | 1.16          |
| (1,68)   | 1:7:A:ILE:HD11  | 1:74:A:ALA:H    | 10       | 1.16          |
| (1,68)   | 1:7:A:ILE:HD11  | 1:74:A:ALA:H    | 13       | 1.16          |
| (1,68)   | 1:7:A:ILE:HD11  | 1:74:A:ALA:H    | 16       | 1.16          |
| (1,1533) | 1:52:A:GLY:HA2  | 1:53:A:PHE:HE1  | 4        | 1.15          |
| (1,1533) | 1:52:A:GLY:HA3  | 1:53:A:PHE:HE1  | 4        | 1.15          |
| (1,1533) | 1:52:A:GLY:HA2  | 1:53:A:PHE:HE1  | 6        | 1.15          |
| (1,1533) | 1:52:A:GLY:HA3  | 1:53:A:PHE:HE1  | 6        | 1.15          |
| (1,1533) | 1:52:A:GLY:HA2  | 1:53:A:PHE:HE1  | 18       | 1.15          |
| (1,1533) | 1:52:A:GLY:HA3  | 1:53:A:PHE:HE1  | 18       | 1.15          |
| (1,1357) | 1:76:A:VAL:H    | 1:76:A:VAL:HG21 | 13       | 1.15          |
| (1,1109) | 1:19:A:ILE:H    | 1:53:A:PHE:HD2  | 11       | 1.15          |
| (1,846)  | 1:72:A:ASP:HA   | 1:76:A:VAL:HG21 | 7        | 1.15          |
| (1,765)  | 1:60:A:ILE:HD12 | 1:63:A:CYS:HB3  | 15       | 1.15          |
| (1,765)  | 1:60:A:ILE:HD12 | 1:63:A:CYS:HB2  | 15       | 1.15          |
| (1,542)  | 1:39:A:VAL:HG21 | 1:43:A:MET:HB3  | 15       | 1.15          |
| (1,493)  | 1:39:A:VAL:HG21 | 1:40:A:GLN:HB2  | 18       | 1.15          |
| (1,467)  | 1:39:A:VAL:HA   | 1:69:A:LEU:HD23 | 5        | 1.15          |
| (1,363)  | 1:27:A:ALA:HB1  | 1:28:A:LEU:HD21 | 11       | 1.15          |
| (1,264)  | 1:19:A:ILE:HG21 | 1:19:A:ILE:HD13 | 2        | 1.15          |
| (1,205)  | 1:18:A:LYS:HB3  | 1:53:A:PHE:HD2  | 7        | 1.15          |
| (1,205)  | 1:18:A:LYS:HB2  | 1:53:A:PHE:HD2  | 7        | 1.15          |
| (1,205)  | 1:18:A:LYS:HB3  | 1:53:A:PHE:HD2  | 19       | 1.15          |
| (1,205)  | 1:18:A:LYS:HB2  | 1:53:A:PHE:HD2  | 19       | 1.15          |
| (1,1467) | 1:33:A:SER:HB2  | 1:34:A:THR:HG23 | 18       | 1.14          |
| (1,1467) | 1:33:A:SER:HB3  | 1:34:A:THR:HG23 | 18       | 1.14          |
| (1,1467) | 1:33:A:SER:HB2  | 1:34:A:THR:HG23 | 20       | 1.14          |
| (1,1467) | 1:33:A:SER:HB3  | 1:34:A:THR:HG23 | 20       | 1.14          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1357) | 1:76:A:VAL:H    | 1:76:A:VAL:HG21 | 9        | 1.14          |
| (1,1357) | 1:76:A:VAL:H    | 1:76:A:VAL:HG21 | 15       | 1.14          |
| (1,765)  | 1:60:A:ILE:HD12 | 1:63:A:CYS:HB3  | 9        | 1.14          |
| (1,765)  | 1:60:A:ILE:HD12 | 1:63:A:CYS:HB2  | 9        | 1.14          |
| (1,576)  | 1:46:A:ILE:HD12 | 1:63:A:CYS:H    | 11       | 1.14          |
| (1,542)  | 1:39:A:VAL:HG21 | 1:43:A:MET:HB3  | 7        | 1.14          |
| (1,542)  | 1:39:A:VAL:HG21 | 1:43:A:MET:HB3  | 17       | 1.14          |
| (1,542)  | 1:39:A:VAL:HG21 | 1:43:A:MET:HB3  | 19       | 1.14          |
| (1,416)  | 1:33:A:SER:HA   | 1:34:A:THR:HG23 | 3        | 1.14          |
| (1,264)  | 1:19:A:ILE:HG21 | 1:19:A:ILE:HD13 | 13       | 1.14          |
| (1,264)  | 1:19:A:ILE:HG21 | 1:19:A:ILE:HD13 | 17       | 1.14          |
| (1,1467) | 1:33:A:SER:HB2  | 1:34:A:THR:HG23 | 2        | 1.13          |
| (1,1467) | 1:33:A:SER:HB3  | 1:34:A:THR:HG23 | 2        | 1.13          |
| (1,1467) | 1:33:A:SER:HB2  | 1:34:A:THR:HG23 | 7        | 1.13          |
| (1,1467) | 1:33:A:SER:HB3  | 1:34:A:THR:HG23 | 7        | 1.13          |
| (1,1357) | 1:76:A:VAL:H    | 1:76:A:VAL:HG21 | 2        | 1.13          |
| (1,1357) | 1:76:A:VAL:H    | 1:76:A:VAL:HG21 | 3        | 1.13          |
| (1,1357) | 1:76:A:VAL:H    | 1:76:A:VAL:HG21 | 5        | 1.13          |
| (1,1357) | 1:76:A:VAL:H    | 1:76:A:VAL:HG21 | 11       | 1.13          |
| (1,1349) | 1:75:A:LYS:H    | 1:76:A:VAL:HG21 | 6        | 1.13          |
| (1,1349) | 1:75:A:LYS:H    | 1:76:A:VAL:HG21 | 13       | 1.13          |
| (1,542)  | 1:39:A:VAL:HG21 | 1:43:A:MET:HB3  | 14       | 1.13          |
| (1,416)  | 1:33:A:SER:HA   | 1:34:A:THR:HG23 | 2        | 1.13          |
| (1,416)  | 1:33:A:SER:HA   | 1:34:A:THR:HG23 | 6        | 1.13          |
| (1,274)  | 1:20:A:SER:HA   | 1:53:A:PHE:HE2  | 5        | 1.13          |
| (1,274)  | 1:20:A:SER:HA   | 1:53:A:PHE:HE2  | 11       | 1.13          |
| (1,264)  | 1:19:A:ILE:HG21 | 1:19:A:ILE:HD13 | 3        | 1.13          |
| (1,68)   | 1:7:A:ILE:HD11  | 1:74:A:ALA:H    | 4        | 1.13          |
| (1,68)   | 1:7:A:ILE:HD11  | 1:74:A:ALA:H    | 6        | 1.13          |
| (1,1533) | 1:52:A:GLY:HA2  | 1:53:A:PHE:HE1  | 2        | 1.12          |
| (1,1533) | 1:52:A:GLY:HA3  | 1:53:A:PHE:HE1  | 2        | 1.12          |
| (1,1533) | 1:52:A:GLY:HA2  | 1:53:A:PHE:HE1  | 8        | 1.12          |
| (1,1533) | 1:52:A:GLY:HA3  | 1:53:A:PHE:HE1  | 8        | 1.12          |
| (1,1533) | 1:52:A:GLY:HA2  | 1:53:A:PHE:HE1  | 17       | 1.12          |
| (1,1533) | 1:52:A:GLY:HA3  | 1:53:A:PHE:HE1  | 17       | 1.12          |
| (1,1532) | 1:52:A:GLY:HA2  | 1:53:A:PHE:HD1  | 11       | 1.12          |
| (1,1532) | 1:52:A:GLY:HA3  | 1:53:A:PHE:HD1  | 11       | 1.12          |
| (1,1467) | 1:33:A:SER:HB2  | 1:34:A:THR:HG23 | 15       | 1.12          |
| (1,1467) | 1:33:A:SER:HB3  | 1:34:A:THR:HG23 | 15       | 1.12          |
| (1,1432) | 1:20:A:SER:HB2  | 1:53:A:PHE:HD2  | 2        | 1.12          |
| (1,1432) | 1:20:A:SER:HB3  | 1:53:A:PHE:HD2  | 2        | 1.12          |
| (1,1357) | 1:76:A:VAL:H    | 1:76:A:VAL:HG21 | 14       | 1.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1357) | 1:76:A:VAL:H    | 1:76:A:VAL:HG21 | 18       | 1.12          |
| (1,1349) | 1:75:A:LYS:H    | 1:76:A:VAL:HG21 | 4        | 1.12          |
| (1,1349) | 1:75:A:LYS:H    | 1:76:A:VAL:HG21 | 16       | 1.12          |
| (1,1109) | 1:19:A:ILE:H    | 1:53:A:PHE:HD2  | 17       | 1.12          |
| (1,846)  | 1:72:A:ASP:HA   | 1:76:A:VAL:HG21 | 10       | 1.12          |
| (1,765)  | 1:60:A:ILE:HD12 | 1:63:A:CYS:HB3  | 16       | 1.12          |
| (1,765)  | 1:60:A:ILE:HD12 | 1:63:A:CYS:HB2  | 16       | 1.12          |
| (1,727)  | 1:5:A:GLU:H     | 1:60:A:ILE:HD13 | 13       | 1.12          |
| (1,578)  | 1:46:A:ILE:HD12 | 1:62:A:PHE:HD1  | 1        | 1.12          |
| (1,578)  | 1:46:A:ILE:HD13 | 1:62:A:PHE:HD1  | 1        | 1.12          |
| (1,542)  | 1:39:A:VAL:HG21 | 1:43:A:MET:HB3  | 9        | 1.12          |
| (1,467)  | 1:39:A:VAL:HA   | 1:69:A:LEU:HD23 | 9        | 1.12          |
| (1,467)  | 1:39:A:VAL:HA   | 1:69:A:LEU:HD23 | 10       | 1.12          |
| (1,467)  | 1:39:A:VAL:HA   | 1:69:A:LEU:HD23 | 11       | 1.12          |
| (1,416)  | 1:33:A:SER:HA   | 1:34:A:THR:HG23 | 18       | 1.12          |
| (1,390)  | 1:10:A:ARG:HB2  | 1:11:A:PHE:HE2  | 13       | 1.12          |
| (1,390)  | 1:10:A:ARG:HB3  | 1:11:A:PHE:HE2  | 13       | 1.12          |
| (1,333)  | 1:11:A:PHE:HE1  | 1:24:A:LEU:HD21 | 6        | 1.12          |
| (1,333)  | 1:11:A:PHE:HE1  | 1:24:A:LEU:HD21 | 10       | 1.12          |
| (1,305)  | 1:11:A:PHE:HE1  | 1:24:A:LEU:HA   | 4        | 1.12          |
| (1,264)  | 1:19:A:ILE:HG21 | 1:19:A:ILE:HD13 | 5        | 1.12          |
| (1,264)  | 1:19:A:ILE:HG21 | 1:19:A:ILE:HD13 | 7        | 1.12          |
| (1,264)  | 1:19:A:ILE:HG21 | 1:19:A:ILE:HD13 | 8        | 1.12          |
| (1,205)  | 1:18:A:LYS:HB3  | 1:53:A:PHE:HD2  | 10       | 1.12          |
| (1,205)  | 1:18:A:LYS:HB2  | 1:53:A:PHE:HD2  | 10       | 1.12          |
| (1,75)   | 1:5:A:GLU:HA    | 1:7:A:ILE:HD13  | 4        | 1.12          |
| (1,68)   | 1:7:A:ILE:HD11  | 1:74:A:ALA:H    | 2        | 1.12          |
| (1,1533) | 1:52:A:GLY:HA2  | 1:53:A:PHE:HE1  | 9        | 1.11          |
| (1,1533) | 1:52:A:GLY:HA3  | 1:53:A:PHE:HE1  | 9        | 1.11          |
| (1,1533) | 1:52:A:GLY:HA2  | 1:53:A:PHE:HE1  | 16       | 1.11          |
| (1,1533) | 1:52:A:GLY:HA3  | 1:53:A:PHE:HE1  | 16       | 1.11          |
| (1,1532) | 1:52:A:GLY:HA2  | 1:53:A:PHE:HD1  | 10       | 1.11          |
| (1,1532) | 1:52:A:GLY:HA3  | 1:53:A:PHE:HD1  | 10       | 1.11          |
| (1,1467) | 1:33:A:SER:HB2  | 1:34:A:THR:HG23 | 19       | 1.11          |
| (1,1467) | 1:33:A:SER:HB3  | 1:34:A:THR:HG23 | 19       | 1.11          |
| (1,1357) | 1:76:A:VAL:H    | 1:76:A:VAL:HG21 | 20       | 1.11          |
| (1,765)  | 1:60:A:ILE:HD12 | 1:63:A:CYS:HB3  | 20       | 1.11          |
| (1,765)  | 1:60:A:ILE:HD12 | 1:63:A:CYS:HB2  | 20       | 1.11          |
| (1,578)  | 1:46:A:ILE:HD12 | 1:62:A:PHE:HD1  | 12       | 1.11          |
| (1,578)  | 1:46:A:ILE:HD13 | 1:62:A:PHE:HD1  | 12       | 1.11          |
| (1,578)  | 1:46:A:ILE:HD12 | 1:62:A:PHE:HD1  | 13       | 1.11          |
| (1,578)  | 1:46:A:ILE:HD13 | 1:62:A:PHE:HD1  | 13       | 1.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,578)  | 1:46:A:ILE:HD12 | 1:62:A:PHE:HD1  | 16       | 1.11          |
| (1,578)  | 1:46:A:ILE:HD13 | 1:62:A:PHE:HD1  | 16       | 1.11          |
| (1,578)  | 1:46:A:ILE:HD12 | 1:62:A:PHE:HD1  | 17       | 1.11          |
| (1,578)  | 1:46:A:ILE:HD13 | 1:62:A:PHE:HD1  | 17       | 1.11          |
| (1,578)  | 1:46:A:ILE:HD12 | 1:62:A:PHE:HD1  | 18       | 1.11          |
| (1,578)  | 1:46:A:ILE:HD13 | 1:62:A:PHE:HD1  | 18       | 1.11          |
| (1,467)  | 1:39:A:VAL:HA   | 1:69:A:LEU:HD23 | 15       | 1.11          |
| (1,416)  | 1:33:A:SER:HA   | 1:34:A:THR:HG23 | 14       | 1.11          |
| (1,390)  | 1:10:A:ARG:HB2  | 1:11:A:PHE:HE2  | 12       | 1.11          |
| (1,390)  | 1:10:A:ARG:HB3  | 1:11:A:PHE:HE2  | 12       | 1.11          |
| (1,345)  | 1:25:A:THR:HG23 | 1:26:A:ASP:HA   | 7        | 1.11          |
| (1,264)  | 1:19:A:ILE:HG21 | 1:19:A:ILE:HD13 | 9        | 1.11          |
| (1,205)  | 1:18:A:LYS:HB3  | 1:53:A:PHE:HD2  | 15       | 1.11          |
| (1,205)  | 1:18:A:LYS:HB2  | 1:53:A:PHE:HD2  | 15       | 1.11          |
| (1,182)  | 1:13:A:THR:HG21 | 1:14:A:ASN:HA   | 8        | 1.11          |
| (1,163)  | 1:12:A:ASP:HB2  | 1:19:A:ILE:HD13 | 12       | 1.11          |
| (1,142)  | 1:10:A:ARG:HD3  | 1:11:A:PHE:HD2  | 9        | 1.11          |
| (1,75)   | 1:5:A:GLU:HA    | 1:7:A:ILE:HD13  | 18       | 1.11          |
| (1,68)   | 1:7:A:ILE:HD11  | 1:74:A:ALA:H    | 1        | 1.11          |
| (1,68)   | 1:7:A:ILE:HD11  | 1:74:A:ALA:H    | 3        | 1.11          |
| (1,68)   | 1:7:A:ILE:HD11  | 1:74:A:ALA:H    | 7        | 1.11          |
| (1,68)   | 1:7:A:ILE:HD11  | 1:74:A:ALA:H    | 15       | 1.11          |
| (1,1533) | 1:52:A:GLY:HA2  | 1:53:A:PHE:HE1  | 14       | 1.1           |
| (1,1533) | 1:52:A:GLY:HA3  | 1:53:A:PHE:HE1  | 14       | 1.1           |
| (1,1533) | 1:52:A:GLY:HA2  | 1:53:A:PHE:HE1  | 20       | 1.1           |
| (1,1533) | 1:52:A:GLY:HA3  | 1:53:A:PHE:HE1  | 20       | 1.1           |
| (1,1532) | 1:52:A:GLY:HA2  | 1:53:A:PHE:HD1  | 7        | 1.1           |
| (1,1532) | 1:52:A:GLY:HA3  | 1:53:A:PHE:HD1  | 7        | 1.1           |
| (1,1532) | 1:52:A:GLY:HA2  | 1:53:A:PHE:HD1  | 19       | 1.1           |
| (1,1532) | 1:52:A:GLY:HA3  | 1:53:A:PHE:HD1  | 19       | 1.1           |
| (1,1357) | 1:76:A:VAL:H    | 1:76:A:VAL:HG21 | 8        | 1.1           |
| (1,1135) | 1:25:A:THR:H    | 1:43:A:MET:HE3  | 5        | 1.1           |
| (1,848)  | 1:31:A:LEU:HB2  | 1:76:A:VAL:HG23 | 8        | 1.1           |
| (1,848)  | 1:31:A:LEU:HB2  | 1:76:A:VAL:HG23 | 16       | 1.1           |
| (1,578)  | 1:46:A:ILE:HD12 | 1:62:A:PHE:HD1  | 2        | 1.1           |
| (1,578)  | 1:46:A:ILE:HD13 | 1:62:A:PHE:HD1  | 2        | 1.1           |
| (1,578)  | 1:46:A:ILE:HD12 | 1:62:A:PHE:HD1  | 4        | 1.1           |
| (1,578)  | 1:46:A:ILE:HD13 | 1:62:A:PHE:HD1  | 4        | 1.1           |
| (1,578)  | 1:46:A:ILE:HD12 | 1:62:A:PHE:HD1  | 6        | 1.1           |
| (1,578)  | 1:46:A:ILE:HD13 | 1:62:A:PHE:HD1  | 6        | 1.1           |
| (1,578)  | 1:46:A:ILE:HD12 | 1:62:A:PHE:HD1  | 9        | 1.1           |
| (1,578)  | 1:46:A:ILE:HD13 | 1:62:A:PHE:HD1  | 9        | 1.1           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,578)  | 1:46:A:ILE:HD12 | 1:62:A:PHE:HD1  | 20       | 1.1           |
| (1,578)  | 1:46:A:ILE:HD13 | 1:62:A:PHE:HD1  | 20       | 1.1           |
| (1,576)  | 1:46:A:ILE:HD12 | 1:63:A:CYS:H    | 20       | 1.1           |
| (1,552)  | 1:39:A:VAL:HG21 | 1:43:A:MET:HG2  | 4        | 1.1           |
| (1,552)  | 1:39:A:VAL:HG21 | 1:43:A:MET:HG3  | 4        | 1.1           |
| (1,552)  | 1:39:A:VAL:HG21 | 1:43:A:MET:HG2  | 20       | 1.1           |
| (1,552)  | 1:39:A:VAL:HG21 | 1:43:A:MET:HG3  | 20       | 1.1           |
| (1,542)  | 1:39:A:VAL:HG21 | 1:43:A:MET:HB3  | 1        | 1.1           |
| (1,542)  | 1:39:A:VAL:HG21 | 1:43:A:MET:HB3  | 10       | 1.1           |
| (1,493)  | 1:39:A:VAL:HG21 | 1:40:A:GLN:HB2  | 12       | 1.1           |
| (1,333)  | 1:11:A:PHE:HE1  | 1:24:A:LEU:HD21 | 3        | 1.1           |
| (1,333)  | 1:11:A:PHE:HE1  | 1:24:A:LEU:HD21 | 7        | 1.1           |
| (1,264)  | 1:19:A:ILE:HG21 | 1:19:A:ILE:HD13 | 1        | 1.1           |
| (1,264)  | 1:19:A:ILE:HG21 | 1:19:A:ILE:HD13 | 14       | 1.1           |
| (1,68)   | 1:7:A:ILE:HD11  | 1:74:A:ALA:H    | 9        | 1.1           |
| (1,68)   | 1:7:A:ILE:HD11  | 1:74:A:ALA:H    | 11       | 1.1           |
| (1,1532) | 1:52:A:GLY:HA2  | 1:53:A:PHE:HD1  | 15       | 1.09          |
| (1,1532) | 1:52:A:GLY:HA3  | 1:53:A:PHE:HD1  | 15       | 1.09          |
| (1,1467) | 1:33:A:SER:HB2  | 1:34:A:THR:HG23 | 8        | 1.09          |
| (1,1467) | 1:33:A:SER:HB3  | 1:34:A:THR:HG23 | 8        | 1.09          |
| (1,1357) | 1:76:A:VAL:H    | 1:76:A:VAL:HG21 | 1        | 1.09          |
| (1,1357) | 1:76:A:VAL:H    | 1:76:A:VAL:HG21 | 10       | 1.09          |
| (1,1357) | 1:76:A:VAL:H    | 1:76:A:VAL:HG21 | 16       | 1.09          |
| (1,850)  | 1:31:A:LEU:HB3  | 1:76:A:VAL:HG23 | 16       | 1.09          |
| (1,809)  | 1:69:A:LEU:HD21 | 1:70:A:MET:HG2  | 4        | 1.09          |
| (1,809)  | 1:69:A:LEU:HD21 | 1:70:A:MET:HG3  | 4        | 1.09          |
| (1,578)  | 1:46:A:ILE:HD12 | 1:62:A:PHE:HD1  | 8        | 1.09          |
| (1,578)  | 1:46:A:ILE:HD13 | 1:62:A:PHE:HD1  | 8        | 1.09          |
| (1,576)  | 1:46:A:ILE:HD12 | 1:63:A:CYS:H    | 18       | 1.09          |
| (1,552)  | 1:39:A:VAL:HG21 | 1:43:A:MET:HG2  | 8        | 1.09          |
| (1,552)  | 1:39:A:VAL:HG21 | 1:43:A:MET:HG3  | 8        | 1.09          |
| (1,542)  | 1:39:A:VAL:HG21 | 1:43:A:MET:HB3  | 16       | 1.09          |
| (1,266)  | 1:12:A:ASP:H    | 1:19:A:ILE:HD13 | 17       | 1.09          |
| (1,264)  | 1:19:A:ILE:HG21 | 1:19:A:ILE:HD13 | 6        | 1.09          |
| (1,264)  | 1:19:A:ILE:HG21 | 1:19:A:ILE:HD13 | 16       | 1.09          |
| (1,264)  | 1:19:A:ILE:HG21 | 1:19:A:ILE:HD13 | 20       | 1.09          |
| (1,205)  | 1:18:A:LYS:HB3  | 1:53:A:PHE:HD2  | 11       | 1.09          |
| (1,205)  | 1:18:A:LYS:HB2  | 1:53:A:PHE:HD2  | 11       | 1.09          |
| (1,68)   | 1:7:A:ILE:HD11  | 1:74:A:ALA:H    | 12       | 1.09          |
| (1,1532) | 1:52:A:GLY:HA2  | 1:53:A:PHE:HD1  | 18       | 1.08          |
| (1,1532) | 1:52:A:GLY:HA3  | 1:53:A:PHE:HD1  | 18       | 1.08          |
| (1,1357) | 1:76:A:VAL:H    | 1:76:A:VAL:HG21 | 4        | 1.08          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1357) | 1:76:A:VAL:H    | 1:76:A:VAL:HG21 | 7        | 1.08          |
| (1,1357) | 1:76:A:VAL:H    | 1:76:A:VAL:HG21 | 19       | 1.08          |
| (1,848)  | 1:31:A:LEU:HB2  | 1:76:A:VAL:HG23 | 5        | 1.08          |
| (1,848)  | 1:31:A:LEU:HB2  | 1:76:A:VAL:HG23 | 13       | 1.08          |
| (1,776)  | 1:62:A:PHE:HD2  | 1:67:A:PRO:HG2  | 5        | 1.08          |
| (1,776)  | 1:62:A:PHE:HD2  | 1:67:A:PRO:HG2  | 8        | 1.08          |
| (1,776)  | 1:62:A:PHE:HD2  | 1:67:A:PRO:HG2  | 20       | 1.08          |
| (1,578)  | 1:46:A:ILE:HD12 | 1:62:A:PHE:HD1  | 5        | 1.08          |
| (1,578)  | 1:46:A:ILE:HD13 | 1:62:A:PHE:HD1  | 5        | 1.08          |
| (1,576)  | 1:46:A:ILE:HD12 | 1:63:A:CYS:H    | 10       | 1.08          |
| (1,576)  | 1:46:A:ILE:HD12 | 1:63:A:CYS:H    | 15       | 1.08          |
| (1,467)  | 1:39:A:VAL:HA   | 1:69:A:LEU:HD23 | 7        | 1.08          |
| (1,416)  | 1:33:A:SER:HA   | 1:34:A:THR:HG23 | 19       | 1.08          |
| (1,345)  | 1:25:A:THR:HG23 | 1:26:A:ASP:HA   | 19       | 1.08          |
| (1,305)  | 1:11:A:PHE:HE1  | 1:24:A:LEU:HA   | 2        | 1.08          |
| (1,305)  | 1:11:A:PHE:HE1  | 1:24:A:LEU:HA   | 6        | 1.08          |
| (1,264)  | 1:19:A:ILE:HG21 | 1:19:A:ILE:HD13 | 18       | 1.08          |
| (1,70)   | 1:7:A:ILE:HD12  | 1:77:A:PHE:HD2  | 16       | 1.08          |
| (1,1467) | 1:33:A:SER:HB2  | 1:34:A:THR:HG23 | 17       | 1.07          |
| (1,1467) | 1:33:A:SER:HB3  | 1:34:A:THR:HG23 | 17       | 1.07          |
| (1,1357) | 1:76:A:VAL:H    | 1:76:A:VAL:HG21 | 6        | 1.07          |
| (1,1357) | 1:76:A:VAL:H    | 1:76:A:VAL:HG21 | 17       | 1.07          |
| (1,776)  | 1:62:A:PHE:HD2  | 1:67:A:PRO:HG2  | 3        | 1.07          |
| (1,776)  | 1:62:A:PHE:HD2  | 1:67:A:PRO:HG2  | 7        | 1.07          |
| (1,776)  | 1:62:A:PHE:HD2  | 1:67:A:PRO:HG2  | 11       | 1.07          |
| (1,776)  | 1:62:A:PHE:HD2  | 1:67:A:PRO:HG2  | 14       | 1.07          |
| (1,776)  | 1:62:A:PHE:HD2  | 1:67:A:PRO:HG2  | 19       | 1.07          |
| (1,578)  | 1:46:A:ILE:HD12 | 1:62:A:PHE:HD1  | 3        | 1.07          |
| (1,578)  | 1:46:A:ILE:HD13 | 1:62:A:PHE:HD1  | 3        | 1.07          |
| (1,578)  | 1:46:A:ILE:HD12 | 1:62:A:PHE:HD1  | 10       | 1.07          |
| (1,578)  | 1:46:A:ILE:HD13 | 1:62:A:PHE:HD1  | 10       | 1.07          |
| (1,578)  | 1:46:A:ILE:HD12 | 1:62:A:PHE:HD1  | 11       | 1.07          |
| (1,578)  | 1:46:A:ILE:HD13 | 1:62:A:PHE:HD1  | 11       | 1.07          |
| (1,578)  | 1:46:A:ILE:HD12 | 1:62:A:PHE:HD1  | 15       | 1.07          |
| (1,578)  | 1:46:A:ILE:HD13 | 1:62:A:PHE:HD1  | 15       | 1.07          |
| (1,576)  | 1:46:A:ILE:HD12 | 1:63:A:CYS:H    | 3        | 1.07          |
| (1,493)  | 1:39:A:VAL:HG21 | 1:40:A:GLN:HB2  | 13       | 1.07          |
| (1,467)  | 1:39:A:VAL:HA   | 1:69:A:LEU:HD23 | 3        | 1.07          |
| (1,416)  | 1:33:A:SER:HA   | 1:34:A:THR:HG23 | 7        | 1.07          |
| (1,345)  | 1:25:A:THR:HG23 | 1:26:A:ASP:HA   | 17       | 1.07          |
| (1,345)  | 1:25:A:THR:HG23 | 1:26:A:ASP:HA   | 20       | 1.07          |
| (1,266)  | 1:12:A:ASP:H    | 1:19:A:ILE:HD13 | 15       | 1.07          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,264)  | 1:19:A:ILE:HG21 | 1:19:A:ILE:HD13 | 10       | 1.07          |
| (1,264)  | 1:19:A:ILE:HG21 | 1:19:A:ILE:HD13 | 19       | 1.07          |
| (1,142)  | 1:10:A:ARG:HD3  | 1:11:A:PHE:HD2  | 1        | 1.07          |
| (1,138)  | 1:10:A:ARG:HD2  | 1:11:A:PHE:HE2  | 13       | 1.07          |
| (1,138)  | 1:10:A:ARG:HD3  | 1:11:A:PHE:HE2  | 13       | 1.07          |
| (1,1532) | 1:52:A:GLY:HA2  | 1:53:A:PHE:HD1  | 5        | 1.06          |
| (1,1532) | 1:52:A:GLY:HA3  | 1:53:A:PHE:HD1  | 5        | 1.06          |
| (1,1467) | 1:33:A:SER:HB2  | 1:34:A:THR:HG23 | 14       | 1.06          |
| (1,1467) | 1:33:A:SER:HB3  | 1:34:A:THR:HG23 | 14       | 1.06          |
| (1,848)  | 1:31:A:LEU:HB2  | 1:76:A:VAL:HG23 | 4        | 1.06          |
| (1,776)  | 1:62:A:PHE:HD2  | 1:67:A:PRO:HG2  | 2        | 1.06          |
| (1,776)  | 1:62:A:PHE:HD2  | 1:67:A:PRO:HG2  | 4        | 1.06          |
| (1,776)  | 1:62:A:PHE:HD2  | 1:67:A:PRO:HG2  | 6        | 1.06          |
| (1,776)  | 1:62:A:PHE:HD2  | 1:67:A:PRO:HG2  | 9        | 1.06          |
| (1,776)  | 1:62:A:PHE:HD2  | 1:67:A:PRO:HG2  | 10       | 1.06          |
| (1,776)  | 1:62:A:PHE:HD2  | 1:67:A:PRO:HG2  | 15       | 1.06          |
| (1,776)  | 1:62:A:PHE:HD2  | 1:67:A:PRO:HG2  | 16       | 1.06          |
| (1,776)  | 1:62:A:PHE:HD2  | 1:67:A:PRO:HG2  | 17       | 1.06          |
| (1,776)  | 1:62:A:PHE:HD2  | 1:67:A:PRO:HG2  | 18       | 1.06          |
| (1,765)  | 1:60:A:ILE:HD12 | 1:63:A:CYS:HB3  | 3        | 1.06          |
| (1,765)  | 1:60:A:ILE:HD12 | 1:63:A:CYS:HB2  | 3        | 1.06          |
| (1,576)  | 1:46:A:ILE:HD12 | 1:63:A:CYS:H    | 6        | 1.06          |
| (1,576)  | 1:46:A:ILE:HD12 | 1:63:A:CYS:H    | 12       | 1.06          |
| (1,467)  | 1:39:A:VAL:HA   | 1:69:A:LEU:HD23 | 19       | 1.06          |
| (1,416)  | 1:33:A:SER:HA   | 1:34:A:THR:HG23 | 8        | 1.06          |
| (1,416)  | 1:33:A:SER:HA   | 1:34:A:THR:HG23 | 15       | 1.06          |
| (1,416)  | 1:33:A:SER:HA   | 1:34:A:THR:HG23 | 17       | 1.06          |
| (1,345)  | 1:25:A:THR:HG23 | 1:26:A:ASP:HA   | 2        | 1.06          |
| (1,266)  | 1:12:A:ASP:H    | 1:19:A:ILE:HD13 | 12       | 1.06          |
| (1,68)   | 1:7:A:ILE:HD11  | 1:74:A:ALA:H    | 17       | 1.06          |
| (1,1532) | 1:52:A:GLY:HA2  | 1:53:A:PHE:HD1  | 1        | 1.05          |
| (1,1532) | 1:52:A:GLY:HA3  | 1:53:A:PHE:HD1  | 1        | 1.05          |
| (1,1467) | 1:33:A:SER:HB2  | 1:34:A:THR:HG23 | 16       | 1.05          |
| (1,1467) | 1:33:A:SER:HB3  | 1:34:A:THR:HG23 | 16       | 1.05          |
| (1,776)  | 1:62:A:PHE:HD2  | 1:67:A:PRO:HG2  | 1        | 1.05          |
| (1,776)  | 1:62:A:PHE:HD2  | 1:67:A:PRO:HG2  | 12       | 1.05          |
| (1,765)  | 1:60:A:ILE:HD12 | 1:63:A:CYS:HB3  | 2        | 1.05          |
| (1,765)  | 1:60:A:ILE:HD12 | 1:63:A:CYS:HB2  | 2        | 1.05          |
| (1,765)  | 1:60:A:ILE:HD12 | 1:63:A:CYS:HB3  | 17       | 1.05          |
| (1,765)  | 1:60:A:ILE:HD12 | 1:63:A:CYS:HB2  | 17       | 1.05          |
| (1,578)  | 1:46:A:ILE:HD12 | 1:62:A:PHE:HD1  | 7        | 1.05          |
| (1,578)  | 1:46:A:ILE:HD13 | 1:62:A:PHE:HD1  | 7        | 1.05          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,578)  | 1:46:A:ILE:HD12 | 1:62:A:PHE:HD1  | 19       | 1.05          |
| (1,578)  | 1:46:A:ILE:HD13 | 1:62:A:PHE:HD1  | 19       | 1.05          |
| (1,576)  | 1:46:A:ILE:HD12 | 1:63:A:CYS:H    | 9        | 1.05          |
| (1,552)  | 1:39:A:VAL:HG21 | 1:43:A:MET:HG2  | 2        | 1.05          |
| (1,552)  | 1:39:A:VAL:HG21 | 1:43:A:MET:HG3  | 2        | 1.05          |
| (1,345)  | 1:25:A:THR:HG23 | 1:26:A:ASP:HA   | 1        | 1.05          |
| (1,345)  | 1:25:A:THR:HG23 | 1:26:A:ASP:HA   | 6        | 1.05          |
| (1,345)  | 1:25:A:THR:HG23 | 1:26:A:ASP:HA   | 18       | 1.05          |
| (1,333)  | 1:11:A:PHE:HE1  | 1:24:A:LEU:HD21 | 12       | 1.05          |
| (1,333)  | 1:11:A:PHE:HE1  | 1:24:A:LEU:HD21 | 17       | 1.05          |
| (1,182)  | 1:13:A:THR:HG21 | 1:14:A:ASN:HA   | 7        | 1.05          |
| (1,1532) | 1:52:A:GLY:HA2  | 1:53:A:PHE:HD1  | 4        | 1.04          |
| (1,1532) | 1:52:A:GLY:HA3  | 1:53:A:PHE:HD1  | 4        | 1.04          |
| (1,1532) | 1:52:A:GLY:HA2  | 1:53:A:PHE:HD1  | 6        | 1.04          |
| (1,1532) | 1:52:A:GLY:HA3  | 1:53:A:PHE:HD1  | 6        | 1.04          |
| (1,1467) | 1:33:A:SER:HB2  | 1:34:A:THR:HG23 | 4        | 1.04          |
| (1,1467) | 1:33:A:SER:HB3  | 1:34:A:THR:HG23 | 4        | 1.04          |
| (1,1432) | 1:20:A:SER:HB2  | 1:53:A:PHE:HD2  | 11       | 1.04          |
| (1,1432) | 1:20:A:SER:HB3  | 1:53:A:PHE:HD2  | 11       | 1.04          |
| (1,1432) | 1:20:A:SER:HB2  | 1:53:A:PHE:HD2  | 17       | 1.04          |
| (1,1432) | 1:20:A:SER:HB3  | 1:53:A:PHE:HD2  | 17       | 1.04          |
| (1,765)  | 1:60:A:ILE:HD12 | 1:63:A:CYS:HB3  | 8        | 1.04          |
| (1,765)  | 1:60:A:ILE:HD12 | 1:63:A:CYS:HB2  | 8        | 1.04          |
| (1,576)  | 1:46:A:ILE:HD12 | 1:63:A:CYS:H    | 1        | 1.04          |
| (1,576)  | 1:46:A:ILE:HD12 | 1:63:A:CYS:H    | 17       | 1.04          |
| (1,552)  | 1:39:A:VAL:HG21 | 1:43:A:MET:HG2  | 3        | 1.04          |
| (1,552)  | 1:39:A:VAL:HG21 | 1:43:A:MET:HG3  | 3        | 1.04          |
| (1,467)  | 1:39:A:VAL:HA   | 1:69:A:LEU:HD23 | 2        | 1.04          |
| (1,467)  | 1:39:A:VAL:HA   | 1:69:A:LEU:HD23 | 4        | 1.04          |
| (1,467)  | 1:39:A:VAL:HA   | 1:69:A:LEU:HD23 | 17       | 1.04          |
| (1,390)  | 1:10:A:ARG:HB2  | 1:11:A:PHE:HE2  | 19       | 1.04          |
| (1,390)  | 1:10:A:ARG:HB3  | 1:11:A:PHE:HE2  | 19       | 1.04          |
| (1,357)  | 1:30:A:THR:HG22 | 1:31:A:LEU:HA   | 20       | 1.04          |
| (1,345)  | 1:25:A:THR:HG23 | 1:26:A:ASP:HA   | 4        | 1.04          |
| (1,345)  | 1:25:A:THR:HG23 | 1:26:A:ASP:HA   | 14       | 1.04          |
| (1,333)  | 1:11:A:PHE:HE1  | 1:24:A:LEU:HD21 | 4        | 1.04          |
| (1,325)  | 1:24:A:LEU:HG   | 1:25:A:THR:HA   | 2        | 1.04          |
| (1,325)  | 1:24:A:LEU:HG   | 1:25:A:THR:HA   | 8        | 1.04          |
| (1,325)  | 1:24:A:LEU:HG   | 1:25:A:THR:HA   | 9        | 1.04          |
| (1,182)  | 1:13:A:THR:HG21 | 1:14:A:ASN:HA   | 17       | 1.04          |
| (1,68)   | 1:7:A:ILE:HD11  | 1:74:A:ALA:H    | 8        | 1.04          |
| (1,68)   | 1:7:A:ILE:HD11  | 1:74:A:ALA:H    | 20       | 1.04          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,809)  | 1:69:A:LEU:HD21 | 1:70:A:MET:HG2  | 17       | 1.03          |
| (1,809)  | 1:69:A:LEU:HD21 | 1:70:A:MET:HG3  | 17       | 1.03          |
| (1,765)  | 1:60:A:ILE:HD12 | 1:63:A:CYS:HB3  | 4        | 1.03          |
| (1,765)  | 1:60:A:ILE:HD12 | 1:63:A:CYS:HB2  | 4        | 1.03          |
| (1,765)  | 1:60:A:ILE:HD12 | 1:63:A:CYS:HB3  | 11       | 1.03          |
| (1,765)  | 1:60:A:ILE:HD12 | 1:63:A:CYS:HB2  | 11       | 1.03          |
| (1,765)  | 1:60:A:ILE:HD12 | 1:63:A:CYS:HB3  | 19       | 1.03          |
| (1,765)  | 1:60:A:ILE:HD12 | 1:63:A:CYS:HB2  | 19       | 1.03          |
| (1,576)  | 1:46:A:ILE:HD12 | 1:63:A:CYS:H    | 4        | 1.03          |
| (1,576)  | 1:46:A:ILE:HD12 | 1:63:A:CYS:H    | 14       | 1.03          |
| (1,493)  | 1:39:A:VAL:HG21 | 1:40:A:GLN:HB2  | 20       | 1.03          |
| (1,390)  | 1:10:A:ARG:HB2  | 1:11:A:PHE:HE2  | 10       | 1.03          |
| (1,390)  | 1:10:A:ARG:HB3  | 1:11:A:PHE:HE2  | 10       | 1.03          |
| (1,363)  | 1:27:A:ALA:HB1  | 1:28:A:LEU:HD21 | 8        | 1.03          |
| (1,363)  | 1:27:A:ALA:HB1  | 1:28:A:LEU:HD21 | 16       | 1.03          |
| (1,345)  | 1:25:A:THR:HG23 | 1:26:A:ASP:HA   | 3        | 1.03          |
| (1,345)  | 1:25:A:THR:HG23 | 1:26:A:ASP:HA   | 8        | 1.03          |
| (1,345)  | 1:25:A:THR:HG23 | 1:26:A:ASP:HA   | 10       | 1.03          |
| (1,345)  | 1:25:A:THR:HG23 | 1:26:A:ASP:HA   | 15       | 1.03          |
| (1,333)  | 1:11:A:PHE:HE1  | 1:24:A:LEU:HD21 | 5        | 1.03          |
| (1,325)  | 1:24:A:LEU:HG   | 1:25:A:THR:HA   | 3        | 1.03          |
| (1,325)  | 1:24:A:LEU:HG   | 1:25:A:THR:HA   | 4        | 1.03          |
| (1,325)  | 1:24:A:LEU:HG   | 1:25:A:THR:HA   | 5        | 1.03          |
| (1,325)  | 1:24:A:LEU:HG   | 1:25:A:THR:HA   | 6        | 1.03          |
| (1,325)  | 1:24:A:LEU:HG   | 1:25:A:THR:HA   | 7        | 1.03          |
| (1,325)  | 1:24:A:LEU:HG   | 1:25:A:THR:HA   | 10       | 1.03          |
| (1,325)  | 1:24:A:LEU:HG   | 1:25:A:THR:HA   | 11       | 1.03          |
| (1,325)  | 1:24:A:LEU:HG   | 1:25:A:THR:HA   | 13       | 1.03          |
| (1,325)  | 1:24:A:LEU:HG   | 1:25:A:THR:HA   | 19       | 1.03          |
| (1,325)  | 1:24:A:LEU:HG   | 1:25:A:THR:HA   | 20       | 1.03          |
| (1,70)   | 1:7:A:ILE:HD12  | 1:77:A:PHE:HD2  | 8        | 1.03          |
| (1,68)   | 1:7:A:ILE:HD11  | 1:74:A:ALA:H    | 5        | 1.03          |
| (1,1532) | 1:52:A:GLY:HA2  | 1:53:A:PHE:HD1  | 2        | 1.02          |
| (1,1532) | 1:52:A:GLY:HA3  | 1:53:A:PHE:HD1  | 2        | 1.02          |
| (1,1532) | 1:52:A:GLY:HA2  | 1:53:A:PHE:HD1  | 8        | 1.02          |
| (1,1532) | 1:52:A:GLY:HA3  | 1:53:A:PHE:HD1  | 8        | 1.02          |
| (1,1532) | 1:52:A:GLY:HA2  | 1:53:A:PHE:HD1  | 17       | 1.02          |
| (1,1532) | 1:52:A:GLY:HA3  | 1:53:A:PHE:HD1  | 17       | 1.02          |
| (1,862)  | 1:4:A:MET:HE3   | 1:7:A:ILE:H     | 11       | 1.02          |
| (1,850)  | 1:31:A:LEU:HB3  | 1:76:A:VAL:HG23 | 5        | 1.02          |
| (1,809)  | 1:69:A:LEU:HD21 | 1:70:A:MET:HG2  | 12       | 1.02          |
| (1,809)  | 1:69:A:LEU:HD21 | 1:70:A:MET:HG3  | 12       | 1.02          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,809)  | 1:69:A:LEU:HD21 | 1:70:A:MET:HG2  | 16       | 1.02          |
| (1,809)  | 1:69:A:LEU:HD21 | 1:70:A:MET:HG3  | 16       | 1.02          |
| (1,765)  | 1:60:A:ILE:HD12 | 1:63:A:CYS:HB3  | 14       | 1.02          |
| (1,765)  | 1:60:A:ILE:HD12 | 1:63:A:CYS:HB2  | 14       | 1.02          |
| (1,576)  | 1:46:A:ILE:HD12 | 1:63:A:CYS:H    | 8        | 1.02          |
| (1,508)  | 1:42:A:MET:HB2  | 1:62:A:PHE:HE1  | 13       | 1.02          |
| (1,476)  | 1:39:A:VAL:HG21 | 1:40:A:GLN:H    | 11       | 1.02          |
| (1,476)  | 1:39:A:VAL:HG21 | 1:40:A:GLN:H    | 14       | 1.02          |
| (1,476)  | 1:39:A:VAL:HG21 | 1:40:A:GLN:H    | 17       | 1.02          |
| (1,467)  | 1:39:A:VAL:HA   | 1:69:A:LEU:HD23 | 8        | 1.02          |
| (1,416)  | 1:33:A:SER:HA   | 1:34:A:THR:HG23 | 4        | 1.02          |
| (1,325)  | 1:24:A:LEU:HG   | 1:25:A:THR:HA   | 12       | 1.02          |
| (1,325)  | 1:24:A:LEU:HG   | 1:25:A:THR:HA   | 14       | 1.02          |
| (1,325)  | 1:24:A:LEU:HG   | 1:25:A:THR:HA   | 16       | 1.02          |
| (1,325)  | 1:24:A:LEU:HG   | 1:25:A:THR:HA   | 17       | 1.02          |
| (1,325)  | 1:24:A:LEU:HG   | 1:25:A:THR:HA   | 18       | 1.02          |
| (1,305)  | 1:11:A:PHE:HE1  | 1:24:A:LEU:HA   | 5        | 1.02          |
| (1,21)   | 1:5:A:GLU:HA    | 1:60:A:ILE:HD13 | 3        | 1.02          |
| (1,1532) | 1:52:A:GLY:HA2  | 1:53:A:PHE:HD1  | 9        | 1.01          |
| (1,1532) | 1:52:A:GLY:HA3  | 1:53:A:PHE:HD1  | 9        | 1.01          |
| (1,1532) | 1:52:A:GLY:HA2  | 1:53:A:PHE:HD1  | 14       | 1.01          |
| (1,1532) | 1:52:A:GLY:HA3  | 1:53:A:PHE:HD1  | 14       | 1.01          |
| (1,1532) | 1:52:A:GLY:HA2  | 1:53:A:PHE:HD1  | 16       | 1.01          |
| (1,1532) | 1:52:A:GLY:HA3  | 1:53:A:PHE:HD1  | 16       | 1.01          |
| (1,1432) | 1:20:A:SER:HB2  | 1:53:A:PHE:HD2  | 5        | 1.01          |
| (1,1432) | 1:20:A:SER:HB3  | 1:53:A:PHE:HD2  | 5        | 1.01          |
| (1,1432) | 1:20:A:SER:HB2  | 1:53:A:PHE:HD2  | 9        | 1.01          |
| (1,1432) | 1:20:A:SER:HB3  | 1:53:A:PHE:HD2  | 9        | 1.01          |
| (1,809)  | 1:69:A:LEU:HD21 | 1:70:A:MET:HG2  | 6        | 1.01          |
| (1,809)  | 1:69:A:LEU:HD21 | 1:70:A:MET:HG3  | 6        | 1.01          |
| (1,776)  | 1:62:A:PHE:HD2  | 1:67:A:PRO:HG2  | 13       | 1.01          |
| (1,576)  | 1:46:A:ILE:HD12 | 1:63:A:CYS:H    | 7        | 1.01          |
| (1,576)  | 1:46:A:ILE:HD12 | 1:63:A:CYS:H    | 16       | 1.01          |
| (1,576)  | 1:46:A:ILE:HD12 | 1:63:A:CYS:H    | 19       | 1.01          |
| (1,508)  | 1:42:A:MET:HB2  | 1:62:A:PHE:HE1  | 14       | 1.01          |
| (1,467)  | 1:39:A:VAL:HA   | 1:69:A:LEU:HD23 | 6        | 1.01          |
| (1,416)  | 1:33:A:SER:HA   | 1:34:A:THR:HG23 | 20       | 1.01          |
| (1,390)  | 1:10:A:ARG:HB2  | 1:11:A:PHE:HE2  | 5        | 1.01          |
| (1,390)  | 1:10:A:ARG:HB3  | 1:11:A:PHE:HE2  | 5        | 1.01          |
| (1,345)  | 1:25:A:THR:HG23 | 1:26:A:ASP:HA   | 16       | 1.01          |
| (1,333)  | 1:11:A:PHE:HE1  | 1:24:A:LEU:HD21 | 13       | 1.01          |
| (1,325)  | 1:24:A:LEU:HG   | 1:25:A:THR:HA   | 1        | 1.01          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,325)  | 1:24:A:LEU:HG   | 1:25:A:THR:HA   | 15       | 1.01          |
| (1,305)  | 1:11:A:PHE:HE1  | 1:24:A:LEU:HA   | 7        | 1.01          |
| (1,305)  | 1:11:A:PHE:HE1  | 1:24:A:LEU:HA   | 16       | 1.01          |
| (1,205)  | 1:18:A:LYS:HB3  | 1:53:A:PHE:HD2  | 14       | 1.01          |
| (1,205)  | 1:18:A:LYS:HB2  | 1:53:A:PHE:HD2  | 14       | 1.01          |
| (1,1532) | 1:52:A:GLY:HA2  | 1:53:A:PHE:HD1  | 20       | 1.0           |
| (1,1532) | 1:52:A:GLY:HA3  | 1:53:A:PHE:HD1  | 20       | 1.0           |
| (1,846)  | 1:72:A:ASP:HA   | 1:76:A:VAL:HG21 | 18       | 1.0           |
| (1,765)  | 1:60:A:ILE:HD12 | 1:63:A:CYS:HB3  | 6        | 1.0           |
| (1,765)  | 1:60:A:ILE:HD12 | 1:63:A:CYS:HB2  | 6        | 1.0           |
| (1,765)  | 1:60:A:ILE:HD12 | 1:63:A:CYS:HB3  | 13       | 1.0           |
| (1,765)  | 1:60:A:ILE:HD12 | 1:63:A:CYS:HB2  | 13       | 1.0           |
| (1,727)  | 1:5:A:GLU:H     | 1:60:A:ILE:HD13 | 14       | 1.0           |
| (1,576)  | 1:46:A:ILE:HD12 | 1:63:A:CYS:H    | 2        | 1.0           |
| (1,552)  | 1:39:A:VAL:HG21 | 1:43:A:MET:HG2  | 19       | 1.0           |
| (1,552)  | 1:39:A:VAL:HG21 | 1:43:A:MET:HG3  | 19       | 1.0           |
| (1,476)  | 1:39:A:VAL:HG21 | 1:40:A:GLN:H    | 3        | 1.0           |
| (1,476)  | 1:39:A:VAL:HG21 | 1:40:A:GLN:H    | 16       | 1.0           |
| (1,476)  | 1:39:A:VAL:HG21 | 1:40:A:GLN:H    | 19       | 1.0           |
| (1,305)  | 1:11:A:PHE:HE1  | 1:24:A:LEU:HA   | 11       | 1.0           |
| (1,205)  | 1:18:A:LYS:HB3  | 1:53:A:PHE:HD2  | 18       | 1.0           |
| (1,205)  | 1:18:A:LYS:HB2  | 1:53:A:PHE:HD2  | 18       | 1.0           |
| (1,182)  | 1:13:A:THR:HG21 | 1:14:A:ASN:HA   | 16       | 1.0           |
| (1,138)  | 1:10:A:ARG:HD2  | 1:11:A:PHE:HE2  | 19       | 1.0           |
| (1,138)  | 1:10:A:ARG:HD3  | 1:11:A:PHE:HE2  | 19       | 1.0           |
| (1,1467) | 1:33:A:SER:HB2  | 1:34:A:THR:HG23 | 9        | 0.99          |
| (1,1467) | 1:33:A:SER:HB3  | 1:34:A:THR:HG23 | 9        | 0.99          |
| (1,1432) | 1:20:A:SER:HB2  | 1:53:A:PHE:HD2  | 8        | 0.99          |
| (1,1432) | 1:20:A:SER:HB3  | 1:53:A:PHE:HD2  | 8        | 0.99          |
| (1,1108) | 1:8:A:PHE:HE1   | 1:19:A:ILE:H    | 6        | 0.99          |
| (1,865)  | 1:4:A:MET:HE3   | 1:74:A:ALA:HB2  | 15       | 0.99          |
| (1,476)  | 1:39:A:VAL:HG21 | 1:40:A:GLN:H    | 1        | 0.99          |
| (1,476)  | 1:39:A:VAL:HG21 | 1:40:A:GLN:H    | 4        | 0.99          |
| (1,476)  | 1:39:A:VAL:HG21 | 1:40:A:GLN:H    | 6        | 0.99          |
| (1,476)  | 1:39:A:VAL:HG21 | 1:40:A:GLN:H    | 7        | 0.99          |
| (1,476)  | 1:39:A:VAL:HG21 | 1:40:A:GLN:H    | 8        | 0.99          |
| (1,476)  | 1:39:A:VAL:HG21 | 1:40:A:GLN:H    | 9        | 0.99          |
| (1,476)  | 1:39:A:VAL:HG21 | 1:40:A:GLN:H    | 10       | 0.99          |
| (1,476)  | 1:39:A:VAL:HG21 | 1:40:A:GLN:H    | 15       | 0.99          |
| (1,476)  | 1:39:A:VAL:HG21 | 1:40:A:GLN:H    | 18       | 0.99          |
| (1,390)  | 1:10:A:ARG:HB2  | 1:11:A:PHE:HE2  | 18       | 0.99          |
| (1,390)  | 1:10:A:ARG:HB3  | 1:11:A:PHE:HE2  | 18       | 0.99          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,345)  | 1:25:A:THR:HG23 | 1:26:A:ASP:HA   | 11       | 0.99          |
| (1,305)  | 1:11:A:PHE:HE1  | 1:24:A:LEU:HA   | 8        | 0.99          |
| (1,305)  | 1:11:A:PHE:HE1  | 1:24:A:LEU:HA   | 12       | 0.99          |
| (1,305)  | 1:11:A:PHE:HE1  | 1:24:A:LEU:HA   | 19       | 0.99          |
| (1,142)  | 1:10:A:ARG:HD3  | 1:11:A:PHE:HD2  | 15       | 0.99          |
| (1,138)  | 1:10:A:ARG:HD2  | 1:11:A:PHE:HE2  | 12       | 0.99          |
| (1,138)  | 1:10:A:ARG:HD3  | 1:11:A:PHE:HE2  | 12       | 0.99          |
| (1,1431) | 1:20:A:SER:HB2  | 1:53:A:PHE:HE2  | 14       | 0.98          |
| (1,1431) | 1:20:A:SER:HB3  | 1:53:A:PHE:HE2  | 14       | 0.98          |
| (1,862)  | 1:4:A:MET:HE3   | 1:7:A:ILE:H     | 2        | 0.98          |
| (1,862)  | 1:4:A:MET:HE3   | 1:7:A:ILE:H     | 19       | 0.98          |
| (1,765)  | 1:60:A:ILE:HD12 | 1:63:A:CYS:HB3  | 5        | 0.98          |
| (1,765)  | 1:60:A:ILE:HD12 | 1:63:A:CYS:HB2  | 5        | 0.98          |
| (1,542)  | 1:39:A:VAL:HG21 | 1:43:A:MET:HB3  | 18       | 0.98          |
| (1,476)  | 1:39:A:VAL:HG21 | 1:40:A:GLN:H    | 5        | 0.98          |
| (1,363)  | 1:27:A:ALA:HB1  | 1:28:A:LEU:HD21 | 10       | 0.98          |
| (1,363)  | 1:27:A:ALA:HB1  | 1:28:A:LEU:HD21 | 17       | 0.98          |
| (1,305)  | 1:11:A:PHE:HE1  | 1:24:A:LEU:HA   | 3        | 0.98          |
| (1,161)  | 1:8:A:PHE:HE2   | 1:12:A:ASP:HB2  | 4        | 0.98          |
| (1,142)  | 1:10:A:ARG:HD3  | 1:11:A:PHE:HD2  | 4        | 0.98          |
| (1,809)  | 1:69:A:LEU:HD21 | 1:70:A:MET:HG2  | 13       | 0.97          |
| (1,809)  | 1:69:A:LEU:HD21 | 1:70:A:MET:HG3  | 13       | 0.97          |
| (1,765)  | 1:60:A:ILE:HD12 | 1:63:A:CYS:HB3  | 10       | 0.97          |
| (1,765)  | 1:60:A:ILE:HD12 | 1:63:A:CYS:HB2  | 10       | 0.97          |
| (1,476)  | 1:39:A:VAL:HG21 | 1:40:A:GLN:H    | 2        | 0.97          |
| (1,390)  | 1:10:A:ARG:HB2  | 1:11:A:PHE:HE2  | 4        | 0.97          |
| (1,390)  | 1:10:A:ARG:HB3  | 1:11:A:PHE:HE2  | 4        | 0.97          |
| (1,390)  | 1:10:A:ARG:HB2  | 1:11:A:PHE:HE2  | 11       | 0.97          |
| (1,390)  | 1:10:A:ARG:HB3  | 1:11:A:PHE:HE2  | 11       | 0.97          |
| (1,363)  | 1:27:A:ALA:HB1  | 1:28:A:LEU:HD21 | 5        | 0.97          |
| (1,324)  | 1:11:A:PHE:HE1  | 1:24:A:LEU:HG   | 14       | 0.97          |
| (1,205)  | 1:18:A:LYS:HB3  | 1:53:A:PHE:HD2  | 1        | 0.97          |
| (1,205)  | 1:18:A:LYS:HB2  | 1:53:A:PHE:HD2  | 1        | 0.97          |
| (1,142)  | 1:10:A:ARG:HD3  | 1:11:A:PHE:HD2  | 14       | 0.97          |
| (1,138)  | 1:10:A:ARG:HD2  | 1:11:A:PHE:HE2  | 11       | 0.97          |
| (1,138)  | 1:10:A:ARG:HD3  | 1:11:A:PHE:HE2  | 11       | 0.97          |
| (1,1295) | 1:60:A:ILE:HD12 | 1:63:A:CYS:H    | 20       | 0.96          |
| (1,765)  | 1:60:A:ILE:HD12 | 1:63:A:CYS:HB3  | 7        | 0.96          |
| (1,765)  | 1:60:A:ILE:HD12 | 1:63:A:CYS:HB2  | 7        | 0.96          |
| (1,552)  | 1:39:A:VAL:HG21 | 1:43:A:MET:HG2  | 7        | 0.96          |
| (1,552)  | 1:39:A:VAL:HG21 | 1:43:A:MET:HG3  | 7        | 0.96          |
| (1,508)  | 1:42:A:MET:HB2  | 1:62:A:PHE:HE1  | 18       | 0.96          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,467)  | 1:39:A:VAL:HA   | 1:69:A:LEU:HD23 | 16       | 0.96          |
| (1,390)  | 1:10:A:ARG:HB2  | 1:11:A:PHE:HE2  | 8        | 0.96          |
| (1,390)  | 1:10:A:ARG:HB3  | 1:11:A:PHE:HE2  | 8        | 0.96          |
| (1,345)  | 1:25:A:THR:HG23 | 1:26:A:ASP:HA   | 9        | 0.96          |
| (1,305)  | 1:11:A:PHE:HE1  | 1:24:A:LEU:HA   | 9        | 0.96          |
| (1,1349) | 1:75:A:LYS:H    | 1:76:A:VAL:HG21 | 12       | 0.95          |
| (1,1295) | 1:60:A:ILE:HD12 | 1:63:A:CYS:H    | 15       | 0.95          |
| (1,476)  | 1:39:A:VAL:HG21 | 1:40:A:GLN:H    | 20       | 0.95          |
| (1,416)  | 1:33:A:SER:HA   | 1:34:A:THR:HG23 | 9        | 0.95          |
| (1,345)  | 1:25:A:THR:HG23 | 1:26:A:ASP:HA   | 5        | 0.95          |
| (1,345)  | 1:25:A:THR:HG23 | 1:26:A:ASP:HA   | 12       | 0.95          |
| (1,345)  | 1:25:A:THR:HG23 | 1:26:A:ASP:HA   | 13       | 0.95          |
| (1,205)  | 1:18:A:LYS:HB3  | 1:53:A:PHE:HD2  | 8        | 0.95          |
| (1,205)  | 1:18:A:LYS:HB2  | 1:53:A:PHE:HD2  | 8        | 0.95          |
| (1,142)  | 1:10:A:ARG:HD3  | 1:11:A:PHE:HD2  | 18       | 0.95          |
| (1,142)  | 1:10:A:ARG:HD3  | 1:11:A:PHE:HD2  | 20       | 0.95          |
| (1,138)  | 1:10:A:ARG:HD2  | 1:11:A:PHE:HE2  | 10       | 0.95          |
| (1,138)  | 1:10:A:ARG:HD3  | 1:11:A:PHE:HE2  | 10       | 0.95          |
| (1,21)   | 1:5:A:GLU:HA    | 1:60:A:ILE:HD13 | 19       | 0.95          |
| (1,1431) | 1:20:A:SER:HB2  | 1:53:A:PHE:HE2  | 1        | 0.94          |
| (1,1431) | 1:20:A:SER:HB3  | 1:53:A:PHE:HE2  | 1        | 0.94          |
| (1,1295) | 1:60:A:ILE:HD12 | 1:63:A:CYS:H    | 16       | 0.94          |
| (1,862)  | 1:4:A:MET:HE3   | 1:7:A:ILE:H     | 7        | 0.94          |
| (1,862)  | 1:4:A:MET:HE3   | 1:7:A:ILE:H     | 12       | 0.94          |
| (1,765)  | 1:60:A:ILE:HD12 | 1:63:A:CYS:HB3  | 12       | 0.94          |
| (1,765)  | 1:60:A:ILE:HD12 | 1:63:A:CYS:HB2  | 12       | 0.94          |
| (1,727)  | 1:5:A:GLU:H     | 1:60:A:ILE:HD13 | 11       | 0.94          |
| (1,390)  | 1:10:A:ARG:HB2  | 1:11:A:PHE:HE2  | 1        | 0.94          |
| (1,390)  | 1:10:A:ARG:HB3  | 1:11:A:PHE:HE2  | 1        | 0.94          |
| (1,390)  | 1:10:A:ARG:HB2  | 1:11:A:PHE:HE2  | 3        | 0.94          |
| (1,390)  | 1:10:A:ARG:HB3  | 1:11:A:PHE:HE2  | 3        | 0.94          |
| (1,363)  | 1:27:A:ALA:HB1  | 1:28:A:LEU:HD21 | 9        | 0.94          |
| (1,324)  | 1:11:A:PHE:HE1  | 1:24:A:LEU:HG   | 6        | 0.94          |
| (1,305)  | 1:11:A:PHE:HE1  | 1:24:A:LEU:HA   | 17       | 0.94          |
| (1,163)  | 1:12:A:ASP:HB2  | 1:19:A:ILE:HD13 | 18       | 0.94          |
| (1,163)  | 1:12:A:ASP:HB2  | 1:19:A:ILE:HD13 | 19       | 0.94          |
| (1,21)   | 1:5:A:GLU:HA    | 1:60:A:ILE:HD13 | 7        | 0.94          |
| (1,1532) | 1:52:A:GLY:HA2  | 1:53:A:PHE:HD1  | 12       | 0.93          |
| (1,1532) | 1:52:A:GLY:HA3  | 1:53:A:PHE:HD1  | 12       | 0.93          |
| (1,1295) | 1:60:A:ILE:HD12 | 1:63:A:CYS:H    | 14       | 0.93          |
| (1,1161) | 1:31:A:LEU:HD21 | 1:32:A:GLY:H    | 3        | 0.93          |
| (1,888)  | 1:46:A:ILE:HD12 | 1:62:A:PHE:H    | 5        | 0.93          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,865)  | 1:4:A:MET:HE3   | 1:74:A:ALA:HB2  | 13       | 0.93          |
| (1,862)  | 1:4:A:MET:HE3   | 1:7:A:ILE:H     | 5        | 0.93          |
| (1,476)  | 1:39:A:VAL:HG21 | 1:40:A:GLN:H    | 12       | 0.93          |
| (1,467)  | 1:39:A:VAL:HA   | 1:69:A:LEU:HD23 | 1        | 0.93          |
| (1,363)  | 1:27:A:ALA:HB1  | 1:28:A:LEU:HD21 | 6        | 0.93          |
| (1,138)  | 1:10:A:ARG:HD2  | 1:11:A:PHE:HE2  | 7        | 0.93          |
| (1,138)  | 1:10:A:ARG:HD3  | 1:11:A:PHE:HE2  | 7        | 0.93          |
| (1,1432) | 1:20:A:SER:HB2  | 1:53:A:PHE:HD2  | 6        | 0.92          |
| (1,1432) | 1:20:A:SER:HB3  | 1:53:A:PHE:HD2  | 6        | 0.92          |
| (1,1295) | 1:60:A:ILE:HD12 | 1:63:A:CYS:H    | 9        | 0.92          |
| (1,1161) | 1:31:A:LEU:HD21 | 1:32:A:GLY:H    | 16       | 0.92          |
| (1,888)  | 1:46:A:ILE:HD12 | 1:62:A:PHE:H    | 11       | 0.92          |
| (1,862)  | 1:4:A:MET:HE3   | 1:7:A:ILE:H     | 6        | 0.92          |
| (1,846)  | 1:72:A:ASP:HA   | 1:76:A:VAL:HG21 | 11       | 0.92          |
| (1,803)  | 1:62:A:PHE:HD2  | 1:70:A:MET:HG2  | 13       | 0.92          |
| (1,765)  | 1:60:A:ILE:HD12 | 1:63:A:CYS:HB3  | 1        | 0.92          |
| (1,765)  | 1:60:A:ILE:HD12 | 1:63:A:CYS:HB2  | 1        | 0.92          |
| (1,390)  | 1:10:A:ARG:HB2  | 1:11:A:PHE:HE2  | 7        | 0.92          |
| (1,390)  | 1:10:A:ARG:HB3  | 1:11:A:PHE:HE2  | 7        | 0.92          |
| (1,363)  | 1:27:A:ALA:HB1  | 1:28:A:LEU:HD21 | 1        | 0.92          |
| (1,324)  | 1:11:A:PHE:HE1  | 1:24:A:LEU:HG   | 9        | 0.92          |
| (1,305)  | 1:11:A:PHE:HE1  | 1:24:A:LEU:HA   | 13       | 0.92          |
| (1,163)  | 1:12:A:ASP:HB2  | 1:19:A:ILE:HD13 | 14       | 0.92          |
| (1,142)  | 1:10:A:ARG:HD3  | 1:11:A:PHE:HD2  | 3        | 0.92          |
| (1,888)  | 1:46:A:ILE:HD12 | 1:62:A:PHE:H    | 13       | 0.91          |
| (1,848)  | 1:31:A:LEU:HB2  | 1:76:A:VAL:HG23 | 1        | 0.91          |
| (1,846)  | 1:72:A:ASP:HA   | 1:76:A:VAL:HG21 | 15       | 0.91          |
| (1,467)  | 1:39:A:VAL:HA   | 1:69:A:LEU:HD23 | 12       | 0.91          |
| (1,390)  | 1:10:A:ARG:HB2  | 1:11:A:PHE:HE2  | 15       | 0.91          |
| (1,390)  | 1:10:A:ARG:HB3  | 1:11:A:PHE:HE2  | 15       | 0.91          |
| (1,390)  | 1:10:A:ARG:HB2  | 1:11:A:PHE:HE2  | 20       | 0.91          |
| (1,390)  | 1:10:A:ARG:HB3  | 1:11:A:PHE:HE2  | 20       | 0.91          |
| (1,363)  | 1:27:A:ALA:HB1  | 1:28:A:LEU:HD21 | 3        | 0.91          |
| (1,324)  | 1:11:A:PHE:HE1  | 1:24:A:LEU:HG   | 2        | 0.91          |
| (1,305)  | 1:11:A:PHE:HE1  | 1:24:A:LEU:HA   | 10       | 0.91          |
| (1,182)  | 1:13:A:THR:HG21 | 1:14:A:ASN:HA   | 13       | 0.91          |
| (1,1532) | 1:52:A:GLY:HA2  | 1:53:A:PHE:HD1  | 3        | 0.9           |
| (1,1532) | 1:52:A:GLY:HA3  | 1:53:A:PHE:HD1  | 3        | 0.9           |
| (1,1467) | 1:33:A:SER:HB2  | 1:34:A:THR:HG23 | 13       | 0.9           |
| (1,1467) | 1:33:A:SER:HB3  | 1:34:A:THR:HG23 | 13       | 0.9           |
| (1,1161) | 1:31:A:LEU:HD21 | 1:32:A:GLY:H    | 2        | 0.9           |
| (1,1161) | 1:31:A:LEU:HD21 | 1:32:A:GLY:H    | 13       | 0.9           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1161) | 1:31:A:LEU:HD21 | 1:32:A:GLY:H    | 15       | 0.9           |
| (1,862)  | 1:4:A:MET:HE3   | 1:7:A:ILE:H     | 4        | 0.9           |
| (1,476)  | 1:39:A:VAL:HG21 | 1:40:A:GLN:H    | 13       | 0.9           |
| (1,416)  | 1:33:A:SER:HA   | 1:34:A:THR:HG23 | 13       | 0.9           |
| (1,324)  | 1:11:A:PHE:HE1  | 1:24:A:LEU:HG   | 7        | 0.9           |
| (1,205)  | 1:18:A:LYS:HB3  | 1:53:A:PHE:HD2  | 2        | 0.9           |
| (1,205)  | 1:18:A:LYS:HB2  | 1:53:A:PHE:HD2  | 2        | 0.9           |
| (1,205)  | 1:18:A:LYS:HB3  | 1:53:A:PHE:HD2  | 5        | 0.9           |
| (1,205)  | 1:18:A:LYS:HB2  | 1:53:A:PHE:HD2  | 5        | 0.9           |
| (1,205)  | 1:18:A:LYS:HB3  | 1:53:A:PHE:HD2  | 9        | 0.9           |
| (1,205)  | 1:18:A:LYS:HB2  | 1:53:A:PHE:HD2  | 9        | 0.9           |
| (1,182)  | 1:13:A:THR:HG21 | 1:14:A:ASN:HA   | 12       | 0.9           |
| (1,182)  | 1:13:A:THR:HG21 | 1:14:A:ASN:HA   | 18       | 0.9           |
| (1,138)  | 1:10:A:ARG:HD2  | 1:11:A:PHE:HE2  | 2        | 0.9           |
| (1,138)  | 1:10:A:ARG:HD3  | 1:11:A:PHE:HE2  | 2        | 0.9           |
| (1,138)  | 1:10:A:ARG:HD2  | 1:11:A:PHE:HE2  | 15       | 0.9           |
| (1,138)  | 1:10:A:ARG:HD3  | 1:11:A:PHE:HE2  | 15       | 0.9           |
| (1,75)   | 1:5:A:GLU:HA    | 1:7:A:ILE:HD13  | 10       | 0.9           |
| (1,1432) | 1:20:A:SER:HB2  | 1:53:A:PHE:HD2  | 4        | 0.89          |
| (1,1432) | 1:20:A:SER:HB3  | 1:53:A:PHE:HD2  | 4        | 0.89          |
| (1,1295) | 1:60:A:ILE:HD12 | 1:63:A:CYS:H    | 13       | 0.89          |
| (1,1161) | 1:31:A:LEU:HD21 | 1:32:A:GLY:H    | 4        | 0.89          |
| (1,1161) | 1:31:A:LEU:HD21 | 1:32:A:GLY:H    | 6        | 0.89          |
| (1,1161) | 1:31:A:LEU:HD21 | 1:32:A:GLY:H    | 9        | 0.89          |
| (1,1161) | 1:31:A:LEU:HD21 | 1:32:A:GLY:H    | 10       | 0.89          |
| (1,809)  | 1:69:A:LEU:HD21 | 1:70:A:MET:HG2  | 1        | 0.89          |
| (1,809)  | 1:69:A:LEU:HD21 | 1:70:A:MET:HG3  | 1        | 0.89          |
| (1,390)  | 1:10:A:ARG:HB2  | 1:11:A:PHE:HE2  | 14       | 0.89          |
| (1,390)  | 1:10:A:ARG:HB3  | 1:11:A:PHE:HE2  | 14       | 0.89          |
| (1,363)  | 1:27:A:ALA:HB1  | 1:28:A:LEU:HD21 | 7        | 0.89          |
| (1,205)  | 1:18:A:LYS:HB3  | 1:53:A:PHE:HD2  | 20       | 0.89          |
| (1,205)  | 1:18:A:LYS:HB2  | 1:53:A:PHE:HD2  | 20       | 0.89          |
| (1,182)  | 1:13:A:THR:HG21 | 1:14:A:ASN:HA   | 9        | 0.89          |
| (1,142)  | 1:10:A:ARG:HD3  | 1:11:A:PHE:HD2  | 12       | 0.89          |
| (1,138)  | 1:10:A:ARG:HD2  | 1:11:A:PHE:HE2  | 1        | 0.89          |
| (1,138)  | 1:10:A:ARG:HD3  | 1:11:A:PHE:HE2  | 1        | 0.89          |
| (1,42)   | 1:62:A:PHE:HE2  | 1:67:A:PRO:HG3  | 8        | 0.89          |
| (1,1161) | 1:31:A:LEU:HD21 | 1:32:A:GLY:H    | 1        | 0.88          |
| (1,1161) | 1:31:A:LEU:HD21 | 1:32:A:GLY:H    | 5        | 0.88          |
| (1,1161) | 1:31:A:LEU:HD21 | 1:32:A:GLY:H    | 7        | 0.88          |
| (1,1161) | 1:31:A:LEU:HD21 | 1:32:A:GLY:H    | 11       | 0.88          |
| (1,1161) | 1:31:A:LEU:HD21 | 1:32:A:GLY:H    | 14       | 0.88          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1161) | 1:31:A:LEU:HD21 | 1:32:A:GLY:H    | 19       | 0.88          |
| (1,862)  | 1:4:A:MET:HE3   | 1:7:A:ILE:H     | 1        | 0.88          |
| (1,862)  | 1:4:A:MET:HE3   | 1:7:A:ILE:H     | 8        | 0.88          |
| (1,848)  | 1:31:A:LEU:HB2  | 1:76:A:VAL:HG23 | 17       | 0.88          |
| (1,846)  | 1:72:A:ASP:HA   | 1:76:A:VAL:HG21 | 2        | 0.88          |
| (1,765)  | 1:60:A:ILE:HD12 | 1:63:A:CYS:HB3  | 18       | 0.88          |
| (1,765)  | 1:60:A:ILE:HD12 | 1:63:A:CYS:HB2  | 18       | 0.88          |
| (1,727)  | 1:5:A:GLU:H     | 1:60:A:ILE:HD13 | 20       | 0.88          |
| (1,467)  | 1:39:A:VAL:HA   | 1:69:A:LEU:HD23 | 14       | 0.88          |
| (1,390)  | 1:10:A:ARG:HB2  | 1:11:A:PHE:HE2  | 2        | 0.88          |
| (1,390)  | 1:10:A:ARG:HB3  | 1:11:A:PHE:HE2  | 2        | 0.88          |
| (1,324)  | 1:11:A:PHE:HE1  | 1:24:A:LEU:HG   | 18       | 0.88          |
| (1,271)  | 1:19:A:ILE:HD11 | 1:54:A:ILE:HG13 | 2        | 0.88          |
| (1,205)  | 1:18:A:LYS:HB3  | 1:53:A:PHE:HD2  | 16       | 0.88          |
| (1,205)  | 1:18:A:LYS:HB2  | 1:53:A:PHE:HD2  | 16       | 0.88          |
| (1,42)   | 1:62:A:PHE:HE2  | 1:67:A:PRO:HG3  | 19       | 0.88          |
| (1,1259) | 1:53:A:PHE:HD2  | 1:54:A:ILE:H    | 3        | 0.87          |
| (1,1161) | 1:31:A:LEU:HD21 | 1:32:A:GLY:H    | 8        | 0.87          |
| (1,1161) | 1:31:A:LEU:HD21 | 1:32:A:GLY:H    | 17       | 0.87          |
| (1,1161) | 1:31:A:LEU:HD21 | 1:32:A:GLY:H    | 18       | 0.87          |
| (1,862)  | 1:4:A:MET:HE3   | 1:7:A:ILE:H     | 15       | 0.87          |
| (1,467)  | 1:39:A:VAL:HA   | 1:69:A:LEU:HD23 | 18       | 0.87          |
| (1,363)  | 1:27:A:ALA:HB1  | 1:28:A:LEU:HD21 | 18       | 0.87          |
| (1,324)  | 1:11:A:PHE:HE1  | 1:24:A:LEU:HG   | 3        | 0.87          |
| (1,324)  | 1:11:A:PHE:HE1  | 1:24:A:LEU:HG   | 10       | 0.87          |
| (1,138)  | 1:10:A:ARG:HD2  | 1:11:A:PHE:HE2  | 16       | 0.87          |
| (1,138)  | 1:10:A:ARG:HD3  | 1:11:A:PHE:HE2  | 16       | 0.87          |
| (1,138)  | 1:10:A:ARG:HD2  | 1:11:A:PHE:HE2  | 18       | 0.87          |
| (1,138)  | 1:10:A:ARG:HD3  | 1:11:A:PHE:HE2  | 18       | 0.87          |
| (1,42)   | 1:62:A:PHE:HE2  | 1:67:A:PRO:HG3  | 3        | 0.87          |
| (1,42)   | 1:62:A:PHE:HE2  | 1:67:A:PRO:HG3  | 7        | 0.87          |
| (1,846)  | 1:72:A:ASP:HA   | 1:76:A:VAL:HG21 | 9        | 0.86          |
| (1,803)  | 1:62:A:PHE:HD2  | 1:70:A:MET:HG2  | 20       | 0.86          |
| (1,727)  | 1:5:A:GLU:H     | 1:60:A:ILE:HD13 | 2        | 0.86          |
| (1,363)  | 1:27:A:ALA:HB1  | 1:28:A:LEU:HD21 | 15       | 0.86          |
| (1,363)  | 1:27:A:ALA:HB1  | 1:28:A:LEU:HD21 | 19       | 0.86          |
| (1,324)  | 1:11:A:PHE:HE1  | 1:24:A:LEU:HG   | 4        | 0.86          |
| (1,42)   | 1:62:A:PHE:HE2  | 1:67:A:PRO:HG3  | 2        | 0.86          |
| (1,1432) | 1:20:A:SER:HB2  | 1:53:A:PHE:HD2  | 20       | 0.85          |
| (1,1432) | 1:20:A:SER:HB3  | 1:53:A:PHE:HD2  | 20       | 0.85          |
| (1,1161) | 1:31:A:LEU:HD21 | 1:32:A:GLY:H    | 12       | 0.85          |
| (1,862)  | 1:4:A:MET:HE3   | 1:7:A:ILE:H     | 13       | 0.85          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,850)  | 1:31:A:LEU:HB3  | 1:76:A:VAL:HG23 | 6        | 0.85          |
| (1,727)  | 1:5:A:GLU:H     | 1:60:A:ILE:HD13 | 8        | 0.85          |
| (1,390)  | 1:10:A:ARG:HB2  | 1:11:A:PHE:HE2  | 16       | 0.85          |
| (1,390)  | 1:10:A:ARG:HB3  | 1:11:A:PHE:HE2  | 16       | 0.85          |
| (1,390)  | 1:10:A:ARG:HB2  | 1:11:A:PHE:HE2  | 17       | 0.85          |
| (1,390)  | 1:10:A:ARG:HB3  | 1:11:A:PHE:HE2  | 17       | 0.85          |
| (1,324)  | 1:11:A:PHE:HE1  | 1:24:A:LEU:HG   | 17       | 0.85          |
| (1,305)  | 1:11:A:PHE:HE1  | 1:24:A:LEU:HA   | 1        | 0.85          |
| (1,182)  | 1:13:A:THR:HG21 | 1:14:A:ASN:HA   | 2        | 0.85          |
| (1,1431) | 1:20:A:SER:HB2  | 1:53:A:PHE:HE2  | 18       | 0.84          |
| (1,1431) | 1:20:A:SER:HB3  | 1:53:A:PHE:HE2  | 18       | 0.84          |
| (1,1295) | 1:60:A:ILE:HD12 | 1:63:A:CYS:H    | 17       | 0.84          |
| (1,1259) | 1:53:A:PHE:HD2  | 1:54:A:ILE:H    | 12       | 0.84          |
| (1,1259) | 1:53:A:PHE:HD2  | 1:54:A:ILE:H    | 13       | 0.84          |
| (1,834)  | 1:31:A:LEU:HD13 | 1:31:A:LEU:HD22 | 1        | 0.84          |
| (1,472)  | 1:62:A:PHE:HE2  | 1:69:A:LEU:HD21 | 7        | 0.84          |
| (1,467)  | 1:39:A:VAL:HA   | 1:69:A:LEU:HD23 | 13       | 0.84          |
| (1,324)  | 1:11:A:PHE:HE1  | 1:24:A:LEU:HG   | 1        | 0.84          |
| (1,182)  | 1:13:A:THR:HG21 | 1:14:A:ASN:HA   | 20       | 0.84          |
| (1,142)  | 1:10:A:ARG:HD3  | 1:11:A:PHE:HD2  | 5        | 0.84          |
| (1,1259) | 1:53:A:PHE:HD2  | 1:54:A:ILE:H    | 6        | 0.83          |
| (1,1108) | 1:8:A:PHE:HE1   | 1:19:A:ILE:H    | 4        | 0.83          |
| (1,888)  | 1:46:A:ILE:HD12 | 1:62:A:PHE:H    | 20       | 0.83          |
| (1,834)  | 1:31:A:LEU:HD13 | 1:31:A:LEU:HD22 | 10       | 0.83          |
| (1,803)  | 1:62:A:PHE:HD2  | 1:70:A:MET:HG2  | 5        | 0.83          |
| (1,508)  | 1:42:A:MET:HB2  | 1:62:A:PHE:HE1  | 1        | 0.83          |
| (1,390)  | 1:10:A:ARG:HB2  | 1:11:A:PHE:HE2  | 6        | 0.83          |
| (1,390)  | 1:10:A:ARG:HB3  | 1:11:A:PHE:HE2  | 6        | 0.83          |
| (1,271)  | 1:19:A:ILE:HD11 | 1:54:A:ILE:HG13 | 1        | 0.83          |
| (1,271)  | 1:19:A:ILE:HD11 | 1:54:A:ILE:HG13 | 15       | 0.83          |
| (1,163)  | 1:12:A:ASP:HB2  | 1:19:A:ILE:HD13 | 13       | 0.83          |
| (1,42)   | 1:62:A:PHE:HE2  | 1:67:A:PRO:HG3  | 4        | 0.83          |
| (1,42)   | 1:62:A:PHE:HE2  | 1:67:A:PRO:HG3  | 16       | 0.83          |
| (1,1333) | 1:69:A:LEU:HD21 | 1:70:A:MET:H    | 5        | 0.82          |
| (1,1333) | 1:69:A:LEU:HD21 | 1:70:A:MET:H    | 10       | 0.82          |
| (1,1333) | 1:69:A:LEU:HD21 | 1:70:A:MET:H    | 11       | 0.82          |
| (1,1295) | 1:60:A:ILE:HD12 | 1:63:A:CYS:H    | 11       | 0.82          |
| (1,1295) | 1:60:A:ILE:HD12 | 1:63:A:CYS:H    | 12       | 0.82          |
| (1,1259) | 1:53:A:PHE:HD2  | 1:54:A:ILE:H    | 4        | 0.82          |
| (1,1259) | 1:53:A:PHE:HD2  | 1:54:A:ILE:H    | 8        | 0.82          |
| (1,1259) | 1:53:A:PHE:HD2  | 1:54:A:ILE:H    | 17       | 0.82          |
| (1,1161) | 1:31:A:LEU:HD21 | 1:32:A:GLY:H    | 20       | 0.82          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,853)  | 1:69:A:LEU:HB2  | 1:70:A:MET:HE3  | 5        | 0.82          |
| (1,791)  | 1:67:A:PRO:HB2  | 1:69:A:LEU:HG   | 14       | 0.82          |
| (1,791)  | 1:67:A:PRO:HB2  | 1:69:A:LEU:HG   | 18       | 0.82          |
| (1,472)  | 1:62:A:PHE:HE2  | 1:69:A:LEU:HD21 | 19       | 0.82          |
| (1,324)  | 1:11:A:PHE:HE1  | 1:24:A:LEU:HG   | 16       | 0.82          |
| (1,324)  | 1:11:A:PHE:HE1  | 1:24:A:LEU:HG   | 19       | 0.82          |
| (1,305)  | 1:11:A:PHE:HE1  | 1:24:A:LEU:HA   | 14       | 0.82          |
| (1,305)  | 1:11:A:PHE:HE1  | 1:24:A:LEU:HA   | 15       | 0.82          |
| (1,42)   | 1:62:A:PHE:HE2  | 1:67:A:PRO:HG3  | 10       | 0.82          |
| (1,42)   | 1:62:A:PHE:HE2  | 1:67:A:PRO:HG3  | 11       | 0.82          |
| (1,1432) | 1:20:A:SER:HB2  | 1:53:A:PHE:HD2  | 19       | 0.81          |
| (1,1432) | 1:20:A:SER:HB3  | 1:53:A:PHE:HD2  | 19       | 0.81          |
| (1,1333) | 1:69:A:LEU:HD21 | 1:70:A:MET:H    | 15       | 0.81          |
| (1,1259) | 1:53:A:PHE:HD2  | 1:54:A:ILE:H    | 9        | 0.81          |
| (1,1259) | 1:53:A:PHE:HD2  | 1:54:A:ILE:H    | 14       | 0.81          |
| (1,888)  | 1:46:A:ILE:HD12 | 1:62:A:PHE:H    | 12       | 0.81          |
| (1,853)  | 1:69:A:LEU:HB2  | 1:70:A:MET:HE3  | 11       | 0.81          |
| (1,834)  | 1:31:A:LEU:HD13 | 1:31:A:LEU:HD22 | 3        | 0.81          |
| (1,727)  | 1:5:A:GLU:H     | 1:60:A:ILE:HD13 | 10       | 0.81          |
| (1,472)  | 1:62:A:PHE:HE2  | 1:69:A:LEU:HD21 | 3        | 0.81          |
| (1,184)  | 1:25:A:THR:HG22 | 1:40:A:GLN:HB2  | 20       | 0.81          |
| (1,142)  | 1:10:A:ARG:HD3  | 1:11:A:PHE:HD2  | 19       | 0.81          |
| (1,42)   | 1:62:A:PHE:HE2  | 1:67:A:PRO:HG3  | 9        | 0.81          |
| (1,42)   | 1:62:A:PHE:HE2  | 1:67:A:PRO:HG3  | 15       | 0.81          |
| (1,1432) | 1:20:A:SER:HB2  | 1:53:A:PHE:HD2  | 10       | 0.8           |
| (1,1432) | 1:20:A:SER:HB3  | 1:53:A:PHE:HD2  | 10       | 0.8           |
| (1,1333) | 1:69:A:LEU:HD21 | 1:70:A:MET:H    | 19       | 0.8           |
| (1,1333) | 1:69:A:LEU:HD21 | 1:70:A:MET:H    | 20       | 0.8           |
| (1,1259) | 1:53:A:PHE:HD2  | 1:54:A:ILE:H    | 16       | 0.8           |
| (1,1259) | 1:53:A:PHE:HD2  | 1:54:A:ILE:H    | 20       | 0.8           |
| (1,862)  | 1:4:A:MET:HE3   | 1:7:A:ILE:H     | 18       | 0.8           |
| (1,846)  | 1:72:A:ASP:HA   | 1:76:A:VAL:HG21 | 3        | 0.8           |
| (1,834)  | 1:31:A:LEU:HD13 | 1:31:A:LEU:HD22 | 7        | 0.8           |
| (1,809)  | 1:69:A:LEU:HD21 | 1:70:A:MET:HG2  | 18       | 0.8           |
| (1,809)  | 1:69:A:LEU:HD21 | 1:70:A:MET:HG3  | 18       | 0.8           |
| (1,727)  | 1:5:A:GLU:H     | 1:60:A:ILE:HD13 | 15       | 0.8           |
| (1,727)  | 1:5:A:GLU:H     | 1:60:A:ILE:HD13 | 18       | 0.8           |
| (1,508)  | 1:42:A:MET:HB2  | 1:62:A:PHE:HE1  | 6        | 0.8           |
| (1,390)  | 1:10:A:ARG:HB2  | 1:11:A:PHE:HE2  | 9        | 0.8           |
| (1,390)  | 1:10:A:ARG:HB3  | 1:11:A:PHE:HE2  | 9        | 0.8           |
| (1,363)  | 1:27:A:ALA:HB1  | 1:28:A:LEU:HD21 | 20       | 0.8           |
| (1,42)   | 1:62:A:PHE:HE2  | 1:67:A:PRO:HG3  | 5        | 0.8           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,42)   | 1:62:A:PHE:HE2  | 1:67:A:PRO:HG3  | 6        | 0.8           |
| (1,42)   | 1:62:A:PHE:HE2  | 1:67:A:PRO:HG3  | 17       | 0.8           |
| (1,1533) | 1:52:A:GLY:HA2  | 1:53:A:PHE:HE1  | 3        | 0.79          |
| (1,1533) | 1:52:A:GLY:HA3  | 1:53:A:PHE:HE1  | 3        | 0.79          |
| (1,1333) | 1:69:A:LEU:HD21 | 1:70:A:MET:H    | 7        | 0.79          |
| (1,1259) | 1:53:A:PHE:HD2  | 1:54:A:ILE:H    | 2        | 0.79          |
| (1,866)  | 1:4:A:MET:HE3   | 1:7:A:ILE:HD11  | 20       | 0.79          |
| (1,866)  | 1:4:A:MET:HE3   | 1:7:A:ILE:HD13  | 20       | 0.79          |
| (1,853)  | 1:69:A:LEU:HB2  | 1:70:A:MET:HE3  | 15       | 0.79          |
| (1,848)  | 1:31:A:LEU:HB2  | 1:76:A:VAL:HG23 | 7        | 0.79          |
| (1,848)  | 1:31:A:LEU:HB2  | 1:76:A:VAL:HG23 | 12       | 0.79          |
| (1,834)  | 1:31:A:LEU:HD13 | 1:31:A:LEU:HD22 | 4        | 0.79          |
| (1,834)  | 1:31:A:LEU:HD13 | 1:31:A:LEU:HD22 | 19       | 0.79          |
| (1,809)  | 1:69:A:LEU:HD21 | 1:70:A:MET:HG2  | 14       | 0.79          |
| (1,809)  | 1:69:A:LEU:HD21 | 1:70:A:MET:HG3  | 14       | 0.79          |
| (1,803)  | 1:62:A:PHE:HD2  | 1:70:A:MET:HG2  | 11       | 0.79          |
| (1,803)  | 1:62:A:PHE:HD2  | 1:70:A:MET:HG2  | 14       | 0.79          |
| (1,727)  | 1:5:A:GLU:H     | 1:60:A:ILE:HD13 | 16       | 0.79          |
| (1,324)  | 1:11:A:PHE:HE1  | 1:24:A:LEU:HG   | 20       | 0.79          |
| (1,182)  | 1:13:A:THR:HG21 | 1:14:A:ASN:HA   | 6        | 0.79          |
| (1,163)  | 1:12:A:ASP:HB2  | 1:19:A:ILE:HD13 | 9        | 0.79          |
| (1,142)  | 1:10:A:ARG:HD3  | 1:11:A:PHE:HD2  | 10       | 0.79          |
| (1,42)   | 1:62:A:PHE:HE2  | 1:67:A:PRO:HG3  | 20       | 0.79          |
| (1,1333) | 1:69:A:LEU:HD21 | 1:70:A:MET:H    | 3        | 0.78          |
| (1,1333) | 1:69:A:LEU:HD21 | 1:70:A:MET:H    | 8        | 0.78          |
| (1,1259) | 1:53:A:PHE:HD2  | 1:54:A:ILE:H    | 11       | 0.78          |
| (1,888)  | 1:46:A:ILE:HD12 | 1:62:A:PHE:H    | 10       | 0.78          |
| (1,853)  | 1:69:A:LEU:HB2  | 1:70:A:MET:HE3  | 8        | 0.78          |
| (1,853)  | 1:69:A:LEU:HB2  | 1:70:A:MET:HE3  | 10       | 0.78          |
| (1,834)  | 1:31:A:LEU:HD13 | 1:31:A:LEU:HD22 | 9        | 0.78          |
| (1,834)  | 1:31:A:LEU:HD13 | 1:31:A:LEU:HD22 | 20       | 0.78          |
| (1,803)  | 1:62:A:PHE:HD2  | 1:70:A:MET:HG2  | 10       | 0.78          |
| (1,803)  | 1:62:A:PHE:HD2  | 1:70:A:MET:HG2  | 15       | 0.78          |
| (1,472)  | 1:62:A:PHE:HE2  | 1:69:A:LEU:HD21 | 10       | 0.78          |
| (1,417)  | 1:28:A:LEU:HD22 | 1:33:A:SER:HA   | 2        | 0.78          |
| (1,271)  | 1:19:A:ILE:HD11 | 1:54:A:ILE:HG13 | 20       | 0.78          |
| (1,268)  | 1:19:A:ILE:HD11 | 1:59:A:PHE:HD2  | 5        | 0.78          |
| (1,163)  | 1:12:A:ASP:HB2  | 1:19:A:ILE:HD13 | 4        | 0.78          |
| (1,142)  | 1:10:A:ARG:HD3  | 1:11:A:PHE:HD2  | 6        | 0.78          |
| (1,138)  | 1:10:A:ARG:HD2  | 1:11:A:PHE:HE2  | 3        | 0.78          |
| (1,138)  | 1:10:A:ARG:HD3  | 1:11:A:PHE:HE2  | 3        | 0.78          |
| (1,42)   | 1:62:A:PHE:HE2  | 1:67:A:PRO:HG3  | 12       | 0.78          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1575) | 1:72:A:ASP:HB2  | 1:73:A:VAL:HG22 | 11       | 0.77          |
| (1,1575) | 1:72:A:ASP:HB3  | 1:73:A:VAL:HG22 | 11       | 0.77          |
| (1,1431) | 1:20:A:SER:HB2  | 1:53:A:PHE:HE2  | 7        | 0.77          |
| (1,1431) | 1:20:A:SER:HB3  | 1:53:A:PHE:HE2  | 7        | 0.77          |
| (1,1295) | 1:60:A:ILE:HD12 | 1:63:A:CYS:H    | 2        | 0.77          |
| (1,1295) | 1:60:A:ILE:HD12 | 1:63:A:CYS:H    | 5        | 0.77          |
| (1,1259) | 1:53:A:PHE:HD2  | 1:54:A:ILE:H    | 1        | 0.77          |
| (1,1259) | 1:53:A:PHE:HD2  | 1:54:A:ILE:H    | 15       | 0.77          |
| (1,1259) | 1:53:A:PHE:HD2  | 1:54:A:ILE:H    | 18       | 0.77          |
| (1,888)  | 1:46:A:ILE:HD12 | 1:62:A:PHE:H    | 18       | 0.77          |
| (1,862)  | 1:4:A:MET:HE3   | 1:7:A:ILE:H     | 3        | 0.77          |
| (1,853)  | 1:69:A:LEU:HB2  | 1:70:A:MET:HE3  | 9        | 0.77          |
| (1,834)  | 1:31:A:LEU:HD13 | 1:31:A:LEU:HD22 | 2        | 0.77          |
| (1,834)  | 1:31:A:LEU:HD13 | 1:31:A:LEU:HD22 | 6        | 0.77          |
| (1,834)  | 1:31:A:LEU:HD13 | 1:31:A:LEU:HD22 | 11       | 0.77          |
| (1,834)  | 1:31:A:LEU:HD13 | 1:31:A:LEU:HD22 | 13       | 0.77          |
| (1,834)  | 1:31:A:LEU:HD13 | 1:31:A:LEU:HD22 | 15       | 0.77          |
| (1,834)  | 1:31:A:LEU:HD13 | 1:31:A:LEU:HD22 | 16       | 0.77          |
| (1,834)  | 1:31:A:LEU:HD13 | 1:31:A:LEU:HD22 | 17       | 0.77          |
| (1,508)  | 1:42:A:MET:HB2  | 1:62:A:PHE:HE1  | 4        | 0.77          |
| (1,508)  | 1:42:A:MET:HB2  | 1:62:A:PHE:HE1  | 12       | 0.77          |
| (1,324)  | 1:11:A:PHE:HE1  | 1:24:A:LEU:HG   | 5        | 0.77          |
| (1,138)  | 1:10:A:ARG:HD2  | 1:11:A:PHE:HE2  | 4        | 0.77          |
| (1,138)  | 1:10:A:ARG:HD3  | 1:11:A:PHE:HE2  | 4        | 0.77          |
| (1,138)  | 1:10:A:ARG:HD2  | 1:11:A:PHE:HE2  | 5        | 0.77          |
| (1,138)  | 1:10:A:ARG:HD3  | 1:11:A:PHE:HE2  | 5        | 0.77          |
| (1,42)   | 1:62:A:PHE:HE2  | 1:67:A:PRO:HG3  | 1        | 0.77          |
| (1,1575) | 1:72:A:ASP:HB2  | 1:73:A:VAL:HG22 | 8        | 0.76          |
| (1,1575) | 1:72:A:ASP:HB3  | 1:73:A:VAL:HG22 | 8        | 0.76          |
| (1,1432) | 1:20:A:SER:HB2  | 1:53:A:PHE:HD2  | 3        | 0.76          |
| (1,1432) | 1:20:A:SER:HB3  | 1:53:A:PHE:HD2  | 3        | 0.76          |
| (1,1295) | 1:60:A:ILE:HD12 | 1:63:A:CYS:H    | 4        | 0.76          |
| (1,1259) | 1:53:A:PHE:HD2  | 1:54:A:ILE:H    | 5        | 0.76          |
| (1,1259) | 1:53:A:PHE:HD2  | 1:54:A:ILE:H    | 7        | 0.76          |
| (1,1259) | 1:53:A:PHE:HD2  | 1:54:A:ILE:H    | 10       | 0.76          |
| (1,1259) | 1:53:A:PHE:HD2  | 1:54:A:ILE:H    | 19       | 0.76          |
| (1,888)  | 1:46:A:ILE:HD12 | 1:62:A:PHE:H    | 3        | 0.76          |
| (1,866)  | 1:4:A:MET:HE3   | 1:7:A:ILE:HD11  | 14       | 0.76          |
| (1,866)  | 1:4:A:MET:HE3   | 1:7:A:ILE:HD13  | 14       | 0.76          |
| (1,834)  | 1:31:A:LEU:HD13 | 1:31:A:LEU:HD22 | 5        | 0.76          |
| (1,834)  | 1:31:A:LEU:HD13 | 1:31:A:LEU:HD22 | 8        | 0.76          |
| (1,834)  | 1:31:A:LEU:HD13 | 1:31:A:LEU:HD22 | 12       | 0.76          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,803)  | 1:62:A:PHE:HD2  | 1:70:A:MET:HG2  | 18       | 0.76          |
| (1,727)  | 1:5:A:GLU:H     | 1:60:A:ILE:HD13 | 9        | 0.76          |
| (1,590)  | 1:11:A:PHE:HB2  | 1:11:A:PHE:HE1  | 1        | 0.76          |
| (1,590)  | 1:11:A:PHE:HB2  | 1:11:A:PHE:HE1  | 6        | 0.76          |
| (1,590)  | 1:11:A:PHE:HB2  | 1:11:A:PHE:HE1  | 7        | 0.76          |
| (1,590)  | 1:11:A:PHE:HB2  | 1:11:A:PHE:HE1  | 9        | 0.76          |
| (1,590)  | 1:11:A:PHE:HB2  | 1:11:A:PHE:HE1  | 14       | 0.76          |
| (1,590)  | 1:11:A:PHE:HB2  | 1:11:A:PHE:HE1  | 15       | 0.76          |
| (1,590)  | 1:11:A:PHE:HB2  | 1:11:A:PHE:HE1  | 17       | 0.76          |
| (1,590)  | 1:11:A:PHE:HB2  | 1:11:A:PHE:HE1  | 18       | 0.76          |
| (1,590)  | 1:11:A:PHE:HB2  | 1:11:A:PHE:HE1  | 20       | 0.76          |
| (1,504)  | 1:25:A:THR:HG22 | 1:40:A:GLN:HG3  | 20       | 0.76          |
| (1,472)  | 1:62:A:PHE:HE2  | 1:69:A:LEU:HD21 | 11       | 0.76          |
| (1,324)  | 1:11:A:PHE:HE1  | 1:24:A:LEU:HG   | 15       | 0.76          |
| (1,271)  | 1:19:A:ILE:HD11 | 1:54:A:ILE:HG13 | 18       | 0.76          |
| (1,184)  | 1:25:A:THR:HG22 | 1:40:A:GLN:HB2  | 13       | 0.76          |
| (1,184)  | 1:25:A:THR:HG22 | 1:40:A:GLN:HB2  | 14       | 0.76          |
| (1,138)  | 1:10:A:ARG:HD2  | 1:11:A:PHE:HE2  | 14       | 0.76          |
| (1,138)  | 1:10:A:ARG:HD3  | 1:11:A:PHE:HE2  | 14       | 0.76          |
| (1,1295) | 1:60:A:ILE:HD12 | 1:63:A:CYS:H    | 3        | 0.75          |
| (1,1295) | 1:60:A:ILE:HD12 | 1:63:A:CYS:H    | 8        | 0.75          |
| (1,848)  | 1:31:A:LEU:HB2  | 1:76:A:VAL:HG23 | 19       | 0.75          |
| (1,834)  | 1:31:A:LEU:HD13 | 1:31:A:LEU:HD22 | 14       | 0.75          |
| (1,834)  | 1:31:A:LEU:HD13 | 1:31:A:LEU:HD22 | 18       | 0.75          |
| (1,727)  | 1:5:A:GLU:H     | 1:60:A:ILE:HD13 | 5        | 0.75          |
| (1,590)  | 1:11:A:PHE:HB2  | 1:11:A:PHE:HE1  | 2        | 0.75          |
| (1,590)  | 1:11:A:PHE:HB2  | 1:11:A:PHE:HE1  | 3        | 0.75          |
| (1,590)  | 1:11:A:PHE:HB2  | 1:11:A:PHE:HE1  | 4        | 0.75          |
| (1,590)  | 1:11:A:PHE:HB2  | 1:11:A:PHE:HE1  | 5        | 0.75          |
| (1,590)  | 1:11:A:PHE:HB2  | 1:11:A:PHE:HE1  | 8        | 0.75          |
| (1,590)  | 1:11:A:PHE:HB2  | 1:11:A:PHE:HE1  | 10       | 0.75          |
| (1,590)  | 1:11:A:PHE:HB2  | 1:11:A:PHE:HE1  | 11       | 0.75          |
| (1,590)  | 1:11:A:PHE:HB2  | 1:11:A:PHE:HE1  | 16       | 0.75          |
| (1,590)  | 1:11:A:PHE:HB2  | 1:11:A:PHE:HE1  | 19       | 0.75          |
| (1,508)  | 1:42:A:MET:HB2  | 1:62:A:PHE:HE1  | 16       | 0.75          |
| (1,472)  | 1:62:A:PHE:HE2  | 1:69:A:LEU:HD21 | 5        | 0.75          |
| (1,472)  | 1:62:A:PHE:HE2  | 1:69:A:LEU:HD21 | 8        | 0.75          |
| (1,472)  | 1:62:A:PHE:HE2  | 1:69:A:LEU:HD21 | 15       | 0.75          |
| (1,305)  | 1:11:A:PHE:HE1  | 1:24:A:LEU:HA   | 20       | 0.75          |
| (1,271)  | 1:19:A:ILE:HD11 | 1:54:A:ILE:HG13 | 19       | 0.75          |
| (1,138)  | 1:10:A:ARG:HD2  | 1:11:A:PHE:HE2  | 20       | 0.75          |
| (1,138)  | 1:10:A:ARG:HD3  | 1:11:A:PHE:HE2  | 20       | 0.75          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1532) | 1:52:A:GLY:HA2  | 1:53:A:PHE:HD1  | 13       | 0.74          |
| (1,1532) | 1:52:A:GLY:HA3  | 1:53:A:PHE:HD1  | 13       | 0.74          |
| (1,1295) | 1:60:A:ILE:HD12 | 1:63:A:CYS:H    | 6        | 0.74          |
| (1,1173) | 1:34:A:THR:HG23 | 1:35:A:SER:H    | 3        | 0.74          |
| (1,888)  | 1:46:A:ILE:HD12 | 1:62:A:PHE:H    | 15       | 0.74          |
| (1,853)  | 1:69:A:LEU:HB2  | 1:70:A:MET:HE3  | 19       | 0.74          |
| (1,853)  | 1:69:A:LEU:HB2  | 1:70:A:MET:HE3  | 20       | 0.74          |
| (1,803)  | 1:62:A:PHE:HD2  | 1:70:A:MET:HG2  | 6        | 0.74          |
| (1,590)  | 1:11:A:PHE:HB2  | 1:11:A:PHE:HE1  | 12       | 0.74          |
| (1,590)  | 1:11:A:PHE:HB2  | 1:11:A:PHE:HE1  | 13       | 0.74          |
| (1,363)  | 1:27:A:ALA:HB1  | 1:28:A:LEU:HD21 | 14       | 0.74          |
| (1,324)  | 1:11:A:PHE:HE1  | 1:24:A:LEU:HG   | 8        | 0.74          |
| (1,305)  | 1:11:A:PHE:HE1  | 1:24:A:LEU:HA   | 18       | 0.74          |
| (1,271)  | 1:19:A:ILE:HD11 | 1:54:A:ILE:HG13 | 5        | 0.74          |
| (1,271)  | 1:19:A:ILE:HD11 | 1:54:A:ILE:HG13 | 7        | 0.74          |
| (1,266)  | 1:12:A:ASP:H    | 1:19:A:ILE:HD13 | 19       | 0.74          |
| (1,1295) | 1:60:A:ILE:HD12 | 1:63:A:CYS:H    | 18       | 0.73          |
| (1,1173) | 1:34:A:THR:HG23 | 1:35:A:SER:H    | 5        | 0.73          |
| (1,888)  | 1:46:A:ILE:HD12 | 1:62:A:PHE:H    | 1        | 0.73          |
| (1,888)  | 1:46:A:ILE:HD12 | 1:62:A:PHE:H    | 6        | 0.73          |
| (1,850)  | 1:31:A:LEU:HB3  | 1:76:A:VAL:HG23 | 4        | 0.73          |
| (1,850)  | 1:31:A:LEU:HB3  | 1:76:A:VAL:HG23 | 8        | 0.73          |
| (1,727)  | 1:5:A:GLU:H     | 1:60:A:ILE:HD13 | 17       | 0.73          |
| (1,508)  | 1:42:A:MET:HB2  | 1:62:A:PHE:HE1  | 5        | 0.73          |
| (1,508)  | 1:42:A:MET:HB2  | 1:62:A:PHE:HE1  | 11       | 0.73          |
| (1,508)  | 1:42:A:MET:HB2  | 1:62:A:PHE:HE1  | 17       | 0.73          |
| (1,508)  | 1:42:A:MET:HB2  | 1:62:A:PHE:HE1  | 20       | 0.73          |
| (1,271)  | 1:19:A:ILE:HD11 | 1:54:A:ILE:HG13 | 6        | 0.73          |
| (1,271)  | 1:19:A:ILE:HD11 | 1:54:A:ILE:HG13 | 9        | 0.73          |
| (1,271)  | 1:19:A:ILE:HD11 | 1:54:A:ILE:HG13 | 10       | 0.73          |
| (1,271)  | 1:19:A:ILE:HD11 | 1:54:A:ILE:HG13 | 12       | 0.73          |
| (1,271)  | 1:19:A:ILE:HD11 | 1:54:A:ILE:HG13 | 14       | 0.73          |
| (1,271)  | 1:19:A:ILE:HD11 | 1:54:A:ILE:HG13 | 16       | 0.73          |
| (1,268)  | 1:19:A:ILE:HD11 | 1:59:A:PHE:HD2  | 1        | 0.73          |
| (1,184)  | 1:25:A:THR:HG22 | 1:40:A:GLN:HB2  | 7        | 0.73          |
| (1,142)  | 1:10:A:ARG:HD3  | 1:11:A:PHE:HD2  | 17       | 0.73          |
| (1,1533) | 1:52:A:GLY:HA2  | 1:53:A:PHE:HE1  | 12       | 0.72          |
| (1,1533) | 1:52:A:GLY:HA3  | 1:53:A:PHE:HE1  | 12       | 0.72          |
| (1,888)  | 1:46:A:ILE:HD12 | 1:62:A:PHE:H    | 4        | 0.72          |
| (1,888)  | 1:46:A:ILE:HD12 | 1:62:A:PHE:H    | 14       | 0.72          |
| (1,853)  | 1:69:A:LEU:HB2  | 1:70:A:MET:HE3  | 2        | 0.72          |
| (1,853)  | 1:69:A:LEU:HB2  | 1:70:A:MET:HE3  | 3        | 0.72          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,853)  | 1:69:A:LEU:HB2  | 1:70:A:MET:HE3  | 7        | 0.72          |
| (1,850)  | 1:31:A:LEU:HB3  | 1:76:A:VAL:HG23 | 13       | 0.72          |
| (1,848)  | 1:31:A:LEU:HB2  | 1:76:A:VAL:HG23 | 3        | 0.72          |
| (1,848)  | 1:31:A:LEU:HB2  | 1:76:A:VAL:HG23 | 10       | 0.72          |
| (1,803)  | 1:62:A:PHE:HD2  | 1:70:A:MET:HG2  | 1        | 0.72          |
| (1,508)  | 1:42:A:MET:HB2  | 1:62:A:PHE:HE1  | 9        | 0.72          |
| (1,508)  | 1:42:A:MET:HB2  | 1:62:A:PHE:HE1  | 15       | 0.72          |
| (1,472)  | 1:62:A:PHE:HE2  | 1:69:A:LEU:HD21 | 20       | 0.72          |
| (1,324)  | 1:11:A:PHE:HE1  | 1:24:A:LEU:HG   | 11       | 0.72          |
| (1,271)  | 1:19:A:ILE:HD11 | 1:54:A:ILE:HG13 | 4        | 0.72          |
| (1,271)  | 1:19:A:ILE:HD11 | 1:54:A:ILE:HG13 | 11       | 0.72          |
| (1,271)  | 1:19:A:ILE:HD11 | 1:54:A:ILE:HG13 | 13       | 0.72          |
| (1,268)  | 1:19:A:ILE:HD11 | 1:59:A:PHE:HD2  | 12       | 0.72          |
| (1,266)  | 1:12:A:ASP:H    | 1:19:A:ILE:HD13 | 2        | 0.72          |
| (1,184)  | 1:25:A:THR:HG22 | 1:40:A:GLN:HB2  | 2        | 0.72          |
| (1,184)  | 1:25:A:THR:HG22 | 1:40:A:GLN:HB2  | 5        | 0.72          |
| (1,163)  | 1:12:A:ASP:HB2  | 1:19:A:ILE:HD13 | 2        | 0.72          |
| (1,1173) | 1:34:A:THR:HG23 | 1:35:A:SER:H    | 11       | 0.71          |
| (1,803)  | 1:62:A:PHE:HD2  | 1:70:A:MET:HG2  | 7        | 0.71          |
| (1,803)  | 1:62:A:PHE:HD2  | 1:70:A:MET:HG2  | 19       | 0.71          |
| (1,791)  | 1:67:A:PRO:HB2  | 1:69:A:LEU:HG   | 1        | 0.71          |
| (1,504)  | 1:25:A:THR:HG22 | 1:40:A:GLN:HG3  | 13       | 0.71          |
| (1,271)  | 1:19:A:ILE:HD11 | 1:54:A:ILE:HG13 | 3        | 0.71          |
| (1,271)  | 1:19:A:ILE:HD11 | 1:54:A:ILE:HG13 | 17       | 0.71          |
| (1,266)  | 1:12:A:ASP:H    | 1:19:A:ILE:HD13 | 11       | 0.71          |
| (1,266)  | 1:12:A:ASP:H    | 1:19:A:ILE:HD13 | 14       | 0.71          |
| (1,184)  | 1:25:A:THR:HG22 | 1:40:A:GLN:HB2  | 12       | 0.71          |
| (1,138)  | 1:10:A:ARG:HD2  | 1:11:A:PHE:HE2  | 6        | 0.71          |
| (1,138)  | 1:10:A:ARG:HD3  | 1:11:A:PHE:HE2  | 6        | 0.71          |
| (1,74)   | 1:7:A:ILE:HD11  | 1:74:A:ALA:HB1  | 10       | 0.71          |
| (1,74)   | 1:7:A:ILE:HD11  | 1:74:A:ALA:HB2  | 10       | 0.71          |
| (1,42)   | 1:62:A:PHE:HE2  | 1:67:A:PRO:HG3  | 14       | 0.71          |
| (1,42)   | 1:62:A:PHE:HE2  | 1:67:A:PRO:HG3  | 18       | 0.71          |
| (1,1575) | 1:72:A:ASP:HB2  | 1:73:A:VAL:HG22 | 20       | 0.7           |
| (1,1575) | 1:72:A:ASP:HB3  | 1:73:A:VAL:HG22 | 20       | 0.7           |
| (1,1295) | 1:60:A:ILE:HD12 | 1:63:A:CYS:H    | 1        | 0.7           |
| (1,1295) | 1:60:A:ILE:HD12 | 1:63:A:CYS:H    | 19       | 0.7           |
| (1,888)  | 1:46:A:ILE:HD12 | 1:62:A:PHE:H    | 2        | 0.7           |
| (1,888)  | 1:46:A:ILE:HD12 | 1:62:A:PHE:H    | 8        | 0.7           |
| (1,888)  | 1:46:A:ILE:HD12 | 1:62:A:PHE:H    | 9        | 0.7           |
| (1,862)  | 1:4:A:MET:HE3   | 1:7:A:ILE:H     | 9        | 0.7           |
| (1,803)  | 1:62:A:PHE:HD2  | 1:70:A:MET:HG2  | 17       | 0.7           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,508)  | 1:42:A:MET:HB2  | 1:62:A:PHE:HE1  | 10       | 0.7           |
| (1,472)  | 1:62:A:PHE:HE2  | 1:69:A:LEU:HD21 | 2        | 0.7           |
| (1,142)  | 1:10:A:ARG:HD3  | 1:11:A:PHE:HD2  | 8        | 0.7           |
| (1,138)  | 1:10:A:ARG:HD2  | 1:11:A:PHE:HE2  | 8        | 0.7           |
| (1,138)  | 1:10:A:ARG:HD3  | 1:11:A:PHE:HE2  | 8        | 0.7           |
| (1,74)   | 1:7:A:ILE:HD11  | 1:74:A:ALA:HB1  | 2        | 0.7           |
| (1,74)   | 1:7:A:ILE:HD11  | 1:74:A:ALA:HB2  | 2        | 0.7           |
| (1,74)   | 1:7:A:ILE:HD11  | 1:74:A:ALA:HB1  | 9        | 0.7           |
| (1,74)   | 1:7:A:ILE:HD11  | 1:74:A:ALA:HB2  | 9        | 0.7           |
| (1,1333) | 1:69:A:LEU:HD21 | 1:70:A:MET:H    | 2        | 0.69          |
| (1,1295) | 1:60:A:ILE:HD12 | 1:63:A:CYS:H    | 10       | 0.69          |
| (1,888)  | 1:46:A:ILE:HD12 | 1:62:A:PHE:H    | 17       | 0.69          |
| (1,862)  | 1:4:A:MET:HE3   | 1:7:A:ILE:H     | 10       | 0.69          |
| (1,862)  | 1:4:A:MET:HE3   | 1:7:A:ILE:H     | 16       | 0.69          |
| (1,803)  | 1:62:A:PHE:HD2  | 1:70:A:MET:HG2  | 4        | 0.69          |
| (1,791)  | 1:67:A:PRO:HB2  | 1:69:A:LEU:HG   | 13       | 0.69          |
| (1,508)  | 1:42:A:MET:HB2  | 1:62:A:PHE:HE1  | 2        | 0.69          |
| (1,417)  | 1:28:A:LEU:HD22 | 1:33:A:SER:HA   | 4        | 0.69          |
| (1,319)  | 1:11:A:PHE:HD1  | 1:24:A:LEU:HB2  | 3        | 0.69          |
| (1,319)  | 1:11:A:PHE:HD1  | 1:24:A:LEU:HB2  | 6        | 0.69          |
| (1,271)  | 1:19:A:ILE:HD11 | 1:54:A:ILE:HG13 | 8        | 0.69          |
| (1,184)  | 1:25:A:THR:HG22 | 1:40:A:GLN:HB2  | 6        | 0.69          |
| (1,163)  | 1:12:A:ASP:HB2  | 1:19:A:ILE:HD13 | 16       | 0.69          |
| (1,163)  | 1:12:A:ASP:HB2  | 1:19:A:ILE:HD13 | 20       | 0.69          |
| (1,961)  | 1:60:A:ILE:H    | 1:60:A:ILE:HD12 | 15       | 0.68          |
| (1,861)  | 1:4:A:MET:H     | 1:4:A:MET:HE3   | 16       | 0.68          |
| (1,803)  | 1:62:A:PHE:HD2  | 1:70:A:MET:HG2  | 3        | 0.68          |
| (1,800)  | 1:62:A:PHE:HE2  | 1:70:A:MET:HG3  | 18       | 0.68          |
| (1,791)  | 1:67:A:PRO:HB2  | 1:69:A:LEU:HG   | 12       | 0.68          |
| (1,652)  | 1:46:A:ILE:HB   | 1:54:A:ILE:HD13 | 15       | 0.68          |
| (1,508)  | 1:42:A:MET:HB2  | 1:62:A:PHE:HE1  | 3        | 0.68          |
| (1,508)  | 1:42:A:MET:HB2  | 1:62:A:PHE:HE1  | 8        | 0.68          |
| (1,324)  | 1:11:A:PHE:HE1  | 1:24:A:LEU:HG   | 12       | 0.68          |
| (1,268)  | 1:19:A:ILE:HD11 | 1:59:A:PHE:HD2  | 8        | 0.68          |
| (1,268)  | 1:19:A:ILE:HD11 | 1:59:A:PHE:HD2  | 11       | 0.68          |
| (1,184)  | 1:25:A:THR:HG22 | 1:40:A:GLN:HB2  | 4        | 0.68          |
| (1,182)  | 1:13:A:THR:HG21 | 1:14:A:ASN:HA   | 3        | 0.68          |
| (1,163)  | 1:12:A:ASP:HB2  | 1:19:A:ILE:HD13 | 11       | 0.68          |
| (1,138)  | 1:10:A:ARG:HD2  | 1:11:A:PHE:HE2  | 17       | 0.68          |
| (1,138)  | 1:10:A:ARG:HD3  | 1:11:A:PHE:HE2  | 17       | 0.68          |
| (1,78)   | 1:8:A:PHE:HA    | 1:8:A:PHE:HD1   | 4        | 0.68          |
| (1,78)   | 1:8:A:PHE:HA    | 1:8:A:PHE:HD1   | 6        | 0.68          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,74)   | 1:7:A:ILE:HD11  | 1:74:A:ALA:HB1  | 4        | 0.68          |
| (1,74)   | 1:7:A:ILE:HD11  | 1:74:A:ALA:HB2  | 4        | 0.68          |
| (1,74)   | 1:7:A:ILE:HD11  | 1:74:A:ALA:HB1  | 16       | 0.68          |
| (1,74)   | 1:7:A:ILE:HD11  | 1:74:A:ALA:HB2  | 16       | 0.68          |
| (1,1173) | 1:34:A:THR:HG23 | 1:35:A:SER:H    | 10       | 0.67          |
| (1,727)  | 1:5:A:GLU:H     | 1:60:A:ILE:HD13 | 1        | 0.67          |
| (1,508)  | 1:42:A:MET:HB2  | 1:62:A:PHE:HE1  | 7        | 0.67          |
| (1,508)  | 1:42:A:MET:HB2  | 1:62:A:PHE:HE1  | 19       | 0.67          |
| (1,319)  | 1:11:A:PHE:HD1  | 1:24:A:LEU:HB2  | 10       | 0.67          |
| (1,319)  | 1:11:A:PHE:HD1  | 1:24:A:LEU:HB2  | 14       | 0.67          |
| (1,319)  | 1:11:A:PHE:HD1  | 1:24:A:LEU:HB2  | 18       | 0.67          |
| (1,184)  | 1:25:A:THR:HG22 | 1:40:A:GLN:HB2  | 11       | 0.67          |
| (1,184)  | 1:25:A:THR:HG22 | 1:40:A:GLN:HB2  | 19       | 0.67          |
| (1,74)   | 1:7:A:ILE:HD11  | 1:74:A:ALA:HB1  | 17       | 0.67          |
| (1,74)   | 1:7:A:ILE:HD11  | 1:74:A:ALA:HB2  | 17       | 0.67          |
| (1,1333) | 1:69:A:LEU:HD21 | 1:70:A:MET:H    | 9        | 0.66          |
| (1,888)  | 1:46:A:ILE:HD12 | 1:62:A:PHE:H    | 16       | 0.66          |
| (1,862)  | 1:4:A:MET:HE3   | 1:7:A:ILE:H     | 17       | 0.66          |
| (1,803)  | 1:62:A:PHE:HD2  | 1:70:A:MET:HG2  | 16       | 0.66          |
| (1,610)  | 1:51:A:ASP:H    | 1:52:A:GLY:HA3  | 10       | 0.66          |
| (1,610)  | 1:51:A:ASP:H    | 1:52:A:GLY:HA3  | 18       | 0.66          |
| (1,504)  | 1:25:A:THR:HG22 | 1:40:A:GLN:HG3  | 7        | 0.66          |
| (1,319)  | 1:11:A:PHE:HD1  | 1:24:A:LEU:HB2  | 4        | 0.66          |
| (1,319)  | 1:11:A:PHE:HD1  | 1:24:A:LEU:HB2  | 9        | 0.66          |
| (1,266)  | 1:12:A:ASP:H    | 1:19:A:ILE:HD13 | 18       | 0.66          |
| (1,184)  | 1:25:A:THR:HG22 | 1:40:A:GLN:HB2  | 1        | 0.66          |
| (1,184)  | 1:25:A:THR:HG22 | 1:40:A:GLN:HB2  | 17       | 0.66          |
| (1,182)  | 1:13:A:THR:HG21 | 1:14:A:ASN:HA   | 15       | 0.66          |
| (1,74)   | 1:7:A:ILE:HD11  | 1:74:A:ALA:HB1  | 11       | 0.66          |
| (1,74)   | 1:7:A:ILE:HD11  | 1:74:A:ALA:HB2  | 11       | 0.66          |
| (1,74)   | 1:7:A:ILE:HD11  | 1:74:A:ALA:HB1  | 19       | 0.66          |
| (1,74)   | 1:7:A:ILE:HD11  | 1:74:A:ALA:HB2  | 19       | 0.66          |
| (1,7)    | 1:3:A:ASP:HB2   | 1:4:A:MET:HE3   | 15       | 0.66          |
| (1,7)    | 1:3:A:ASP:HB3   | 1:4:A:MET:HE3   | 15       | 0.66          |
| (1,1295) | 1:60:A:ILE:HD12 | 1:63:A:CYS:H    | 7        | 0.65          |
| (1,1173) | 1:34:A:THR:HG23 | 1:35:A:SER:H    | 1        | 0.65          |
| (1,888)  | 1:46:A:ILE:HD12 | 1:62:A:PHE:H    | 7        | 0.65          |
| (1,888)  | 1:46:A:ILE:HD12 | 1:62:A:PHE:H    | 19       | 0.65          |
| (1,803)  | 1:62:A:PHE:HD2  | 1:70:A:MET:HG2  | 8        | 0.65          |
| (1,803)  | 1:62:A:PHE:HD2  | 1:70:A:MET:HG2  | 12       | 0.65          |
| (1,700)  | 1:62:A:PHE:HA   | 1:62:A:PHE:HD2  | 19       | 0.65          |
| (1,652)  | 1:46:A:ILE:HB   | 1:54:A:ILE:HD13 | 20       | 0.65          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,610)  | 1:51:A:ASP:H    | 1:52:A:GLY:HA3  | 3        | 0.65          |
| (1,610)  | 1:51:A:ASP:H    | 1:52:A:GLY:HA3  | 4        | 0.65          |
| (1,610)  | 1:51:A:ASP:H    | 1:52:A:GLY:HA3  | 7        | 0.65          |
| (1,610)  | 1:51:A:ASP:H    | 1:52:A:GLY:HA3  | 13       | 0.65          |
| (1,610)  | 1:51:A:ASP:H    | 1:52:A:GLY:HA3  | 19       | 0.65          |
| (1,74)   | 1:7:A:ILE:HD11  | 1:74:A:ALA:HB1  | 3        | 0.65          |
| (1,74)   | 1:7:A:ILE:HD11  | 1:74:A:ALA:HB2  | 3        | 0.65          |
| (1,74)   | 1:7:A:ILE:HD11  | 1:74:A:ALA:HB1  | 14       | 0.65          |
| (1,74)   | 1:7:A:ILE:HD11  | 1:74:A:ALA:HB2  | 14       | 0.65          |
| (1,7)    | 1:3:A:ASP:HB2   | 1:4:A:MET:HE3   | 9        | 0.65          |
| (1,7)    | 1:3:A:ASP:HB3   | 1:4:A:MET:HE3   | 9        | 0.65          |
| (1,1472) | 1:34:A:THR:HG23 | 1:35:A:SER:HB2  | 11       | 0.64          |
| (1,1472) | 1:34:A:THR:HG23 | 1:35:A:SER:HB3  | 11       | 0.64          |
| (1,1333) | 1:69:A:LEU:HD21 | 1:70:A:MET:H    | 4        | 0.64          |
| (1,961)  | 1:60:A:ILE:H    | 1:60:A:ILE:HD12 | 18       | 0.64          |
| (1,865)  | 1:4:A:MET:HE3   | 1:74:A:ALA:HB2  | 16       | 0.64          |
| (1,865)  | 1:4:A:MET:HE3   | 1:74:A:ALA:HB2  | 20       | 0.64          |
| (1,853)  | 1:69:A:LEU:HB2  | 1:70:A:MET:HE3  | 16       | 0.64          |
| (1,848)  | 1:31:A:LEU:HB2  | 1:76:A:VAL:HG23 | 11       | 0.64          |
| (1,802)  | 1:62:A:PHE:HE2  | 1:70:A:MET:HG2  | 13       | 0.64          |
| (1,700)  | 1:62:A:PHE:HA   | 1:62:A:PHE:HD2  | 3        | 0.64          |
| (1,700)  | 1:62:A:PHE:HA   | 1:62:A:PHE:HD2  | 7        | 0.64          |
| (1,610)  | 1:51:A:ASP:H    | 1:52:A:GLY:HA3  | 2        | 0.64          |
| (1,610)  | 1:51:A:ASP:H    | 1:52:A:GLY:HA3  | 6        | 0.64          |
| (1,610)  | 1:51:A:ASP:H    | 1:52:A:GLY:HA3  | 8        | 0.64          |
| (1,610)  | 1:51:A:ASP:H    | 1:52:A:GLY:HA3  | 15       | 0.64          |
| (1,610)  | 1:51:A:ASP:H    | 1:52:A:GLY:HA3  | 17       | 0.64          |
| (1,319)  | 1:11:A:PHE:HD1  | 1:24:A:LEU:HB2  | 16       | 0.64          |
| (1,268)  | 1:19:A:ILE:HD11 | 1:59:A:PHE:HD2  | 2        | 0.64          |
| (1,266)  | 1:12:A:ASP:H    | 1:19:A:ILE:HD13 | 9        | 0.64          |
| (1,184)  | 1:25:A:THR:HG22 | 1:40:A:GLN:HB2  | 9        | 0.64          |
| (1,184)  | 1:25:A:THR:HG22 | 1:40:A:GLN:HB2  | 10       | 0.64          |
| (1,184)  | 1:25:A:THR:HG22 | 1:40:A:GLN:HB2  | 18       | 0.64          |
| (1,74)   | 1:7:A:ILE:HD11  | 1:74:A:ALA:HB1  | 7        | 0.64          |
| (1,74)   | 1:7:A:ILE:HD11  | 1:74:A:ALA:HB2  | 7        | 0.64          |
| (1,74)   | 1:7:A:ILE:HD11  | 1:74:A:ALA:HB1  | 12       | 0.64          |
| (1,74)   | 1:7:A:ILE:HD11  | 1:74:A:ALA:HB2  | 12       | 0.64          |
| (1,74)   | 1:7:A:ILE:HD11  | 1:74:A:ALA:HB1  | 13       | 0.64          |
| (1,74)   | 1:7:A:ILE:HD11  | 1:74:A:ALA:HB2  | 13       | 0.64          |
| (1,74)   | 1:7:A:ILE:HD11  | 1:74:A:ALA:HB1  | 15       | 0.64          |
| (1,74)   | 1:7:A:ILE:HD11  | 1:74:A:ALA:HB2  | 15       | 0.64          |
| (1,42)   | 1:62:A:PHE:HE2  | 1:67:A:PRO:HG3  | 13       | 0.64          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1472) | 1:34:A:THR:HG23 | 1:35:A:SER:HB2  | 10       | 0.63          |
| (1,1472) | 1:34:A:THR:HG23 | 1:35:A:SER:HB3  | 10       | 0.63          |
| (1,800)  | 1:62:A:PHE:HE2  | 1:70:A:MET:HG3  | 14       | 0.63          |
| (1,759)  | 1:4:A:MET:HE2   | 1:63:A:CYS:HB3  | 14       | 0.63          |
| (1,700)  | 1:62:A:PHE:HA   | 1:62:A:PHE:HD2  | 2        | 0.63          |
| (1,695)  | 1:46:A:ILE:HD11 | 1:58:A:GLU:HB3  | 10       | 0.63          |
| (1,610)  | 1:51:A:ASP:H    | 1:52:A:GLY:HA3  | 1        | 0.63          |
| (1,610)  | 1:51:A:ASP:H    | 1:52:A:GLY:HA3  | 5        | 0.63          |
| (1,610)  | 1:51:A:ASP:H    | 1:52:A:GLY:HA3  | 9        | 0.63          |
| (1,610)  | 1:51:A:ASP:H    | 1:52:A:GLY:HA3  | 16       | 0.63          |
| (1,610)  | 1:51:A:ASP:H    | 1:52:A:GLY:HA3  | 20       | 0.63          |
| (1,472)  | 1:62:A:PHE:HE2  | 1:69:A:LEU:HD21 | 9        | 0.63          |
| (1,324)  | 1:11:A:PHE:HE1  | 1:24:A:LEU:HG   | 13       | 0.63          |
| (1,319)  | 1:11:A:PHE:HD1  | 1:24:A:LEU:HB2  | 7        | 0.63          |
| (1,277)  | 1:44:A:ALA:HA   | 1:50:A:GLY:H    | 12       | 0.63          |
| (1,184)  | 1:25:A:THR:HG22 | 1:40:A:GLN:HB2  | 3        | 0.63          |
| (1,184)  | 1:25:A:THR:HG22 | 1:40:A:GLN:HB2  | 15       | 0.63          |
| (1,163)  | 1:12:A:ASP:HB2  | 1:19:A:ILE:HD13 | 5        | 0.63          |
| (1,1575) | 1:72:A:ASP:HB2  | 1:73:A:VAL:HG22 | 3        | 0.62          |
| (1,1575) | 1:72:A:ASP:HB3  | 1:73:A:VAL:HG22 | 3        | 0.62          |
| (1,1575) | 1:72:A:ASP:HB2  | 1:73:A:VAL:HG22 | 15       | 0.62          |
| (1,1575) | 1:72:A:ASP:HB3  | 1:73:A:VAL:HG22 | 15       | 0.62          |
| (1,1333) | 1:69:A:LEU:HD21 | 1:70:A:MET:H    | 6        | 0.62          |
| (1,1173) | 1:34:A:THR:HG23 | 1:35:A:SER:H    | 12       | 0.62          |
| (1,961)  | 1:60:A:ILE:H    | 1:60:A:ILE:HD12 | 19       | 0.62          |
| (1,803)  | 1:62:A:PHE:HD2  | 1:70:A:MET:HG2  | 9        | 0.62          |
| (1,791)  | 1:67:A:PRO:HB2  | 1:69:A:LEU:HG   | 16       | 0.62          |
| (1,700)  | 1:62:A:PHE:HA   | 1:62:A:PHE:HD2  | 8        | 0.62          |
| (1,610)  | 1:51:A:ASP:H    | 1:52:A:GLY:HA3  | 11       | 0.62          |
| (1,610)  | 1:51:A:ASP:H    | 1:52:A:GLY:HA3  | 12       | 0.62          |
| (1,610)  | 1:51:A:ASP:H    | 1:52:A:GLY:HA3  | 14       | 0.62          |
| (1,504)  | 1:25:A:THR:HG22 | 1:40:A:GLN:HG3  | 5        | 0.62          |
| (1,504)  | 1:25:A:THR:HG22 | 1:40:A:GLN:HG3  | 12       | 0.62          |
| (1,504)  | 1:25:A:THR:HG22 | 1:40:A:GLN:HG3  | 19       | 0.62          |
| (1,384)  | 1:28:A:LEU:H    | 1:28:A:LEU:HD21 | 12       | 0.62          |
| (1,266)  | 1:12:A:ASP:H    | 1:19:A:ILE:HD13 | 20       | 0.62          |
| (1,184)  | 1:25:A:THR:HG22 | 1:40:A:GLN:HB2  | 8        | 0.62          |
| (1,74)   | 1:7:A:ILE:HD11  | 1:74:A:ALA:HB1  | 6        | 0.62          |
| (1,74)   | 1:7:A:ILE:HD11  | 1:74:A:ALA:HB2  | 6        | 0.62          |
| (1,961)  | 1:60:A:ILE:H    | 1:60:A:ILE:HD12 | 13       | 0.61          |
| (1,961)  | 1:60:A:ILE:H    | 1:60:A:ILE:HD12 | 14       | 0.61          |
| (1,961)  | 1:60:A:ILE:H    | 1:60:A:ILE:HD12 | 20       | 0.61          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,803)  | 1:62:A:PHE:HD2  | 1:70:A:MET:HG2  | 2        | 0.61          |
| (1,791)  | 1:67:A:PRO:HB2  | 1:69:A:LEU:HG   | 17       | 0.61          |
| (1,728)  | 1:60:A:ILE:HD12 | 1:61:A:SER:H    | 14       | 0.61          |
| (1,700)  | 1:62:A:PHE:HA   | 1:62:A:PHE:HD2  | 10       | 0.61          |
| (1,695)  | 1:46:A:ILE:HD11 | 1:58:A:GLU:HB3  | 15       | 0.61          |
| (1,417)  | 1:28:A:LEU:HD22 | 1:33:A:SER:HA   | 12       | 0.61          |
| (1,384)  | 1:28:A:LEU:H    | 1:28:A:LEU:HD21 | 2        | 0.61          |
| (1,277)  | 1:44:A:ALA:HA   | 1:50:A:GLY:H    | 11       | 0.61          |
| (1,184)  | 1:25:A:THR:HG22 | 1:40:A:GLN:HB2  | 16       | 0.61          |
| (1,163)  | 1:12:A:ASP:HB2  | 1:19:A:ILE:HD13 | 1        | 0.61          |
| (1,74)   | 1:7:A:ILE:HD11  | 1:74:A:ALA:HB1  | 18       | 0.61          |
| (1,74)   | 1:7:A:ILE:HD11  | 1:74:A:ALA:HB2  | 18       | 0.61          |
| (1,1472) | 1:34:A:THR:HG23 | 1:35:A:SER:HB2  | 2        | 0.6           |
| (1,1472) | 1:34:A:THR:HG23 | 1:35:A:SER:HB3  | 2        | 0.6           |
| (1,1472) | 1:34:A:THR:HG23 | 1:35:A:SER:HB2  | 12       | 0.6           |
| (1,1472) | 1:34:A:THR:HG23 | 1:35:A:SER:HB3  | 12       | 0.6           |
| (1,1333) | 1:69:A:LEU:HD21 | 1:70:A:MET:H    | 17       | 0.6           |
| (1,989)  | 1:46:A:ILE:HD11 | 1:59:A:PHE:H    | 5        | 0.6           |
| (1,961)  | 1:60:A:ILE:H    | 1:60:A:ILE:HD12 | 7        | 0.6           |
| (1,961)  | 1:60:A:ILE:H    | 1:60:A:ILE:HD12 | 9        | 0.6           |
| (1,961)  | 1:60:A:ILE:H    | 1:60:A:ILE:HD12 | 16       | 0.6           |
| (1,853)  | 1:69:A:LEU:HB2  | 1:70:A:MET:HE3  | 12       | 0.6           |
| (1,801)  | 1:62:A:PHE:HD2  | 1:70:A:MET:HG3  | 5        | 0.6           |
| (1,801)  | 1:62:A:PHE:HD2  | 1:70:A:MET:HG3  | 20       | 0.6           |
| (1,800)  | 1:62:A:PHE:HE2  | 1:70:A:MET:HG3  | 9        | 0.6           |
| (1,800)  | 1:62:A:PHE:HE2  | 1:70:A:MET:HG3  | 12       | 0.6           |
| (1,800)  | 1:62:A:PHE:HE2  | 1:70:A:MET:HG3  | 20       | 0.6           |
| (1,791)  | 1:67:A:PRO:HB2  | 1:69:A:LEU:HG   | 6        | 0.6           |
| (1,728)  | 1:60:A:ILE:HD12 | 1:61:A:SER:H    | 15       | 0.6           |
| (1,700)  | 1:62:A:PHE:HA   | 1:62:A:PHE:HD2  | 4        | 0.6           |
| (1,700)  | 1:62:A:PHE:HA   | 1:62:A:PHE:HD2  | 15       | 0.6           |
| (1,504)  | 1:25:A:THR:HG22 | 1:40:A:GLN:HG3  | 11       | 0.6           |
| (1,504)  | 1:25:A:THR:HG22 | 1:40:A:GLN:HG3  | 14       | 0.6           |
| (1,401)  | 1:30:A:THR:HB   | 1:31:A:LEU:HD21 | 9        | 0.6           |
| (1,384)  | 1:28:A:LEU:H    | 1:28:A:LEU:HD21 | 4        | 0.6           |
| (1,319)  | 1:11:A:PHE:HD1  | 1:24:A:LEU:HB2  | 1        | 0.6           |
| (1,319)  | 1:11:A:PHE:HD1  | 1:24:A:LEU:HB2  | 19       | 0.6           |
| (1,961)  | 1:60:A:ILE:H    | 1:60:A:ILE:HD12 | 10       | 0.59          |
| (1,961)  | 1:60:A:ILE:H    | 1:60:A:ILE:HD12 | 12       | 0.59          |
| (1,791)  | 1:67:A:PRO:HB2  | 1:69:A:LEU:HG   | 4        | 0.59          |
| (1,728)  | 1:60:A:ILE:HD12 | 1:61:A:SER:H    | 20       | 0.59          |
| (1,700)  | 1:62:A:PHE:HA   | 1:62:A:PHE:HD2  | 9        | 0.59          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,652)  | 1:46:A:ILE:HB   | 1:54:A:ILE:HD13 | 16       | 0.59          |
| (1,652)  | 1:46:A:ILE:HB   | 1:54:A:ILE:HD13 | 17       | 0.59          |
| (1,504)  | 1:25:A:THR:HG22 | 1:40:A:GLN:HG3  | 2        | 0.59          |
| (1,504)  | 1:25:A:THR:HG22 | 1:40:A:GLN:HG3  | 3        | 0.59          |
| (1,401)  | 1:30:A:THR:HB   | 1:31:A:LEU:HD21 | 15       | 0.59          |
| (1,319)  | 1:11:A:PHE:HD1  | 1:24:A:LEU:HB2  | 2        | 0.59          |
| (1,268)  | 1:19:A:ILE:HD11 | 1:59:A:PHE:HD2  | 4        | 0.59          |
| (1,74)   | 1:7:A:ILE:HD11  | 1:74:A:ALA:HB1  | 5        | 0.59          |
| (1,74)   | 1:7:A:ILE:HD11  | 1:74:A:ALA:HB2  | 5        | 0.59          |
| (1,1575) | 1:72:A:ASP:HB2  | 1:73:A:VAL:HG22 | 14       | 0.58          |
| (1,1575) | 1:72:A:ASP:HB3  | 1:73:A:VAL:HG22 | 14       | 0.58          |
| (1,961)  | 1:60:A:ILE:H    | 1:60:A:ILE:HD12 | 6        | 0.58          |
| (1,961)  | 1:60:A:ILE:H    | 1:60:A:ILE:HD12 | 11       | 0.58          |
| (1,800)  | 1:62:A:PHE:HE2  | 1:70:A:MET:HG3  | 5        | 0.58          |
| (1,759)  | 1:4:A:MET:HE2   | 1:63:A:CYS:HB3  | 20       | 0.58          |
| (1,727)  | 1:5:A:GLU:H     | 1:60:A:ILE:HD13 | 6        | 0.58          |
| (1,700)  | 1:62:A:PHE:HA   | 1:62:A:PHE:HD2  | 11       | 0.58          |
| (1,676)  | 1:8:A:PHE:HE1   | 1:56:A:PHE:HB2  | 4        | 0.58          |
| (1,652)  | 1:46:A:ILE:HB   | 1:54:A:ILE:HD13 | 9        | 0.58          |
| (1,652)  | 1:46:A:ILE:HB   | 1:54:A:ILE:HD13 | 14       | 0.58          |
| (1,504)  | 1:25:A:THR:HG22 | 1:40:A:GLN:HG3  | 4        | 0.58          |
| (1,504)  | 1:25:A:THR:HG22 | 1:40:A:GLN:HG3  | 8        | 0.58          |
| (1,504)  | 1:25:A:THR:HG22 | 1:40:A:GLN:HG3  | 17       | 0.58          |
| (1,384)  | 1:28:A:LEU:H    | 1:28:A:LEU:HD21 | 13       | 0.58          |
| (1,266)  | 1:12:A:ASP:H    | 1:19:A:ILE:HD13 | 13       | 0.58          |
| (1,74)   | 1:7:A:ILE:HD11  | 1:74:A:ALA:HB1  | 1        | 0.58          |
| (1,74)   | 1:7:A:ILE:HD11  | 1:74:A:ALA:HB2  | 1        | 0.58          |
| (1,74)   | 1:7:A:ILE:HD11  | 1:74:A:ALA:HB1  | 20       | 0.58          |
| (1,74)   | 1:7:A:ILE:HD11  | 1:74:A:ALA:HB2  | 20       | 0.58          |
| (1,16)   | 1:42:A:MET:HG2  | 1:62:A:PHE:HE1  | 14       | 0.58          |
| (1,1575) | 1:72:A:ASP:HB2  | 1:73:A:VAL:HG22 | 1        | 0.57          |
| (1,1575) | 1:72:A:ASP:HB3  | 1:73:A:VAL:HG22 | 1        | 0.57          |
| (1,1168) | 1:28:A:LEU:HD21 | 1:33:A:SER:H    | 16       | 0.57          |
| (1,961)  | 1:60:A:ILE:H    | 1:60:A:ILE:HD12 | 1        | 0.57          |
| (1,961)  | 1:60:A:ILE:H    | 1:60:A:ILE:HD12 | 2        | 0.57          |
| (1,961)  | 1:60:A:ILE:H    | 1:60:A:ILE:HD12 | 3        | 0.57          |
| (1,961)  | 1:60:A:ILE:H    | 1:60:A:ILE:HD12 | 4        | 0.57          |
| (1,961)  | 1:60:A:ILE:H    | 1:60:A:ILE:HD12 | 17       | 0.57          |
| (1,801)  | 1:62:A:PHE:HD2  | 1:70:A:MET:HG3  | 11       | 0.57          |
| (1,727)  | 1:5:A:GLU:H     | 1:60:A:ILE:HD13 | 4        | 0.57          |
| (1,700)  | 1:62:A:PHE:HA   | 1:62:A:PHE:HD2  | 5        | 0.57          |
| (1,700)  | 1:62:A:PHE:HA   | 1:62:A:PHE:HD2  | 6        | 0.57          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,695)  | 1:46:A:ILE:HD11 | 1:58:A:GLU:HB3  | 18       | 0.57          |
| (1,652)  | 1:46:A:ILE:HB   | 1:54:A:ILE:HD13 | 19       | 0.57          |
| (1,504)  | 1:25:A:THR:HG22 | 1:40:A:GLN:HG3  | 1        | 0.57          |
| (1,504)  | 1:25:A:THR:HG22 | 1:40:A:GLN:HG3  | 18       | 0.57          |
| (1,319)  | 1:11:A:PHE:HD1  | 1:24:A:LEU:HB2  | 5        | 0.57          |
| (1,277)  | 1:44:A:ALA:HA   | 1:50:A:GLY:H    | 7        | 0.57          |
| (1,268)  | 1:19:A:ILE:HD11 | 1:59:A:PHE:HD2  | 6        | 0.57          |
| (1,74)   | 1:7:A:ILE:HD11  | 1:74:A:ALA:HB1  | 8        | 0.57          |
| (1,74)   | 1:7:A:ILE:HD11  | 1:74:A:ALA:HB2  | 8        | 0.57          |
| (1,70)   | 1:7:A:ILE:HD12  | 1:77:A:PHE:HD2  | 13       | 0.57          |
| (1,1575) | 1:72:A:ASP:HB2  | 1:73:A:VAL:HG22 | 19       | 0.56          |
| (1,1575) | 1:72:A:ASP:HB3  | 1:73:A:VAL:HG22 | 19       | 0.56          |
| (1,1168) | 1:28:A:LEU:HD21 | 1:33:A:SER:H    | 20       | 0.56          |
| (1,961)  | 1:60:A:ILE:H    | 1:60:A:ILE:HD12 | 5        | 0.56          |
| (1,961)  | 1:60:A:ILE:H    | 1:60:A:ILE:HD12 | 8        | 0.56          |
| (1,856)  | 1:70:A:MET:HG3  | 1:70:A:MET:HE3  | 18       | 0.56          |
| (1,728)  | 1:60:A:ILE:HD12 | 1:61:A:SER:H    | 13       | 0.56          |
| (1,700)  | 1:62:A:PHE:HA   | 1:62:A:PHE:HD2  | 16       | 0.56          |
| (1,700)  | 1:62:A:PHE:HA   | 1:62:A:PHE:HD2  | 17       | 0.56          |
| (1,700)  | 1:62:A:PHE:HA   | 1:62:A:PHE:HD2  | 20       | 0.56          |
| (1,504)  | 1:25:A:THR:HG22 | 1:40:A:GLN:HG3  | 6        | 0.56          |
| (1,401)  | 1:30:A:THR:HB   | 1:31:A:LEU:HD21 | 1        | 0.56          |
| (1,384)  | 1:28:A:LEU:H    | 1:28:A:LEU:HD21 | 11       | 0.56          |
| (1,370)  | 1:62:A:PHE:HD2  | 1:69:A:LEU:HB2  | 14       | 0.56          |
| (1,370)  | 1:62:A:PHE:HD2  | 1:69:A:LEU:HB3  | 14       | 0.56          |
| (1,277)  | 1:44:A:ALA:HA   | 1:50:A:GLY:H    | 19       | 0.56          |
| (1,70)   | 1:7:A:ILE:HD12  | 1:77:A:PHE:HD2  | 12       | 0.56          |
| (1,1333) | 1:69:A:LEU:HD21 | 1:70:A:MET:H    | 16       | 0.55          |
| (1,865)  | 1:4:A:MET:HE3   | 1:74:A:ALA:HB2  | 9        | 0.55          |
| (1,802)  | 1:62:A:PHE:HE2  | 1:70:A:MET:HG2  | 14       | 0.55          |
| (1,802)  | 1:62:A:PHE:HE2  | 1:70:A:MET:HG2  | 18       | 0.55          |
| (1,801)  | 1:62:A:PHE:HD2  | 1:70:A:MET:HG3  | 15       | 0.55          |
| (1,800)  | 1:62:A:PHE:HE2  | 1:70:A:MET:HG3  | 11       | 0.55          |
| (1,800)  | 1:62:A:PHE:HE2  | 1:70:A:MET:HG3  | 13       | 0.55          |
| (1,800)  | 1:62:A:PHE:HE2  | 1:70:A:MET:HG3  | 17       | 0.55          |
| (1,791)  | 1:67:A:PRO:HB2  | 1:69:A:LEU:HG   | 5        | 0.55          |
| (1,791)  | 1:67:A:PRO:HB2  | 1:69:A:LEU:HG   | 10       | 0.55          |
| (1,676)  | 1:8:A:PHE:HE1   | 1:56:A:PHE:HB2  | 6        | 0.55          |
| (1,652)  | 1:46:A:ILE:HB   | 1:54:A:ILE:HD13 | 7        | 0.55          |
| (1,401)  | 1:30:A:THR:HB   | 1:31:A:LEU:HD21 | 13       | 0.55          |
| (1,319)  | 1:11:A:PHE:HD1  | 1:24:A:LEU:HB2  | 17       | 0.55          |
| (1,266)  | 1:12:A:ASP:H    | 1:19:A:ILE:HD13 | 3        | 0.55          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,266)  | 1:12:A:ASP:H    | 1:19:A:ILE:HD13 | 5        | 0.55          |
| (1,62)   | 1:7:A:ILE:HB    | 1:7:A:ILE:HD13  | 6        | 0.55          |
| (1,16)   | 1:42:A:MET:HG2  | 1:62:A:PHE:HE1  | 18       | 0.55          |
| (1,1575) | 1:72:A:ASP:HB2  | 1:73:A:VAL:HG22 | 9        | 0.54          |
| (1,1575) | 1:72:A:ASP:HB3  | 1:73:A:VAL:HG22 | 9        | 0.54          |
| (1,1173) | 1:34:A:THR:HG23 | 1:35:A:SER:H    | 14       | 0.54          |
| (1,861)  | 1:4:A:MET:H     | 1:4:A:MET:HE3   | 9        | 0.54          |
| (1,856)  | 1:70:A:MET:HG3  | 1:70:A:MET:HE3  | 1        | 0.54          |
| (1,856)  | 1:70:A:MET:HG3  | 1:70:A:MET:HE3  | 12       | 0.54          |
| (1,856)  | 1:70:A:MET:HG3  | 1:70:A:MET:HE3  | 14       | 0.54          |
| (1,791)  | 1:67:A:PRO:HB2  | 1:69:A:LEU:HG   | 2        | 0.54          |
| (1,791)  | 1:67:A:PRO:HB2  | 1:69:A:LEU:HG   | 9        | 0.54          |
| (1,791)  | 1:67:A:PRO:HB2  | 1:69:A:LEU:HG   | 15       | 0.54          |
| (1,791)  | 1:67:A:PRO:HB2  | 1:69:A:LEU:HG   | 20       | 0.54          |
| (1,700)  | 1:62:A:PHE:HA   | 1:62:A:PHE:HD2  | 1        | 0.54          |
| (1,700)  | 1:62:A:PHE:HA   | 1:62:A:PHE:HD2  | 12       | 0.54          |
| (1,652)  | 1:46:A:ILE:HB   | 1:54:A:ILE:HD13 | 3        | 0.54          |
| (1,504)  | 1:25:A:THR:HG22 | 1:40:A:GLN:HG3  | 10       | 0.54          |
| (1,504)  | 1:25:A:THR:HG22 | 1:40:A:GLN:HG3  | 15       | 0.54          |
| (1,401)  | 1:30:A:THR:HB   | 1:31:A:LEU:HD21 | 17       | 0.54          |
| (1,401)  | 1:30:A:THR:HB   | 1:31:A:LEU:HD21 | 19       | 0.54          |
| (1,387)  | 1:24:A:LEU:HD22 | 1:28:A:LEU:HD23 | 6        | 0.54          |
| (1,313)  | 1:69:A:LEU:HB2  | 1:69:A:LEU:HD21 | 3        | 0.54          |
| (1,62)   | 1:7:A:ILE:HB    | 1:7:A:ILE:HD13  | 1        | 0.54          |
| (1,62)   | 1:7:A:ILE:HB    | 1:7:A:ILE:HD13  | 7        | 0.54          |
| (1,62)   | 1:7:A:ILE:HB    | 1:7:A:ILE:HD13  | 8        | 0.54          |
| (1,62)   | 1:7:A:ILE:HB    | 1:7:A:ILE:HD13  | 18       | 0.54          |
| (1,62)   | 1:7:A:ILE:HB    | 1:7:A:ILE:HD13  | 19       | 0.54          |
| (1,16)   | 1:42:A:MET:HG2  | 1:62:A:PHE:HE1  | 13       | 0.54          |
| (1,989)  | 1:46:A:ILE:HD11 | 1:59:A:PHE:H    | 11       | 0.53          |
| (1,856)  | 1:70:A:MET:HG3  | 1:70:A:MET:HE3  | 2        | 0.53          |
| (1,856)  | 1:70:A:MET:HG3  | 1:70:A:MET:HE3  | 9        | 0.53          |
| (1,802)  | 1:62:A:PHE:HE2  | 1:70:A:MET:HG2  | 20       | 0.53          |
| (1,800)  | 1:62:A:PHE:HE2  | 1:70:A:MET:HG3  | 2        | 0.53          |
| (1,800)  | 1:62:A:PHE:HE2  | 1:70:A:MET:HG3  | 15       | 0.53          |
| (1,791)  | 1:67:A:PRO:HB2  | 1:69:A:LEU:HG   | 19       | 0.53          |
| (1,728)  | 1:60:A:ILE:HD12 | 1:61:A:SER:H    | 16       | 0.53          |
| (1,727)  | 1:5:A:GLU:H     | 1:60:A:ILE:HD13 | 19       | 0.53          |
| (1,695)  | 1:46:A:ILE:HD11 | 1:58:A:GLU:HB3  | 7        | 0.53          |
| (1,652)  | 1:46:A:ILE:HB   | 1:54:A:ILE:HD13 | 6        | 0.53          |
| (1,652)  | 1:46:A:ILE:HB   | 1:54:A:ILE:HD13 | 18       | 0.53          |
| (1,417)  | 1:28:A:LEU:HD22 | 1:33:A:SER:HA   | 13       | 0.53          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,401)  | 1:30:A:THR:HB   | 1:31:A:LEU:HD21 | 4        | 0.53          |
| (1,401)  | 1:30:A:THR:HB   | 1:31:A:LEU:HD21 | 11       | 0.53          |
| (1,370)  | 1:62:A:PHE:HD2  | 1:69:A:LEU:HB2  | 18       | 0.53          |
| (1,370)  | 1:62:A:PHE:HD2  | 1:69:A:LEU:HB3  | 18       | 0.53          |
| (1,277)  | 1:44:A:ALA:HA   | 1:50:A:GLY:H    | 2        | 0.53          |
| (1,277)  | 1:44:A:ALA:HA   | 1:50:A:GLY:H    | 3        | 0.53          |
| (1,277)  | 1:44:A:ALA:HA   | 1:50:A:GLY:H    | 8        | 0.53          |
| (1,277)  | 1:44:A:ALA:HA   | 1:50:A:GLY:H    | 10       | 0.53          |
| (1,235)  | 1:53:A:PHE:HB3  | 1:53:A:PHE:HD2  | 13       | 0.53          |
| (1,235)  | 1:53:A:PHE:HB2  | 1:53:A:PHE:HD1  | 13       | 0.53          |
| (1,62)   | 1:7:A:ILE:HB    | 1:7:A:ILE:HD13  | 3        | 0.53          |
| (1,989)  | 1:46:A:ILE:HD11 | 1:59:A:PHE:H    | 18       | 0.52          |
| (1,865)  | 1:4:A:MET:HE3   | 1:74:A:ALA:HB2  | 14       | 0.52          |
| (1,856)  | 1:70:A:MET:HG3  | 1:70:A:MET:HE3  | 3        | 0.52          |
| (1,856)  | 1:70:A:MET:HG3  | 1:70:A:MET:HE3  | 16       | 0.52          |
| (1,801)  | 1:62:A:PHE:HD2  | 1:70:A:MET:HG3  | 18       | 0.52          |
| (1,791)  | 1:67:A:PRO:HB2  | 1:69:A:LEU:HG   | 11       | 0.52          |
| (1,728)  | 1:60:A:ILE:HD12 | 1:61:A:SER:H    | 9        | 0.52          |
| (1,313)  | 1:69:A:LEU:HB2  | 1:69:A:LEU:HD21 | 19       | 0.52          |
| (1,277)  | 1:44:A:ALA:HA   | 1:50:A:GLY:H    | 13       | 0.52          |
| (1,277)  | 1:44:A:ALA:HA   | 1:50:A:GLY:H    | 20       | 0.52          |
| (1,235)  | 1:53:A:PHE:HB3  | 1:53:A:PHE:HD2  | 12       | 0.52          |
| (1,235)  | 1:53:A:PHE:HB2  | 1:53:A:PHE:HD1  | 12       | 0.52          |
| (1,70)   | 1:7:A:ILE:HD12  | 1:77:A:PHE:HD2  | 1        | 0.52          |
| (1,62)   | 1:7:A:ILE:HB    | 1:7:A:ILE:HD13  | 2        | 0.52          |
| (1,62)   | 1:7:A:ILE:HB    | 1:7:A:ILE:HD13  | 4        | 0.52          |
| (1,62)   | 1:7:A:ILE:HB    | 1:7:A:ILE:HD13  | 5        | 0.52          |
| (1,62)   | 1:7:A:ILE:HB    | 1:7:A:ILE:HD13  | 9        | 0.52          |
| (1,62)   | 1:7:A:ILE:HB    | 1:7:A:ILE:HD13  | 11       | 0.52          |
| (1,62)   | 1:7:A:ILE:HB    | 1:7:A:ILE:HD13  | 12       | 0.52          |
| (1,62)   | 1:7:A:ILE:HB    | 1:7:A:ILE:HD13  | 15       | 0.52          |
| (1,1575) | 1:72:A:ASP:HB2  | 1:73:A:VAL:HG22 | 18       | 0.51          |
| (1,1575) | 1:72:A:ASP:HB3  | 1:73:A:VAL:HG22 | 18       | 0.51          |
| (1,1472) | 1:34:A:THR:HG23 | 1:35:A:SER:HB2  | 14       | 0.51          |
| (1,1472) | 1:34:A:THR:HG23 | 1:35:A:SER:HB3  | 14       | 0.51          |
| (1,1168) | 1:28:A:LEU:HD21 | 1:33:A:SER:H    | 5        | 0.51          |
| (1,898)  | 1:25:A:THR:HG23 | 1:27:A:ALA:H    | 20       | 0.51          |
| (1,856)  | 1:70:A:MET:HG3  | 1:70:A:MET:HE3  | 8        | 0.51          |
| (1,856)  | 1:70:A:MET:HG3  | 1:70:A:MET:HE3  | 13       | 0.51          |
| (1,856)  | 1:70:A:MET:HG3  | 1:70:A:MET:HE3  | 17       | 0.51          |
| (1,853)  | 1:69:A:LEU:HB2  | 1:70:A:MET:HE3  | 13       | 0.51          |
| (1,802)  | 1:62:A:PHE:HE2  | 1:70:A:MET:HG2  | 12       | 0.51          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,801)  | 1:62:A:PHE:HD2  | 1:70:A:MET:HG3  | 10       | 0.51          |
| (1,791)  | 1:67:A:PRO:HB2  | 1:69:A:LEU:HG   | 3        | 0.51          |
| (1,791)  | 1:67:A:PRO:HB2  | 1:69:A:LEU:HG   | 7        | 0.51          |
| (1,652)  | 1:46:A:ILE:HB   | 1:54:A:ILE:HD13 | 8        | 0.51          |
| (1,411)  | 1:30:A:THR:HG22 | 1:31:A:LEU:HG   | 5        | 0.51          |
| (1,401)  | 1:30:A:THR:HB   | 1:31:A:LEU:HD21 | 10       | 0.51          |
| (1,387)  | 1:24:A:LEU:HD22 | 1:28:A:LEU:HD23 | 10       | 0.51          |
| (1,384)  | 1:28:A:LEU:H    | 1:28:A:LEU:HD21 | 16       | 0.51          |
| (1,319)  | 1:11:A:PHE:HD1  | 1:24:A:LEU:HB2  | 8        | 0.51          |
| (1,313)  | 1:69:A:LEU:HB2  | 1:69:A:LEU:HD21 | 7        | 0.51          |
| (1,313)  | 1:69:A:LEU:HB2  | 1:69:A:LEU:HD21 | 8        | 0.51          |
| (1,313)  | 1:69:A:LEU:HB2  | 1:69:A:LEU:HD21 | 11       | 0.51          |
| (1,277)  | 1:44:A:ALA:HA   | 1:50:A:GLY:H    | 4        | 0.51          |
| (1,277)  | 1:44:A:ALA:HA   | 1:50:A:GLY:H    | 15       | 0.51          |
| (1,277)  | 1:44:A:ALA:HA   | 1:50:A:GLY:H    | 18       | 0.51          |
| (1,268)  | 1:19:A:ILE:HD11 | 1:59:A:PHE:HD2  | 18       | 0.51          |
| (1,266)  | 1:12:A:ASP:H    | 1:19:A:ILE:HD13 | 16       | 0.51          |
| (1,62)   | 1:7:A:ILE:HB    | 1:7:A:ILE:HD13  | 13       | 0.51          |
| (1,62)   | 1:7:A:ILE:HB    | 1:7:A:ILE:HD13  | 16       | 0.51          |
| (1,62)   | 1:7:A:ILE:HB    | 1:7:A:ILE:HD13  | 20       | 0.51          |
| (1,1432) | 1:20:A:SER:HB2  | 1:53:A:PHE:HD2  | 14       | 0.5           |
| (1,1432) | 1:20:A:SER:HB3  | 1:53:A:PHE:HD2  | 14       | 0.5           |
| (1,1395) | 1:7:A:ILE:HG12  | 1:77:A:PHE:HD2  | 20       | 0.5           |
| (1,1395) | 1:7:A:ILE:HG13  | 1:77:A:PHE:HD2  | 20       | 0.5           |
| (1,1333) | 1:69:A:LEU:HD21 | 1:70:A:MET:H    | 12       | 0.5           |
| (1,1168) | 1:28:A:LEU:HD21 | 1:33:A:SER:H    | 14       | 0.5           |
| (1,989)  | 1:46:A:ILE:HD11 | 1:59:A:PHE:H    | 13       | 0.5           |
| (1,898)  | 1:25:A:THR:HG23 | 1:27:A:ALA:H    | 19       | 0.5           |
| (1,861)  | 1:4:A:MET:H     | 1:4:A:MET:HE3   | 14       | 0.5           |
| (1,856)  | 1:70:A:MET:HG3  | 1:70:A:MET:HE3  | 4        | 0.5           |
| (1,801)  | 1:62:A:PHE:HD2  | 1:70:A:MET:HG3  | 9        | 0.5           |
| (1,800)  | 1:62:A:PHE:HE2  | 1:70:A:MET:HG3  | 4        | 0.5           |
| (1,791)  | 1:67:A:PRO:HB2  | 1:69:A:LEU:HG   | 8        | 0.5           |
| (1,728)  | 1:60:A:ILE:HD12 | 1:61:A:SER:H    | 12       | 0.5           |
| (1,695)  | 1:46:A:ILE:HD11 | 1:58:A:GLU:HB3  | 5        | 0.5           |
| (1,504)  | 1:25:A:THR:HG22 | 1:40:A:GLN:HG3  | 9        | 0.5           |
| (1,472)  | 1:62:A:PHE:HE2  | 1:69:A:LEU:HD21 | 4        | 0.5           |
| (1,401)  | 1:30:A:THR:HB   | 1:31:A:LEU:HD21 | 6        | 0.5           |
| (1,401)  | 1:30:A:THR:HB   | 1:31:A:LEU:HD21 | 18       | 0.5           |
| (1,384)  | 1:28:A:LEU:H    | 1:28:A:LEU:HD21 | 8        | 0.5           |
| (1,384)  | 1:28:A:LEU:H    | 1:28:A:LEU:HD21 | 17       | 0.5           |
| (1,370)  | 1:62:A:PHE:HD2  | 1:69:A:LEU:HB2  | 13       | 0.5           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,370)  | 1:62:A:PHE:HD2  | 1:69:A:LEU:HB3  | 13       | 0.5           |
| (1,313)  | 1:69:A:LEU:HB2  | 1:69:A:LEU:HD21 | 2        | 0.5           |
| (1,313)  | 1:69:A:LEU:HB2  | 1:69:A:LEU:HD21 | 10       | 0.5           |
| (1,313)  | 1:69:A:LEU:HB2  | 1:69:A:LEU:HD21 | 15       | 0.5           |
| (1,277)  | 1:44:A:ALA:HA   | 1:50:A:GLY:H    | 6        | 0.5           |
| (1,62)   | 1:7:A:ILE:HB    | 1:7:A:ILE:HD13  | 14       | 0.5           |
| (1,62)   | 1:7:A:ILE:HB    | 1:7:A:ILE:HD13  | 17       | 0.5           |
| (1,1168) | 1:28:A:LEU:HD21 | 1:33:A:SER:H    | 3        | 0.49          |
| (1,898)  | 1:25:A:THR:HG23 | 1:27:A:ALA:H    | 6        | 0.49          |
| (1,898)  | 1:25:A:THR:HG23 | 1:27:A:ALA:H    | 7        | 0.49          |
| (1,898)  | 1:25:A:THR:HG23 | 1:27:A:ALA:H    | 15       | 0.49          |
| (1,898)  | 1:25:A:THR:HG23 | 1:27:A:ALA:H    | 17       | 0.49          |
| (1,853)  | 1:69:A:LEU:HB2  | 1:70:A:MET:HE3  | 4        | 0.49          |
| (1,802)  | 1:62:A:PHE:HE2  | 1:70:A:MET:HG2  | 5        | 0.49          |
| (1,801)  | 1:62:A:PHE:HD2  | 1:70:A:MET:HG3  | 14       | 0.49          |
| (1,727)  | 1:5:A:GLU:H     | 1:60:A:ILE:HD13 | 3        | 0.49          |
| (1,504)  | 1:25:A:THR:HG22 | 1:40:A:GLN:HG3  | 16       | 0.49          |
| (1,401)  | 1:30:A:THR:HB   | 1:31:A:LEU:HD21 | 8        | 0.49          |
| (1,387)  | 1:24:A:LEU:HD22 | 1:28:A:LEU:HD23 | 3        | 0.49          |
| (1,319)  | 1:11:A:PHE:HD1  | 1:24:A:LEU:HB2  | 11       | 0.49          |
| (1,313)  | 1:69:A:LEU:HB2  | 1:69:A:LEU:HD21 | 9        | 0.49          |
| (1,313)  | 1:69:A:LEU:HB2  | 1:69:A:LEU:HD21 | 20       | 0.49          |
| (1,266)  | 1:12:A:ASP:H    | 1:19:A:ILE:HD13 | 1        | 0.49          |
| (1,62)   | 1:7:A:ILE:HB    | 1:7:A:ILE:HD13  | 10       | 0.49          |
| (1,1395) | 1:7:A:ILE:HG12  | 1:77:A:PHE:HD2  | 4        | 0.48          |
| (1,1395) | 1:7:A:ILE:HG13  | 1:77:A:PHE:HD2  | 4        | 0.48          |
| (1,1333) | 1:69:A:LEU:HD21 | 1:70:A:MET:H    | 13       | 0.48          |
| (1,898)  | 1:25:A:THR:HG23 | 1:27:A:ALA:H    | 1        | 0.48          |
| (1,898)  | 1:25:A:THR:HG23 | 1:27:A:ALA:H    | 2        | 0.48          |
| (1,898)  | 1:25:A:THR:HG23 | 1:27:A:ALA:H    | 4        | 0.48          |
| (1,898)  | 1:25:A:THR:HG23 | 1:27:A:ALA:H    | 10       | 0.48          |
| (1,898)  | 1:25:A:THR:HG23 | 1:27:A:ALA:H    | 14       | 0.48          |
| (1,898)  | 1:25:A:THR:HG23 | 1:27:A:ALA:H    | 18       | 0.48          |
| (1,856)  | 1:70:A:MET:HG3  | 1:70:A:MET:HE3  | 7        | 0.48          |
| (1,856)  | 1:70:A:MET:HG3  | 1:70:A:MET:HE3  | 15       | 0.48          |
| (1,856)  | 1:70:A:MET:HG3  | 1:70:A:MET:HE3  | 20       | 0.48          |
| (1,853)  | 1:69:A:LEU:HB2  | 1:70:A:MET:HE3  | 17       | 0.48          |
| (1,800)  | 1:62:A:PHE:HE2  | 1:70:A:MET:HG3  | 10       | 0.48          |
| (1,727)  | 1:5:A:GLU:H     | 1:60:A:ILE:HD13 | 7        | 0.48          |
| (1,700)  | 1:62:A:PHE:HA   | 1:62:A:PHE:HD2  | 18       | 0.48          |
| (1,401)  | 1:30:A:THR:HB   | 1:31:A:LEU:HD21 | 7        | 0.48          |
| (1,401)  | 1:30:A:THR:HB   | 1:31:A:LEU:HD21 | 12       | 0.48          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,384)  | 1:28:A:LEU:H    | 1:28:A:LEU:HD21 | 5        | 0.48          |
| (1,319)  | 1:11:A:PHE:HD1  | 1:24:A:LEU:HB2  | 20       | 0.48          |
| (1,313)  | 1:69:A:LEU:HB2  | 1:69:A:LEU:HD21 | 5        | 0.48          |
| (1,277)  | 1:44:A:ALA:HA   | 1:50:A:GLY:H    | 5        | 0.48          |
| (1,277)  | 1:44:A:ALA:HA   | 1:50:A:GLY:H    | 9        | 0.48          |
| (1,277)  | 1:44:A:ALA:HA   | 1:50:A:GLY:H    | 16       | 0.48          |
| (1,70)   | 1:7:A:ILE:HD12  | 1:77:A:PHE:HD2  | 7        | 0.48          |
| (1,1333) | 1:69:A:LEU:HD21 | 1:70:A:MET:H    | 1        | 0.47          |
| (1,989)  | 1:46:A:ILE:HD11 | 1:59:A:PHE:H    | 10       | 0.47          |
| (1,898)  | 1:25:A:THR:HG23 | 1:27:A:ALA:H    | 3        | 0.47          |
| (1,898)  | 1:25:A:THR:HG23 | 1:27:A:ALA:H    | 8        | 0.47          |
| (1,856)  | 1:70:A:MET:HG3  | 1:70:A:MET:HE3  | 5        | 0.47          |
| (1,850)  | 1:31:A:LEU:HB3  | 1:76:A:VAL:HG23 | 1        | 0.47          |
| (1,802)  | 1:62:A:PHE:HE2  | 1:70:A:MET:HG2  | 1        | 0.47          |
| (1,801)  | 1:62:A:PHE:HD2  | 1:70:A:MET:HG3  | 13       | 0.47          |
| (1,800)  | 1:62:A:PHE:HE2  | 1:70:A:MET:HG3  | 1        | 0.47          |
| (1,728)  | 1:60:A:ILE:HD12 | 1:61:A:SER:H    | 17       | 0.47          |
| (1,652)  | 1:46:A:ILE:HB   | 1:54:A:ILE:HD13 | 13       | 0.47          |
| (1,384)  | 1:28:A:LEU:H    | 1:28:A:LEU:HD21 | 10       | 0.47          |
| (1,319)  | 1:11:A:PHE:HD1  | 1:24:A:LEU:HB2  | 13       | 0.47          |
| (1,319)  | 1:11:A:PHE:HD1  | 1:24:A:LEU:HB2  | 15       | 0.47          |
| (1,277)  | 1:44:A:ALA:HA   | 1:50:A:GLY:H    | 1        | 0.47          |
| (1,1432) | 1:20:A:SER:HB2  | 1:53:A:PHE:HD2  | 1        | 0.46          |
| (1,1432) | 1:20:A:SER:HB3  | 1:53:A:PHE:HD2  | 1        | 0.46          |
| (1,1395) | 1:7:A:ILE:HG12  | 1:77:A:PHE:HD2  | 14       | 0.46          |
| (1,1395) | 1:7:A:ILE:HG13  | 1:77:A:PHE:HD2  | 14       | 0.46          |
| (1,1173) | 1:34:A:THR:HG23 | 1:35:A:SER:H    | 6        | 0.46          |
| (1,898)  | 1:25:A:THR:HG23 | 1:27:A:ALA:H    | 9        | 0.46          |
| (1,898)  | 1:25:A:THR:HG23 | 1:27:A:ALA:H    | 11       | 0.46          |
| (1,898)  | 1:25:A:THR:HG23 | 1:27:A:ALA:H    | 13       | 0.46          |
| (1,898)  | 1:25:A:THR:HG23 | 1:27:A:ALA:H    | 16       | 0.46          |
| (1,856)  | 1:70:A:MET:HG3  | 1:70:A:MET:HE3  | 6        | 0.46          |
| (1,856)  | 1:70:A:MET:HG3  | 1:70:A:MET:HE3  | 10       | 0.46          |
| (1,856)  | 1:70:A:MET:HG3  | 1:70:A:MET:HE3  | 11       | 0.46          |
| (1,856)  | 1:70:A:MET:HG3  | 1:70:A:MET:HE3  | 19       | 0.46          |
| (1,850)  | 1:31:A:LEU:HB3  | 1:76:A:VAL:HG23 | 3        | 0.46          |
| (1,848)  | 1:31:A:LEU:HB2  | 1:76:A:VAL:HG23 | 2        | 0.46          |
| (1,802)  | 1:62:A:PHE:HE2  | 1:70:A:MET:HG2  | 17       | 0.46          |
| (1,801)  | 1:62:A:PHE:HD2  | 1:70:A:MET:HG3  | 7        | 0.46          |
| (1,800)  | 1:62:A:PHE:HE2  | 1:70:A:MET:HG3  | 7        | 0.46          |
| (1,700)  | 1:62:A:PHE:HA   | 1:62:A:PHE:HD2  | 13       | 0.46          |
| (1,700)  | 1:62:A:PHE:HA   | 1:62:A:PHE:HD2  | 14       | 0.46          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,652)  | 1:46:A:ILE:HB   | 1:54:A:ILE:HD13 | 1        | 0.46          |
| (1,652)  | 1:46:A:ILE:HB   | 1:54:A:ILE:HD13 | 4        | 0.46          |
| (1,401)  | 1:30:A:THR:HB   | 1:31:A:LEU:HD21 | 2        | 0.46          |
| (1,387)  | 1:24:A:LEU:HD22 | 1:28:A:LEU:HD23 | 5        | 0.46          |
| (1,387)  | 1:24:A:LEU:HD22 | 1:28:A:LEU:HD23 | 7        | 0.46          |
| (1,387)  | 1:24:A:LEU:HD22 | 1:28:A:LEU:HD23 | 17       | 0.46          |
| (1,384)  | 1:28:A:LEU:H    | 1:28:A:LEU:HD21 | 1        | 0.46          |
| (1,370)  | 1:62:A:PHE:HD2  | 1:69:A:LEU:HB2  | 1        | 0.46          |
| (1,370)  | 1:62:A:PHE:HD2  | 1:69:A:LEU:HB3  | 1        | 0.46          |
| (1,370)  | 1:62:A:PHE:HD2  | 1:69:A:LEU:HB2  | 5        | 0.46          |
| (1,370)  | 1:62:A:PHE:HD2  | 1:69:A:LEU:HB3  | 5        | 0.46          |
| (1,370)  | 1:62:A:PHE:HD2  | 1:69:A:LEU:HB2  | 20       | 0.46          |
| (1,370)  | 1:62:A:PHE:HD2  | 1:69:A:LEU:HB3  | 20       | 0.46          |
| (1,277)  | 1:44:A:ALA:HA   | 1:50:A:GLY:H    | 14       | 0.46          |
| (1,277)  | 1:44:A:ALA:HA   | 1:50:A:GLY:H    | 17       | 0.46          |
| (1,235)  | 1:53:A:PHE:HB3  | 1:53:A:PHE:HD2  | 3        | 0.46          |
| (1,235)  | 1:53:A:PHE:HB2  | 1:53:A:PHE:HD1  | 3        | 0.46          |
| (1,1333) | 1:69:A:LEU:HD21 | 1:70:A:MET:H    | 14       | 0.45          |
| (1,1253) | 1:53:A:PHE:H    | 1:53:A:PHE:HD1  | 12       | 0.45          |
| (1,898)  | 1:25:A:THR:HG23 | 1:27:A:ALA:H    | 12       | 0.45          |
| (1,861)  | 1:4:A:MET:H     | 1:4:A:MET:HE3   | 17       | 0.45          |
| (1,861)  | 1:4:A:MET:H     | 1:4:A:MET:HE3   | 20       | 0.45          |
| (1,850)  | 1:31:A:LEU:HB3  | 1:76:A:VAL:HG23 | 17       | 0.45          |
| (1,802)  | 1:62:A:PHE:HE2  | 1:70:A:MET:HG2  | 11       | 0.45          |
| (1,801)  | 1:62:A:PHE:HD2  | 1:70:A:MET:HG3  | 2        | 0.45          |
| (1,728)  | 1:60:A:ILE:HD12 | 1:61:A:SER:H    | 18       | 0.45          |
| (1,695)  | 1:46:A:ILE:HD11 | 1:58:A:GLU:HB3  | 19       | 0.45          |
| (1,652)  | 1:46:A:ILE:HB   | 1:54:A:ILE:HD13 | 5        | 0.45          |
| (1,387)  | 1:24:A:LEU:HD22 | 1:28:A:LEU:HD23 | 13       | 0.45          |
| (1,384)  | 1:28:A:LEU:H    | 1:28:A:LEU:HD21 | 6        | 0.45          |
| (1,384)  | 1:28:A:LEU:H    | 1:28:A:LEU:HD21 | 9        | 0.45          |
| (1,319)  | 1:11:A:PHE:HD1  | 1:24:A:LEU:HB2  | 12       | 0.45          |
| (1,199)  | 1:8:A:PHE:HE1   | 1:18:A:LYS:HA   | 6        | 0.45          |
| (1,70)   | 1:7:A:ILE:HD12  | 1:77:A:PHE:HD2  | 5        | 0.45          |
| (1,1472) | 1:34:A:THR:HG23 | 1:35:A:SER:HB2  | 3        | 0.44          |
| (1,1472) | 1:34:A:THR:HG23 | 1:35:A:SER:HB3  | 3        | 0.44          |
| (1,1173) | 1:34:A:THR:HG23 | 1:35:A:SER:H    | 7        | 0.44          |
| (1,989)  | 1:46:A:ILE:HD11 | 1:59:A:PHE:H    | 20       | 0.44          |
| (1,898)  | 1:25:A:THR:HG23 | 1:27:A:ALA:H    | 5        | 0.44          |
| (1,865)  | 1:4:A:MET:HE3   | 1:74:A:ALA:HB2  | 17       | 0.44          |
| (1,800)  | 1:62:A:PHE:HE2  | 1:70:A:MET:HG3  | 3        | 0.44          |
| (1,728)  | 1:60:A:ILE:HD12 | 1:61:A:SER:H    | 11       | 0.44          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,695)  | 1:46:A:ILE:HD11 | 1:58:A:GLU:HB3  | 11       | 0.44          |
| (1,695)  | 1:46:A:ILE:HD11 | 1:58:A:GLU:HB3  | 13       | 0.44          |
| (1,411)  | 1:30:A:THR:HG22 | 1:31:A:LEU:HG   | 9        | 0.44          |
| (1,387)  | 1:24:A:LEU:HD22 | 1:28:A:LEU:HD23 | 4        | 0.44          |
| (1,384)  | 1:28:A:LEU:H    | 1:28:A:LEU:HD21 | 3        | 0.44          |
| (1,384)  | 1:28:A:LEU:H    | 1:28:A:LEU:HD21 | 7        | 0.44          |
| (1,384)  | 1:28:A:LEU:H    | 1:28:A:LEU:HD21 | 18       | 0.44          |
| (1,382)  | 1:24:A:LEU:HG   | 1:28:A:LEU:HG   | 2        | 0.44          |
| (1,365)  | 1:28:A:LEU:HA   | 1:28:A:LEU:HD21 | 4        | 0.44          |
| (1,365)  | 1:28:A:LEU:HA   | 1:28:A:LEU:HD21 | 12       | 0.44          |
| (1,313)  | 1:69:A:LEU:HB2  | 1:69:A:LEU:HD21 | 4        | 0.44          |
| (1,235)  | 1:53:A:PHE:HB3  | 1:53:A:PHE:HD2  | 7        | 0.44          |
| (1,235)  | 1:53:A:PHE:HB2  | 1:53:A:PHE:HD1  | 7        | 0.44          |
| (1,235)  | 1:53:A:PHE:HB3  | 1:53:A:PHE:HD2  | 10       | 0.44          |
| (1,235)  | 1:53:A:PHE:HB2  | 1:53:A:PHE:HD1  | 10       | 0.44          |
| (1,235)  | 1:53:A:PHE:HB3  | 1:53:A:PHE:HD2  | 11       | 0.44          |
| (1,235)  | 1:53:A:PHE:HB2  | 1:53:A:PHE:HD1  | 11       | 0.44          |
| (1,1395) | 1:7:A:ILE:HG12  | 1:77:A:PHE:HD2  | 17       | 0.43          |
| (1,1395) | 1:7:A:ILE:HG13  | 1:77:A:PHE:HD2  | 17       | 0.43          |
| (1,1333) | 1:69:A:LEU:HD21 | 1:70:A:MET:H    | 18       | 0.43          |
| (1,1293) | 1:60:A:ILE:HG21 | 1:63:A:CYS:H    | 3        | 0.43          |
| (1,1293) | 1:60:A:ILE:HG21 | 1:63:A:CYS:H    | 8        | 0.43          |
| (1,1293) | 1:60:A:ILE:HG21 | 1:63:A:CYS:H    | 11       | 0.43          |
| (1,853)  | 1:69:A:LEU:HB2  | 1:70:A:MET:HE3  | 1        | 0.43          |
| (1,853)  | 1:69:A:LEU:HB2  | 1:70:A:MET:HE3  | 18       | 0.43          |
| (1,802)  | 1:62:A:PHE:HE2  | 1:70:A:MET:HG2  | 6        | 0.43          |
| (1,801)  | 1:62:A:PHE:HD2  | 1:70:A:MET:HG3  | 3        | 0.43          |
| (1,800)  | 1:62:A:PHE:HE2  | 1:70:A:MET:HG3  | 6        | 0.43          |
| (1,800)  | 1:62:A:PHE:HE2  | 1:70:A:MET:HG3  | 16       | 0.43          |
| (1,695)  | 1:46:A:ILE:HD11 | 1:58:A:GLU:HB3  | 3        | 0.43          |
| (1,384)  | 1:28:A:LEU:H    | 1:28:A:LEU:HD21 | 15       | 0.43          |
| (1,384)  | 1:28:A:LEU:H    | 1:28:A:LEU:HD21 | 19       | 0.43          |
| (1,382)  | 1:24:A:LEU:HG   | 1:28:A:LEU:HG   | 8        | 0.43          |
| (1,370)  | 1:62:A:PHE:HD2  | 1:69:A:LEU:HB2  | 10       | 0.43          |
| (1,370)  | 1:62:A:PHE:HD2  | 1:69:A:LEU:HB3  | 10       | 0.43          |
| (1,235)  | 1:53:A:PHE:HB3  | 1:53:A:PHE:HD2  | 15       | 0.43          |
| (1,235)  | 1:53:A:PHE:HB2  | 1:53:A:PHE:HD1  | 15       | 0.43          |
| (1,235)  | 1:53:A:PHE:HB3  | 1:53:A:PHE:HD2  | 18       | 0.43          |
| (1,235)  | 1:53:A:PHE:HB2  | 1:53:A:PHE:HD1  | 18       | 0.43          |
| (1,235)  | 1:53:A:PHE:HB3  | 1:53:A:PHE:HD2  | 19       | 0.43          |
| (1,235)  | 1:53:A:PHE:HB2  | 1:53:A:PHE:HD1  | 19       | 0.43          |
| (1,1293) | 1:60:A:ILE:HG21 | 1:63:A:CYS:H    | 2        | 0.42          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1293) | 1:60:A:ILE:HG21 | 1:63:A:CYS:H    | 19       | 0.42          |
| (1,1253) | 1:53:A:PHE:H    | 1:53:A:PHE:HD1  | 11       | 0.42          |
| (1,1190) | 1:25:A:THR:HG22 | 1:40:A:GLN:H    | 20       | 0.42          |
| (1,989)  | 1:46:A:ILE:HD11 | 1:59:A:PHE:H    | 7        | 0.42          |
| (1,989)  | 1:46:A:ILE:HD11 | 1:59:A:PHE:H    | 15       | 0.42          |
| (1,802)  | 1:62:A:PHE:HE2  | 1:70:A:MET:HG2  | 4        | 0.42          |
| (1,802)  | 1:62:A:PHE:HE2  | 1:70:A:MET:HG2  | 15       | 0.42          |
| (1,802)  | 1:62:A:PHE:HE2  | 1:70:A:MET:HG2  | 16       | 0.42          |
| (1,801)  | 1:62:A:PHE:HD2  | 1:70:A:MET:HG3  | 17       | 0.42          |
| (1,384)  | 1:28:A:LEU:H    | 1:28:A:LEU:HD21 | 20       | 0.42          |
| (1,382)  | 1:24:A:LEU:HG   | 1:28:A:LEU:HG   | 4        | 0.42          |
| (1,382)  | 1:24:A:LEU:HG   | 1:28:A:LEU:HG   | 6        | 0.42          |
| (1,382)  | 1:24:A:LEU:HG   | 1:28:A:LEU:HG   | 7        | 0.42          |
| (1,382)  | 1:24:A:LEU:HG   | 1:28:A:LEU:HG   | 9        | 0.42          |
| (1,382)  | 1:24:A:LEU:HG   | 1:28:A:LEU:HG   | 10       | 0.42          |
| (1,365)  | 1:28:A:LEU:HA   | 1:28:A:LEU:HD21 | 2        | 0.42          |
| (1,1533) | 1:52:A:GLY:HA2  | 1:53:A:PHE:HE1  | 13       | 0.41          |
| (1,1533) | 1:52:A:GLY:HA3  | 1:53:A:PHE:HE1  | 13       | 0.41          |
| (1,1293) | 1:60:A:ILE:HG21 | 1:63:A:CYS:H    | 6        | 0.41          |
| (1,1293) | 1:60:A:ILE:HG21 | 1:63:A:CYS:H    | 7        | 0.41          |
| (1,1253) | 1:53:A:PHE:H    | 1:53:A:PHE:HD1  | 7        | 0.41          |
| (1,1253) | 1:53:A:PHE:H    | 1:53:A:PHE:HD1  | 10       | 0.41          |
| (1,989)  | 1:46:A:ILE:HD11 | 1:59:A:PHE:H    | 12       | 0.41          |
| (1,989)  | 1:46:A:ILE:HD11 | 1:59:A:PHE:H    | 19       | 0.41          |
| (1,848)  | 1:31:A:LEU:HB2  | 1:76:A:VAL:HG23 | 15       | 0.41          |
| (1,848)  | 1:31:A:LEU:HB2  | 1:76:A:VAL:HG23 | 18       | 0.41          |
| (1,846)  | 1:72:A:ASP:HA   | 1:76:A:VAL:HG21 | 12       | 0.41          |
| (1,802)  | 1:62:A:PHE:HE2  | 1:70:A:MET:HG2  | 9        | 0.41          |
| (1,728)  | 1:60:A:ILE:HD12 | 1:61:A:SER:H    | 5        | 0.41          |
| (1,652)  | 1:46:A:ILE:HB   | 1:54:A:ILE:HD13 | 2        | 0.41          |
| (1,652)  | 1:46:A:ILE:HB   | 1:54:A:ILE:HD13 | 12       | 0.41          |
| (1,433)  | 1:34:A:THR:HA   | 1:34:A:THR:HG23 | 3        | 0.41          |
| (1,412)  | 1:30:A:THR:HG22 | 1:31:A:LEU:HD22 | 5        | 0.41          |
| (1,411)  | 1:30:A:THR:HG22 | 1:31:A:LEU:HG   | 1        | 0.41          |
| (1,382)  | 1:24:A:LEU:HG   | 1:28:A:LEU:HG   | 19       | 0.41          |
| (1,370)  | 1:62:A:PHE:HD2  | 1:69:A:LEU:HB2  | 11       | 0.41          |
| (1,370)  | 1:62:A:PHE:HD2  | 1:69:A:LEU:HB3  | 11       | 0.41          |
| (1,370)  | 1:62:A:PHE:HD2  | 1:69:A:LEU:HB2  | 12       | 0.41          |
| (1,370)  | 1:62:A:PHE:HD2  | 1:69:A:LEU:HB3  | 12       | 0.41          |
| (1,370)  | 1:62:A:PHE:HD2  | 1:69:A:LEU:HB2  | 15       | 0.41          |
| (1,370)  | 1:62:A:PHE:HD2  | 1:69:A:LEU:HB3  | 15       | 0.41          |
| (1,365)  | 1:28:A:LEU:HA   | 1:28:A:LEU:HD21 | 13       | 0.41          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,313)  | 1:69:A:LEU:HB2  | 1:69:A:LEU:HD21 | 6        | 0.41          |
| (1,82)   | 1:8:A:PHE:HA    | 1:19:A:ILE:HD13 | 3        | 0.41          |
| (1,1472) | 1:34:A:THR:HG23 | 1:35:A:SER:HB2  | 6        | 0.4           |
| (1,1472) | 1:34:A:THR:HG23 | 1:35:A:SER:HB3  | 6        | 0.4           |
| (1,1293) | 1:60:A:ILE:HG21 | 1:63:A:CYS:H    | 4        | 0.4           |
| (1,1293) | 1:60:A:ILE:HG21 | 1:63:A:CYS:H    | 5        | 0.4           |
| (1,1293) | 1:60:A:ILE:HG21 | 1:63:A:CYS:H    | 10       | 0.4           |
| (1,1293) | 1:60:A:ILE:HG21 | 1:63:A:CYS:H    | 15       | 0.4           |
| (1,1253) | 1:53:A:PHE:H    | 1:53:A:PHE:HD1  | 13       | 0.4           |
| (1,1253) | 1:53:A:PHE:H    | 1:53:A:PHE:HD1  | 18       | 0.4           |
| (1,1253) | 1:53:A:PHE:H    | 1:53:A:PHE:HD1  | 19       | 0.4           |
| (1,1173) | 1:34:A:THR:HG23 | 1:35:A:SER:H    | 2        | 0.4           |
| (1,1173) | 1:34:A:THR:HG23 | 1:35:A:SER:H    | 20       | 0.4           |
| (1,875)  | 1:7:A:ILE:HD12  | 1:77:A:PHE:H    | 6        | 0.4           |
| (1,866)  | 1:4:A:MET:HE3   | 1:7:A:ILE:HD11  | 10       | 0.4           |
| (1,866)  | 1:4:A:MET:HE3   | 1:7:A:ILE:HD13  | 10       | 0.4           |
| (1,802)  | 1:62:A:PHE:HE2  | 1:70:A:MET:HG2  | 10       | 0.4           |
| (1,801)  | 1:62:A:PHE:HD2  | 1:70:A:MET:HG3  | 4        | 0.4           |
| (1,801)  | 1:62:A:PHE:HD2  | 1:70:A:MET:HG3  | 12       | 0.4           |
| (1,800)  | 1:62:A:PHE:HE2  | 1:70:A:MET:HG3  | 8        | 0.4           |
| (1,728)  | 1:60:A:ILE:HD12 | 1:61:A:SER:H    | 2        | 0.4           |
| (1,433)  | 1:34:A:THR:HA   | 1:34:A:THR:HG23 | 1        | 0.4           |
| (1,433)  | 1:34:A:THR:HA   | 1:34:A:THR:HG23 | 10       | 0.4           |
| (1,411)  | 1:30:A:THR:HG22 | 1:31:A:LEU:HG   | 13       | 0.4           |
| (1,411)  | 1:30:A:THR:HG22 | 1:31:A:LEU:HG   | 19       | 0.4           |
| (1,387)  | 1:24:A:LEU:HD22 | 1:28:A:LEU:HD23 | 18       | 0.4           |
| (1,387)  | 1:24:A:LEU:HD22 | 1:28:A:LEU:HD23 | 20       | 0.4           |
| (1,382)  | 1:24:A:LEU:HG   | 1:28:A:LEU:HG   | 1        | 0.4           |
| (1,382)  | 1:24:A:LEU:HG   | 1:28:A:LEU:HG   | 3        | 0.4           |
| (1,382)  | 1:24:A:LEU:HG   | 1:28:A:LEU:HG   | 13       | 0.4           |
| (1,382)  | 1:24:A:LEU:HG   | 1:28:A:LEU:HG   | 14       | 0.4           |
| (1,382)  | 1:24:A:LEU:HG   | 1:28:A:LEU:HG   | 15       | 0.4           |
| (1,382)  | 1:24:A:LEU:HG   | 1:28:A:LEU:HG   | 18       | 0.4           |
| (1,370)  | 1:62:A:PHE:HD2  | 1:69:A:LEU:HB2  | 6        | 0.4           |
| (1,370)  | 1:62:A:PHE:HD2  | 1:69:A:LEU:HB3  | 6        | 0.4           |
| (1,370)  | 1:62:A:PHE:HD2  | 1:69:A:LEU:HB2  | 17       | 0.4           |
| (1,370)  | 1:62:A:PHE:HD2  | 1:69:A:LEU:HB3  | 17       | 0.4           |
| (1,235)  | 1:53:A:PHE:HB3  | 1:53:A:PHE:HD2  | 1        | 0.4           |
| (1,235)  | 1:53:A:PHE:HB2  | 1:53:A:PHE:HD1  | 1        | 0.4           |
| (1,235)  | 1:53:A:PHE:HB3  | 1:53:A:PHE:HD2  | 2        | 0.4           |
| (1,235)  | 1:53:A:PHE:HB2  | 1:53:A:PHE:HD1  | 2        | 0.4           |
| (1,235)  | 1:53:A:PHE:HB3  | 1:53:A:PHE:HD2  | 4        | 0.4           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,235)  | 1:53:A:PHE:HB2  | 1:53:A:PHE:HD1  | 4        | 0.4           |
| (1,235)  | 1:53:A:PHE:HB3  | 1:53:A:PHE:HD2  | 5        | 0.4           |
| (1,235)  | 1:53:A:PHE:HB2  | 1:53:A:PHE:HD1  | 5        | 0.4           |
| (1,235)  | 1:53:A:PHE:HB3  | 1:53:A:PHE:HD2  | 6        | 0.4           |
| (1,235)  | 1:53:A:PHE:HB2  | 1:53:A:PHE:HD1  | 6        | 0.4           |
| (1,235)  | 1:53:A:PHE:HB3  | 1:53:A:PHE:HD2  | 8        | 0.4           |
| (1,235)  | 1:53:A:PHE:HB2  | 1:53:A:PHE:HD1  | 8        | 0.4           |
| (1,235)  | 1:53:A:PHE:HB3  | 1:53:A:PHE:HD2  | 9        | 0.4           |
| (1,235)  | 1:53:A:PHE:HB2  | 1:53:A:PHE:HD1  | 9        | 0.4           |
| (1,235)  | 1:53:A:PHE:HB3  | 1:53:A:PHE:HD2  | 14       | 0.4           |
| (1,235)  | 1:53:A:PHE:HB2  | 1:53:A:PHE:HD1  | 14       | 0.4           |
| (1,235)  | 1:53:A:PHE:HB3  | 1:53:A:PHE:HD2  | 16       | 0.4           |
| (1,235)  | 1:53:A:PHE:HB2  | 1:53:A:PHE:HD1  | 16       | 0.4           |
| (1,235)  | 1:53:A:PHE:HB3  | 1:53:A:PHE:HD2  | 17       | 0.4           |
| (1,235)  | 1:53:A:PHE:HB2  | 1:53:A:PHE:HD1  | 17       | 0.4           |
| (1,70)   | 1:7:A:ILE:HD12  | 1:77:A:PHE:HD2  | 19       | 0.4           |
| (1,1293) | 1:60:A:ILE:HG21 | 1:63:A:CYS:H    | 9        | 0.39          |
| (1,1253) | 1:53:A:PHE:H    | 1:53:A:PHE:HD1  | 15       | 0.39          |
| (1,1168) | 1:28:A:LEU:HD21 | 1:33:A:SER:H    | 6        | 0.39          |
| (1,853)  | 1:69:A:LEU:HB2  | 1:70:A:MET:HE3  | 6        | 0.39          |
| (1,850)  | 1:31:A:LEU:HB3  | 1:76:A:VAL:HG23 | 7        | 0.39          |
| (1,728)  | 1:60:A:ILE:HD12 | 1:61:A:SER:H    | 10       | 0.39          |
| (1,652)  | 1:46:A:ILE:HB   | 1:54:A:ILE:HD13 | 11       | 0.39          |
| (1,433)  | 1:34:A:THR:HA   | 1:34:A:THR:HG23 | 5        | 0.39          |
| (1,433)  | 1:34:A:THR:HA   | 1:34:A:THR:HG23 | 11       | 0.39          |
| (1,417)  | 1:28:A:LEU:HD22 | 1:33:A:SER:HA   | 11       | 0.39          |
| (1,401)  | 1:30:A:THR:HB   | 1:31:A:LEU:HD21 | 16       | 0.39          |
| (1,382)  | 1:24:A:LEU:HG   | 1:28:A:LEU:HG   | 12       | 0.39          |
| (1,382)  | 1:24:A:LEU:HG   | 1:28:A:LEU:HG   | 16       | 0.39          |
| (1,382)  | 1:24:A:LEU:HG   | 1:28:A:LEU:HG   | 17       | 0.39          |
| (1,370)  | 1:62:A:PHE:HD2  | 1:69:A:LEU:HB2  | 4        | 0.39          |
| (1,370)  | 1:62:A:PHE:HD2  | 1:69:A:LEU:HB3  | 4        | 0.39          |
| (1,370)  | 1:62:A:PHE:HD2  | 1:69:A:LEU:HB2  | 7        | 0.39          |
| (1,370)  | 1:62:A:PHE:HD2  | 1:69:A:LEU:HB3  | 7        | 0.39          |
| (1,370)  | 1:62:A:PHE:HD2  | 1:69:A:LEU:HB2  | 9        | 0.39          |
| (1,370)  | 1:62:A:PHE:HD2  | 1:69:A:LEU:HB3  | 9        | 0.39          |
| (1,365)  | 1:28:A:LEU:HA   | 1:28:A:LEU:HD21 | 11       | 0.39          |
| (1,313)  | 1:69:A:LEU:HB2  | 1:69:A:LEU:HD21 | 17       | 0.39          |
| (1,235)  | 1:53:A:PHE:HB3  | 1:53:A:PHE:HD2  | 20       | 0.39          |
| (1,235)  | 1:53:A:PHE:HB2  | 1:53:A:PHE:HD1  | 20       | 0.39          |
| (1,1293) | 1:60:A:ILE:HG21 | 1:63:A:CYS:H    | 1        | 0.38          |
| (1,1293) | 1:60:A:ILE:HG21 | 1:63:A:CYS:H    | 12       | 0.38          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1293) | 1:60:A:ILE:HG21 | 1:63:A:CYS:H    | 13       | 0.38          |
| (1,1293) | 1:60:A:ILE:HG21 | 1:63:A:CYS:H    | 20       | 0.38          |
| (1,1173) | 1:34:A:THR:HG23 | 1:35:A:SER:H    | 15       | 0.38          |
| (1,1173) | 1:34:A:THR:HG23 | 1:35:A:SER:H    | 18       | 0.38          |
| (1,989)  | 1:46:A:ILE:HD11 | 1:59:A:PHE:H    | 3        | 0.38          |
| (1,801)  | 1:62:A:PHE:HD2  | 1:70:A:MET:HG3  | 8        | 0.38          |
| (1,801)  | 1:62:A:PHE:HD2  | 1:70:A:MET:HG3  | 19       | 0.38          |
| (1,728)  | 1:60:A:ILE:HD12 | 1:61:A:SER:H    | 4        | 0.38          |
| (1,501)  | 1:42:A:MET:HB3  | 1:62:A:PHE:HD1  | 13       | 0.38          |
| (1,472)  | 1:62:A:PHE:HE2  | 1:69:A:LEU:HD21 | 6        | 0.38          |
| (1,437)  | 1:36:A:ALA:HA   | 1:39:A:VAL:HB   | 2        | 0.38          |
| (1,417)  | 1:28:A:LEU:HD22 | 1:33:A:SER:HA   | 8        | 0.38          |
| (1,411)  | 1:30:A:THR:HG22 | 1:31:A:LEU:HG   | 12       | 0.38          |
| (1,411)  | 1:30:A:THR:HG22 | 1:31:A:LEU:HG   | 17       | 0.38          |
| (1,387)  | 1:24:A:LEU:HD22 | 1:28:A:LEU:HD23 | 12       | 0.38          |
| (1,382)  | 1:24:A:LEU:HG   | 1:28:A:LEU:HG   | 5        | 0.38          |
| (1,382)  | 1:24:A:LEU:HG   | 1:28:A:LEU:HG   | 11       | 0.38          |
| (1,382)  | 1:24:A:LEU:HG   | 1:28:A:LEU:HG   | 20       | 0.38          |
| (1,370)  | 1:62:A:PHE:HD2  | 1:69:A:LEU:HB2  | 19       | 0.38          |
| (1,370)  | 1:62:A:PHE:HD2  | 1:69:A:LEU:HB3  | 19       | 0.38          |
| (1,7)    | 1:3:A:ASP:HB2   | 1:4:A:MET:HE3   | 13       | 0.38          |
| (1,7)    | 1:3:A:ASP:HB3   | 1:4:A:MET:HE3   | 13       | 0.38          |
| (1,1293) | 1:60:A:ILE:HG21 | 1:63:A:CYS:H    | 16       | 0.37          |
| (1,1253) | 1:53:A:PHE:H    | 1:53:A:PHE:HD1  | 3        | 0.37          |
| (1,1135) | 1:25:A:THR:H    | 1:43:A:MET:HE3  | 12       | 0.37          |
| (1,800)  | 1:62:A:PHE:HE2  | 1:70:A:MET:HG3  | 19       | 0.37          |
| (1,731)  | 1:60:A:ILE:HA   | 1:60:A:ILE:HD12 | 15       | 0.37          |
| (1,728)  | 1:60:A:ILE:HD12 | 1:61:A:SER:H    | 1        | 0.37          |
| (1,652)  | 1:46:A:ILE:HB   | 1:54:A:ILE:HD13 | 10       | 0.37          |
| (1,501)  | 1:42:A:MET:HB3  | 1:62:A:PHE:HD1  | 14       | 0.37          |
| (1,433)  | 1:34:A:THR:HA   | 1:34:A:THR:HG23 | 16       | 0.37          |
| (1,411)  | 1:30:A:THR:HG22 | 1:31:A:LEU:HG   | 11       | 0.37          |
| (1,411)  | 1:30:A:THR:HG22 | 1:31:A:LEU:HG   | 15       | 0.37          |
| (1,384)  | 1:28:A:LEU:H    | 1:28:A:LEU:HD21 | 14       | 0.37          |
| (1,72)   | 1:7:A:ILE:HA    | 1:7:A:ILE:HD13  | 8        | 0.37          |
| (1,72)   | 1:7:A:ILE:HA    | 1:7:A:ILE:HD13  | 15       | 0.37          |
| (1,1432) | 1:20:A:SER:HB2  | 1:53:A:PHE:HD2  | 18       | 0.36          |
| (1,1432) | 1:20:A:SER:HB3  | 1:53:A:PHE:HD2  | 18       | 0.36          |
| (1,1293) | 1:60:A:ILE:HG21 | 1:63:A:CYS:H    | 17       | 0.36          |
| (1,1238) | 1:48:A:THR:H    | 1:48:A:THR:HG22 | 7        | 0.36          |
| (1,1238) | 1:48:A:THR:H    | 1:48:A:THR:HG22 | 19       | 0.36          |
| (1,1190) | 1:25:A:THR:HG22 | 1:40:A:GLN:H    | 14       | 0.36          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1173) | 1:34:A:THR:HG23 | 1:35:A:SER:H    | 8        | 0.36          |
| (1,1173) | 1:34:A:THR:HG23 | 1:35:A:SER:H    | 16       | 0.36          |
| (1,1173) | 1:34:A:THR:HG23 | 1:35:A:SER:H    | 19       | 0.36          |
| (1,875)  | 1:7:A:ILE:HD12  | 1:77:A:PHE:H    | 16       | 0.36          |
| (1,853)  | 1:69:A:LEU:HB2  | 1:70:A:MET:HE3  | 14       | 0.36          |
| (1,501)  | 1:42:A:MET:HB3  | 1:62:A:PHE:HD1  | 18       | 0.36          |
| (1,437)  | 1:36:A:ALA:HA   | 1:39:A:VAL:HB   | 13       | 0.36          |
| (1,437)  | 1:36:A:ALA:HA   | 1:39:A:VAL:HB   | 14       | 0.36          |
| (1,387)  | 1:24:A:LEU:HD22 | 1:28:A:LEU:HD23 | 2        | 0.36          |
| (1,370)  | 1:62:A:PHE:HD2  | 1:69:A:LEU:HB2  | 2        | 0.36          |
| (1,370)  | 1:62:A:PHE:HD2  | 1:69:A:LEU:HB3  | 2        | 0.36          |
| (1,365)  | 1:28:A:LEU:HA   | 1:28:A:LEU:HD21 | 16       | 0.36          |
| (1,146)  | 1:11:A:PHE:HB2  | 1:11:A:PHE:HD1  | 6        | 0.36          |
| (1,146)  | 1:11:A:PHE:HB2  | 1:11:A:PHE:HD1  | 9        | 0.36          |
| (1,146)  | 1:11:A:PHE:HB2  | 1:11:A:PHE:HD1  | 14       | 0.36          |
| (1,146)  | 1:11:A:PHE:HB2  | 1:11:A:PHE:HD1  | 15       | 0.36          |
| (1,146)  | 1:11:A:PHE:HB2  | 1:11:A:PHE:HD1  | 17       | 0.36          |
| (1,146)  | 1:11:A:PHE:HB2  | 1:11:A:PHE:HD1  | 18       | 0.36          |
| (1,146)  | 1:11:A:PHE:HB2  | 1:11:A:PHE:HD1  | 20       | 0.36          |
| (1,72)   | 1:7:A:ILE:HA    | 1:7:A:ILE:HD13  | 1        | 0.36          |
| (1,1253) | 1:53:A:PHE:H    | 1:53:A:PHE:HD1  | 1        | 0.35          |
| (1,1253) | 1:53:A:PHE:H    | 1:53:A:PHE:HD1  | 4        | 0.35          |
| (1,1253) | 1:53:A:PHE:H    | 1:53:A:PHE:HD1  | 5        | 0.35          |
| (1,1238) | 1:48:A:THR:H    | 1:48:A:THR:HG22 | 3        | 0.35          |
| (1,1238) | 1:48:A:THR:H    | 1:48:A:THR:HG22 | 8        | 0.35          |
| (1,1238) | 1:48:A:THR:H    | 1:48:A:THR:HG22 | 9        | 0.35          |
| (1,1238) | 1:48:A:THR:H    | 1:48:A:THR:HG22 | 14       | 0.35          |
| (1,1238) | 1:48:A:THR:H    | 1:48:A:THR:HG22 | 20       | 0.35          |
| (1,802)  | 1:62:A:PHE:HE2  | 1:70:A:MET:HG2  | 2        | 0.35          |
| (1,802)  | 1:62:A:PHE:HE2  | 1:70:A:MET:HG2  | 7        | 0.35          |
| (1,801)  | 1:62:A:PHE:HD2  | 1:70:A:MET:HG3  | 6        | 0.35          |
| (1,728)  | 1:60:A:ILE:HD12 | 1:61:A:SER:H    | 6        | 0.35          |
| (1,695)  | 1:46:A:ILE:HD11 | 1:58:A:GLU:HB3  | 20       | 0.35          |
| (1,437)  | 1:36:A:ALA:HA   | 1:39:A:VAL:HB   | 12       | 0.35          |
| (1,437)  | 1:36:A:ALA:HA   | 1:39:A:VAL:HB   | 20       | 0.35          |
| (1,433)  | 1:34:A:THR:HA   | 1:34:A:THR:HG23 | 12       | 0.35          |
| (1,411)  | 1:30:A:THR:HG22 | 1:31:A:LEU:HG   | 4        | 0.35          |
| (1,411)  | 1:30:A:THR:HG22 | 1:31:A:LEU:HG   | 8        | 0.35          |
| (1,370)  | 1:62:A:PHE:HD2  | 1:69:A:LEU:HB2  | 3        | 0.35          |
| (1,370)  | 1:62:A:PHE:HD2  | 1:69:A:LEU:HB3  | 3        | 0.35          |
| (1,146)  | 1:11:A:PHE:HB2  | 1:11:A:PHE:HD1  | 1        | 0.35          |
| (1,146)  | 1:11:A:PHE:HB2  | 1:11:A:PHE:HD1  | 2        | 0.35          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,146)  | 1:11:A:PHE:HB2  | 1:11:A:PHE:HD1  | 3        | 0.35          |
| (1,146)  | 1:11:A:PHE:HB2  | 1:11:A:PHE:HD1  | 5        | 0.35          |
| (1,146)  | 1:11:A:PHE:HB2  | 1:11:A:PHE:HD1  | 7        | 0.35          |
| (1,146)  | 1:11:A:PHE:HB2  | 1:11:A:PHE:HD1  | 10       | 0.35          |
| (1,146)  | 1:11:A:PHE:HB2  | 1:11:A:PHE:HD1  | 16       | 0.35          |
| (1,146)  | 1:11:A:PHE:HB2  | 1:11:A:PHE:HD1  | 19       | 0.35          |
| (1,72)   | 1:7:A:ILE:HA    | 1:7:A:ILE:HD13  | 19       | 0.35          |
| (1,1293) | 1:60:A:ILE:HG21 | 1:63:A:CYS:H    | 14       | 0.34          |
| (1,1253) | 1:53:A:PHE:H    | 1:53:A:PHE:HD1  | 2        | 0.34          |
| (1,1253) | 1:53:A:PHE:H    | 1:53:A:PHE:HD1  | 6        | 0.34          |
| (1,1253) | 1:53:A:PHE:H    | 1:53:A:PHE:HD1  | 8        | 0.34          |
| (1,1253) | 1:53:A:PHE:H    | 1:53:A:PHE:HD1  | 9        | 0.34          |
| (1,1253) | 1:53:A:PHE:H    | 1:53:A:PHE:HD1  | 14       | 0.34          |
| (1,1253) | 1:53:A:PHE:H    | 1:53:A:PHE:HD1  | 17       | 0.34          |
| (1,1238) | 1:48:A:THR:H    | 1:48:A:THR:HG22 | 1        | 0.34          |
| (1,1238) | 1:48:A:THR:H    | 1:48:A:THR:HG22 | 2        | 0.34          |
| (1,1238) | 1:48:A:THR:H    | 1:48:A:THR:HG22 | 4        | 0.34          |
| (1,1238) | 1:48:A:THR:H    | 1:48:A:THR:HG22 | 6        | 0.34          |
| (1,1238) | 1:48:A:THR:H    | 1:48:A:THR:HG22 | 16       | 0.34          |
| (1,1238) | 1:48:A:THR:H    | 1:48:A:THR:HG22 | 17       | 0.34          |
| (1,728)  | 1:60:A:ILE:HD12 | 1:61:A:SER:H    | 3        | 0.34          |
| (1,728)  | 1:60:A:ILE:HD12 | 1:61:A:SER:H    | 8        | 0.34          |
| (1,472)  | 1:62:A:PHE:HE2  | 1:69:A:LEU:HD21 | 17       | 0.34          |
| (1,437)  | 1:36:A:ALA:HA   | 1:39:A:VAL:HB   | 4        | 0.34          |
| (1,437)  | 1:36:A:ALA:HA   | 1:39:A:VAL:HB   | 5        | 0.34          |
| (1,437)  | 1:36:A:ALA:HA   | 1:39:A:VAL:HB   | 7        | 0.34          |
| (1,437)  | 1:36:A:ALA:HA   | 1:39:A:VAL:HB   | 9        | 0.34          |
| (1,437)  | 1:36:A:ALA:HA   | 1:39:A:VAL:HB   | 11       | 0.34          |
| (1,437)  | 1:36:A:ALA:HA   | 1:39:A:VAL:HB   | 17       | 0.34          |
| (1,437)  | 1:36:A:ALA:HA   | 1:39:A:VAL:HB   | 19       | 0.34          |
| (1,370)  | 1:62:A:PHE:HD2  | 1:69:A:LEU:HB2  | 16       | 0.34          |
| (1,370)  | 1:62:A:PHE:HD2  | 1:69:A:LEU:HB3  | 16       | 0.34          |
| (1,146)  | 1:11:A:PHE:HB2  | 1:11:A:PHE:HD1  | 4        | 0.34          |
| (1,146)  | 1:11:A:PHE:HB2  | 1:11:A:PHE:HD1  | 8        | 0.34          |
| (1,146)  | 1:11:A:PHE:HB2  | 1:11:A:PHE:HD1  | 11       | 0.34          |
| (1,72)   | 1:7:A:ILE:HA    | 1:7:A:ILE:HD13  | 4        | 0.34          |
| (1,72)   | 1:7:A:ILE:HA    | 1:7:A:ILE:HD13  | 7        | 0.34          |
| (1,72)   | 1:7:A:ILE:HA    | 1:7:A:ILE:HD13  | 9        | 0.34          |
| (1,72)   | 1:7:A:ILE:HA    | 1:7:A:ILE:HD13  | 16       | 0.34          |
| (1,1358) | 1:2:A:ASP:HB2   | 1:3:A:ASP:H     | 17       | 0.33          |
| (1,1358) | 1:2:A:ASP:HB3   | 1:3:A:ASP:H     | 17       | 0.33          |
| (1,1293) | 1:60:A:ILE:HG21 | 1:63:A:CYS:H    | 18       | 0.33          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1253) | 1:53:A:PHE:H    | 1:53:A:PHE:HD1  | 16       | 0.33          |
| (1,1238) | 1:48:A:THR:H    | 1:48:A:THR:HG22 | 11       | 0.33          |
| (1,1238) | 1:48:A:THR:H    | 1:48:A:THR:HG22 | 15       | 0.33          |
| (1,1168) | 1:28:A:LEU:HD21 | 1:33:A:SER:H    | 7        | 0.33          |
| (1,866)  | 1:4:A:MET:HE3   | 1:7:A:ILE:HD11  | 12       | 0.33          |
| (1,866)  | 1:4:A:MET:HE3   | 1:7:A:ILE:HD13  | 12       | 0.33          |
| (1,802)  | 1:62:A:PHE:HE2  | 1:70:A:MET:HG2  | 3        | 0.33          |
| (1,731)  | 1:60:A:ILE:HA   | 1:60:A:ILE:HD12 | 14       | 0.33          |
| (1,731)  | 1:60:A:ILE:HA   | 1:60:A:ILE:HD12 | 20       | 0.33          |
| (1,728)  | 1:60:A:ILE:HD12 | 1:61:A:SER:H    | 19       | 0.33          |
| (1,437)  | 1:36:A:ALA:HA   | 1:39:A:VAL:HB   | 1        | 0.33          |
| (1,437)  | 1:36:A:ALA:HA   | 1:39:A:VAL:HB   | 3        | 0.33          |
| (1,437)  | 1:36:A:ALA:HA   | 1:39:A:VAL:HB   | 6        | 0.33          |
| (1,437)  | 1:36:A:ALA:HA   | 1:39:A:VAL:HB   | 8        | 0.33          |
| (1,437)  | 1:36:A:ALA:HA   | 1:39:A:VAL:HB   | 10       | 0.33          |
| (1,437)  | 1:36:A:ALA:HA   | 1:39:A:VAL:HB   | 15       | 0.33          |
| (1,437)  | 1:36:A:ALA:HA   | 1:39:A:VAL:HB   | 16       | 0.33          |
| (1,437)  | 1:36:A:ALA:HA   | 1:39:A:VAL:HB   | 18       | 0.33          |
| (1,417)  | 1:28:A:LEU:HD22 | 1:33:A:SER:HA   | 6        | 0.33          |
| (1,417)  | 1:28:A:LEU:HD22 | 1:33:A:SER:HA   | 10       | 0.33          |
| (1,411)  | 1:30:A:THR:HG22 | 1:31:A:LEU:HG   | 10       | 0.33          |
| (1,411)  | 1:30:A:THR:HG22 | 1:31:A:LEU:HG   | 18       | 0.33          |
| (1,401)  | 1:30:A:THR:HB   | 1:31:A:LEU:HD21 | 3        | 0.33          |
| (1,370)  | 1:62:A:PHE:HD2  | 1:69:A:LEU:HB2  | 8        | 0.33          |
| (1,370)  | 1:62:A:PHE:HD2  | 1:69:A:LEU:HB3  | 8        | 0.33          |
| (1,365)  | 1:28:A:LEU:HA   | 1:28:A:LEU:HD21 | 8        | 0.33          |
| (1,313)  | 1:69:A:LEU:HB2  | 1:69:A:LEU:HD21 | 16       | 0.33          |
| (1,146)  | 1:11:A:PHE:HB2  | 1:11:A:PHE:HD1  | 12       | 0.33          |
| (1,146)  | 1:11:A:PHE:HB2  | 1:11:A:PHE:HD1  | 13       | 0.33          |
| (1,72)   | 1:7:A:ILE:HA    | 1:7:A:ILE:HD13  | 3        | 0.33          |
| (1,72)   | 1:7:A:ILE:HA    | 1:7:A:ILE:HD13  | 6        | 0.33          |
| (1,72)   | 1:7:A:ILE:HA    | 1:7:A:ILE:HD13  | 13       | 0.33          |
| (1,72)   | 1:7:A:ILE:HA    | 1:7:A:ILE:HD13  | 20       | 0.33          |
| (1,1530) | 1:52:A:GLY:HA2  | 1:53:A:PHE:H    | 10       | 0.32          |
| (1,1530) | 1:52:A:GLY:HA3  | 1:53:A:PHE:H    | 10       | 0.32          |
| (1,1432) | 1:20:A:SER:HB2  | 1:53:A:PHE:HD2  | 7        | 0.32          |
| (1,1432) | 1:20:A:SER:HB3  | 1:53:A:PHE:HD2  | 7        | 0.32          |
| (1,1253) | 1:53:A:PHE:H    | 1:53:A:PHE:HD1  | 20       | 0.32          |
| (1,1190) | 1:25:A:THR:HG22 | 1:40:A:GLN:H    | 13       | 0.32          |
| (1,1125) | 1:21:A:LEU:HG   | 1:22:A:SER:H    | 14       | 0.32          |
| (1,802)  | 1:62:A:PHE:HE2  | 1:70:A:MET:HG2  | 8        | 0.32          |
| (1,802)  | 1:62:A:PHE:HE2  | 1:70:A:MET:HG2  | 19       | 0.32          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,801)  | 1:62:A:PHE:HD2  | 1:70:A:MET:HG3  | 1        | 0.32          |
| (1,731)  | 1:60:A:ILE:HA   | 1:60:A:ILE:HD12 | 16       | 0.32          |
| (1,695)  | 1:46:A:ILE:HD11 | 1:58:A:GLU:HB3  | 9        | 0.32          |
| (1,433)  | 1:34:A:THR:HA   | 1:34:A:THR:HG23 | 2        | 0.32          |
| (1,411)  | 1:30:A:THR:HG22 | 1:31:A:LEU:HG   | 7        | 0.32          |
| (1,411)  | 1:30:A:THR:HG22 | 1:31:A:LEU:HG   | 14       | 0.32          |
| (1,365)  | 1:28:A:LEU:HA   | 1:28:A:LEU:HD21 | 17       | 0.32          |
| (1,332)  | 1:24:A:LEU:HD22 | 1:27:A:ALA:H    | 8        | 0.32          |
| (1,268)  | 1:19:A:ILE:HD11 | 1:59:A:PHE:HD2  | 13       | 0.32          |
| (1,72)   | 1:7:A:ILE:HA    | 1:7:A:ILE:HD13  | 5        | 0.32          |
| (1,72)   | 1:7:A:ILE:HA    | 1:7:A:ILE:HD13  | 11       | 0.32          |
| (1,72)   | 1:7:A:ILE:HA    | 1:7:A:ILE:HD13  | 17       | 0.32          |
| (1,16)   | 1:42:A:MET:HG2  | 1:62:A:PHE:HE1  | 1        | 0.32          |
| (1,1530) | 1:52:A:GLY:HA2  | 1:53:A:PHE:H    | 7        | 0.31          |
| (1,1530) | 1:52:A:GLY:HA3  | 1:53:A:PHE:H    | 7        | 0.31          |
| (1,1530) | 1:52:A:GLY:HA2  | 1:53:A:PHE:H    | 19       | 0.31          |
| (1,1530) | 1:52:A:GLY:HA3  | 1:53:A:PHE:H    | 19       | 0.31          |
| (1,1135) | 1:25:A:THR:H    | 1:43:A:MET:HE3  | 10       | 0.31          |
| (1,1125) | 1:21:A:LEU:HG   | 1:22:A:SER:H    | 1        | 0.31          |
| (1,1125) | 1:21:A:LEU:HG   | 1:22:A:SER:H    | 20       | 0.31          |
| (1,998)  | 1:24:A:LEU:H    | 1:24:A:LEU:HD21 | 2        | 0.31          |
| (1,998)  | 1:24:A:LEU:H    | 1:24:A:LEU:HD21 | 3        | 0.31          |
| (1,998)  | 1:24:A:LEU:H    | 1:24:A:LEU:HD21 | 4        | 0.31          |
| (1,998)  | 1:24:A:LEU:H    | 1:24:A:LEU:HD21 | 6        | 0.31          |
| (1,998)  | 1:24:A:LEU:H    | 1:24:A:LEU:HD21 | 12       | 0.31          |
| (1,998)  | 1:24:A:LEU:H    | 1:24:A:LEU:HD21 | 13       | 0.31          |
| (1,998)  | 1:24:A:LEU:H    | 1:24:A:LEU:HD21 | 20       | 0.31          |
| (1,989)  | 1:46:A:ILE:HD11 | 1:59:A:PHE:H    | 9        | 0.31          |
| (1,866)  | 1:4:A:MET:HE3   | 1:7:A:ILE:HD11  | 11       | 0.31          |
| (1,866)  | 1:4:A:MET:HE3   | 1:7:A:ILE:HD13  | 11       | 0.31          |
| (1,850)  | 1:31:A:LEU:HB3  | 1:76:A:VAL:HG23 | 12       | 0.31          |
| (1,731)  | 1:60:A:ILE:HA   | 1:60:A:ILE:HD12 | 9        | 0.31          |
| (1,728)  | 1:60:A:ILE:HD12 | 1:61:A:SER:H    | 7        | 0.31          |
| (1,411)  | 1:30:A:THR:HG22 | 1:31:A:LEU:HG   | 2        | 0.31          |
| (1,411)  | 1:30:A:THR:HG22 | 1:31:A:LEU:HG   | 6        | 0.31          |
| (1,365)  | 1:28:A:LEU:HA   | 1:28:A:LEU:HD21 | 10       | 0.31          |
| (1,313)  | 1:69:A:LEU:HB2  | 1:69:A:LEU:HD21 | 12       | 0.31          |
| (1,268)  | 1:19:A:ILE:HD11 | 1:59:A:PHE:HD2  | 19       | 0.31          |
| (1,72)   | 1:7:A:ILE:HA    | 1:7:A:ILE:HD13  | 2        | 0.31          |
| (1,72)   | 1:7:A:ILE:HA    | 1:7:A:ILE:HD13  | 14       | 0.31          |
| (1,1530) | 1:52:A:GLY:HA2  | 1:53:A:PHE:H    | 3        | 0.3           |
| (1,1530) | 1:52:A:GLY:HA3  | 1:53:A:PHE:H    | 3        | 0.3           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1530) | 1:52:A:GLY:HA2  | 1:53:A:PHE:H    | 15       | 0.3           |
| (1,1530) | 1:52:A:GLY:HA3  | 1:53:A:PHE:H    | 15       | 0.3           |
| (1,1530) | 1:52:A:GLY:HA2  | 1:53:A:PHE:H    | 18       | 0.3           |
| (1,1530) | 1:52:A:GLY:HA3  | 1:53:A:PHE:H    | 18       | 0.3           |
| (1,1528) | 1:51:A:ASP:H    | 1:52:A:GLY:HA2  | 10       | 0.3           |
| (1,1528) | 1:51:A:ASP:H    | 1:52:A:GLY:HA3  | 10       | 0.3           |
| (1,1528) | 1:51:A:ASP:H    | 1:52:A:GLY:HA2  | 18       | 0.3           |
| (1,1528) | 1:51:A:ASP:H    | 1:52:A:GLY:HA3  | 18       | 0.3           |
| (1,1238) | 1:48:A:THR:H    | 1:48:A:THR:HG22 | 12       | 0.3           |
| (1,1168) | 1:28:A:LEU:HD21 | 1:33:A:SER:H    | 8        | 0.3           |
| (1,1168) | 1:28:A:LEU:HD21 | 1:33:A:SER:H    | 10       | 0.3           |
| (1,998)  | 1:24:A:LEU:H    | 1:24:A:LEU:HD21 | 5        | 0.3           |
| (1,998)  | 1:24:A:LEU:H    | 1:24:A:LEU:HD21 | 7        | 0.3           |
| (1,998)  | 1:24:A:LEU:H    | 1:24:A:LEU:HD21 | 10       | 0.3           |
| (1,998)  | 1:24:A:LEU:H    | 1:24:A:LEU:HD21 | 17       | 0.3           |
| (1,998)  | 1:24:A:LEU:H    | 1:24:A:LEU:HD21 | 18       | 0.3           |
| (1,988)  | 1:34:A:THR:H    | 1:34:A:THR:HG23 | 5        | 0.3           |
| (1,801)  | 1:62:A:PHE:HD2  | 1:70:A:MET:HG3  | 16       | 0.3           |
| (1,572)  | 1:46:A:ILE:HG22 | 1:62:A:PHE:HD1  | 13       | 0.3           |
| (1,572)  | 1:46:A:ILE:HG23 | 1:62:A:PHE:HD1  | 13       | 0.3           |
| (1,433)  | 1:34:A:THR:HA   | 1:34:A:THR:HG23 | 6        | 0.3           |
| (1,433)  | 1:34:A:THR:HA   | 1:34:A:THR:HG23 | 14       | 0.3           |
| (1,332)  | 1:24:A:LEU:HD22 | 1:27:A:ALA:H    | 9        | 0.3           |
| (1,332)  | 1:24:A:LEU:HD22 | 1:27:A:ALA:H    | 19       | 0.3           |
| (1,268)  | 1:19:A:ILE:HD11 | 1:59:A:PHE:HD2  | 7        | 0.3           |
| (1,268)  | 1:19:A:ILE:HD11 | 1:59:A:PHE:HD2  | 14       | 0.3           |
| (1,266)  | 1:12:A:ASP:H    | 1:19:A:ILE:HD13 | 4        | 0.3           |
| (1,72)   | 1:7:A:ILE:HA    | 1:7:A:ILE:HD13  | 12       | 0.3           |
| (1,1528) | 1:51:A:ASP:H    | 1:52:A:GLY:HA2  | 3        | 0.29          |
| (1,1528) | 1:51:A:ASP:H    | 1:52:A:GLY:HA3  | 3        | 0.29          |
| (1,1528) | 1:51:A:ASP:H    | 1:52:A:GLY:HA2  | 7        | 0.29          |
| (1,1528) | 1:51:A:ASP:H    | 1:52:A:GLY:HA3  | 7        | 0.29          |
| (1,1528) | 1:51:A:ASP:H    | 1:52:A:GLY:HA2  | 19       | 0.29          |
| (1,1528) | 1:51:A:ASP:H    | 1:52:A:GLY:HA3  | 19       | 0.29          |
| (1,1173) | 1:34:A:THR:HG23 | 1:35:A:SER:H    | 17       | 0.29          |
| (1,1125) | 1:21:A:LEU:HG   | 1:22:A:SER:H    | 9        | 0.29          |
| (1,1125) | 1:21:A:LEU:HG   | 1:22:A:SER:H    | 17       | 0.29          |
| (1,1125) | 1:21:A:LEU:HG   | 1:22:A:SER:H    | 18       | 0.29          |
| (1,989)  | 1:46:A:ILE:HD11 | 1:59:A:PHE:H    | 1        | 0.29          |
| (1,866)  | 1:4:A:MET:HE3   | 1:7:A:ILE:HD11  | 6        | 0.29          |
| (1,866)  | 1:4:A:MET:HE3   | 1:7:A:ILE:HD13  | 6        | 0.29          |
| (1,731)  | 1:60:A:ILE:HA   | 1:60:A:ILE:HD12 | 13       | 0.29          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,695)  | 1:46:A:ILE:HD11 | 1:58:A:GLU:HB3  | 12       | 0.29          |
| (1,693)  | 1:46:A:ILE:HG21 | 1:58:A:GLU:HB3  | 5        | 0.29          |
| (1,433)  | 1:34:A:THR:HA   | 1:34:A:THR:HG23 | 7        | 0.29          |
| (1,433)  | 1:34:A:THR:HA   | 1:34:A:THR:HG23 | 20       | 0.29          |
| (1,417)  | 1:28:A:LEU:HD22 | 1:33:A:SER:HA   | 3        | 0.29          |
| (1,365)  | 1:28:A:LEU:HA   | 1:28:A:LEU:HD21 | 1        | 0.29          |
| (1,365)  | 1:28:A:LEU:HA   | 1:28:A:LEU:HD21 | 5        | 0.29          |
| (1,332)  | 1:24:A:LEU:HD22 | 1:27:A:ALA:H    | 14       | 0.29          |
| (1,332)  | 1:24:A:LEU:HD22 | 1:27:A:ALA:H    | 16       | 0.29          |
| (1,313)  | 1:69:A:LEU:HB2  | 1:69:A:LEU:HD21 | 1        | 0.29          |
| (1,313)  | 1:69:A:LEU:HB2  | 1:69:A:LEU:HD21 | 13       | 0.29          |
| (1,1528) | 1:51:A:ASP:H    | 1:52:A:GLY:HA2  | 4        | 0.28          |
| (1,1528) | 1:51:A:ASP:H    | 1:52:A:GLY:HA3  | 4        | 0.28          |
| (1,1173) | 1:34:A:THR:HG23 | 1:35:A:SER:H    | 4        | 0.28          |
| (1,1168) | 1:28:A:LEU:HD21 | 1:33:A:SER:H    | 18       | 0.28          |
| (1,1125) | 1:21:A:LEU:HG   | 1:22:A:SER:H    | 3        | 0.28          |
| (1,1125) | 1:21:A:LEU:HG   | 1:22:A:SER:H    | 6        | 0.28          |
| (1,989)  | 1:46:A:ILE:HD11 | 1:59:A:PHE:H    | 4        | 0.28          |
| (1,989)  | 1:46:A:ILE:HD11 | 1:59:A:PHE:H    | 6        | 0.28          |
| (1,988)  | 1:34:A:THR:H    | 1:34:A:THR:HG23 | 10       | 0.28          |
| (1,875)  | 1:7:A:ILE:HD12  | 1:77:A:PHE:H    | 14       | 0.28          |
| (1,875)  | 1:7:A:ILE:HD12  | 1:77:A:PHE:H    | 20       | 0.28          |
| (1,866)  | 1:4:A:MET:HE3   | 1:7:A:ILE:HD11  | 18       | 0.28          |
| (1,866)  | 1:4:A:MET:HE3   | 1:7:A:ILE:HD13  | 18       | 0.28          |
| (1,433)  | 1:34:A:THR:HA   | 1:34:A:THR:HG23 | 15       | 0.28          |
| (1,433)  | 1:34:A:THR:HA   | 1:34:A:THR:HG23 | 18       | 0.28          |
| (1,433)  | 1:34:A:THR:HA   | 1:34:A:THR:HG23 | 19       | 0.28          |
| (1,417)  | 1:28:A:LEU:HD22 | 1:33:A:SER:HA   | 7        | 0.28          |
| (1,365)  | 1:28:A:LEU:HA   | 1:28:A:LEU:HD21 | 9        | 0.28          |
| (1,337)  | 1:24:A:LEU:HD22 | 1:27:A:ALA:HB1  | 1        | 0.28          |
| (1,337)  | 1:24:A:LEU:HD22 | 1:27:A:ALA:HB1  | 16       | 0.28          |
| (1,332)  | 1:24:A:LEU:HD22 | 1:27:A:ALA:H    | 1        | 0.28          |
| (1,332)  | 1:24:A:LEU:HD22 | 1:27:A:ALA:H    | 11       | 0.28          |
| (1,1530) | 1:52:A:GLY:HA2  | 1:53:A:PHE:H    | 13       | 0.27          |
| (1,1530) | 1:52:A:GLY:HA3  | 1:53:A:PHE:H    | 13       | 0.27          |
| (1,1528) | 1:51:A:ASP:H    | 1:52:A:GLY:HA2  | 2        | 0.27          |
| (1,1528) | 1:51:A:ASP:H    | 1:52:A:GLY:HA3  | 2        | 0.27          |
| (1,1528) | 1:51:A:ASP:H    | 1:52:A:GLY:HA2  | 6        | 0.27          |
| (1,1528) | 1:51:A:ASP:H    | 1:52:A:GLY:HA3  | 6        | 0.27          |
| (1,1528) | 1:51:A:ASP:H    | 1:52:A:GLY:HA2  | 8        | 0.27          |
| (1,1528) | 1:51:A:ASP:H    | 1:52:A:GLY:HA3  | 8        | 0.27          |
| (1,1528) | 1:51:A:ASP:H    | 1:52:A:GLY:HA2  | 13       | 0.27          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1528) | 1:51:A:ASP:H    | 1:52:A:GLY:HA3  | 13       | 0.27          |
| (1,1528) | 1:51:A:ASP:H    | 1:52:A:GLY:HA2  | 15       | 0.27          |
| (1,1528) | 1:51:A:ASP:H    | 1:52:A:GLY:HA3  | 15       | 0.27          |
| (1,1528) | 1:51:A:ASP:H    | 1:52:A:GLY:HA2  | 17       | 0.27          |
| (1,1528) | 1:51:A:ASP:H    | 1:52:A:GLY:HA3  | 17       | 0.27          |
| (1,1472) | 1:34:A:THR:HG23 | 1:35:A:SER:HB2  | 7        | 0.27          |
| (1,1472) | 1:34:A:THR:HG23 | 1:35:A:SER:HB3  | 7        | 0.27          |
| (1,1190) | 1:25:A:THR:HG22 | 1:40:A:GLN:H    | 5        | 0.27          |
| (1,1190) | 1:25:A:THR:HG22 | 1:40:A:GLN:H    | 7        | 0.27          |
| (1,1168) | 1:28:A:LEU:HD21 | 1:33:A:SER:H    | 19       | 0.27          |
| (1,1135) | 1:25:A:THR:H    | 1:43:A:MET:HE3  | 2        | 0.27          |
| (1,1135) | 1:25:A:THR:H    | 1:43:A:MET:HE3  | 8        | 0.27          |
| (1,1135) | 1:25:A:THR:H    | 1:43:A:MET:HE3  | 16       | 0.27          |
| (1,1125) | 1:21:A:LEU:HG   | 1:22:A:SER:H    | 2        | 0.27          |
| (1,1125) | 1:21:A:LEU:HG   | 1:22:A:SER:H    | 4        | 0.27          |
| (1,1125) | 1:21:A:LEU:HG   | 1:22:A:SER:H    | 8        | 0.27          |
| (1,1125) | 1:21:A:LEU:HG   | 1:22:A:SER:H    | 16       | 0.27          |
| (1,611)  | 1:52:A:GLY:HA3  | 1:53:A:PHE:HD1  | 11       | 0.27          |
| (1,611)  | 1:52:A:GLY:HA2  | 1:53:A:PHE:HD1  | 11       | 0.27          |
| (1,433)  | 1:34:A:THR:HA   | 1:34:A:THR:HG23 | 8        | 0.27          |
| (1,365)  | 1:28:A:LEU:HA   | 1:28:A:LEU:HD21 | 6        | 0.27          |
| (1,365)  | 1:28:A:LEU:HA   | 1:28:A:LEU:HD21 | 18       | 0.27          |
| (1,337)  | 1:24:A:LEU:HD22 | 1:27:A:ALA:HB1  | 8        | 0.27          |
| (1,337)  | 1:24:A:LEU:HD22 | 1:27:A:ALA:HB1  | 9        | 0.27          |
| (1,332)  | 1:24:A:LEU:HD22 | 1:27:A:ALA:H    | 15       | 0.27          |
| (1,257)  | 1:8:A:PHE:HE1   | 1:19:A:ILE:HG23 | 6        | 0.27          |
| (1,72)   | 1:7:A:ILE:HA    | 1:7:A:ILE:HD13  | 18       | 0.27          |
| (1,1530) | 1:52:A:GLY:HA2  | 1:53:A:PHE:H    | 2        | 0.26          |
| (1,1530) | 1:52:A:GLY:HA3  | 1:53:A:PHE:H    | 2        | 0.26          |
| (1,1528) | 1:51:A:ASP:H    | 1:52:A:GLY:HA2  | 1        | 0.26          |
| (1,1528) | 1:51:A:ASP:H    | 1:52:A:GLY:HA3  | 1        | 0.26          |
| (1,1528) | 1:51:A:ASP:H    | 1:52:A:GLY:HA2  | 9        | 0.26          |
| (1,1528) | 1:51:A:ASP:H    | 1:52:A:GLY:HA3  | 9        | 0.26          |
| (1,1528) | 1:51:A:ASP:H    | 1:52:A:GLY:HA2  | 16       | 0.26          |
| (1,1528) | 1:51:A:ASP:H    | 1:52:A:GLY:HA3  | 16       | 0.26          |
| (1,1472) | 1:34:A:THR:HG23 | 1:35:A:SER:HB2  | 19       | 0.26          |
| (1,1472) | 1:34:A:THR:HG23 | 1:35:A:SER:HB3  | 19       | 0.26          |
| (1,1472) | 1:34:A:THR:HG23 | 1:35:A:SER:HB2  | 20       | 0.26          |
| (1,1472) | 1:34:A:THR:HG23 | 1:35:A:SER:HB3  | 20       | 0.26          |
| (1,1190) | 1:25:A:THR:HG22 | 1:40:A:GLN:H    | 2        | 0.26          |
| (1,1010) | 1:42:A:MET:HG2  | 1:44:A:ALA:H    | 15       | 0.26          |
| (1,989)  | 1:46:A:ILE:HD11 | 1:59:A:PHE:H    | 2        | 0.26          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,989)  | 1:46:A:ILE:HD11 | 1:59:A:PHE:H    | 8        | 0.26          |
| (1,989)  | 1:46:A:ILE:HD11 | 1:59:A:PHE:H    | 14       | 0.26          |
| (1,989)  | 1:46:A:ILE:HD11 | 1:59:A:PHE:H    | 17       | 0.26          |
| (1,988)  | 1:34:A:THR:H    | 1:34:A:THR:HG23 | 11       | 0.26          |
| (1,866)  | 1:4:A:MET:HE3   | 1:7:A:ILE:HD11  | 7        | 0.26          |
| (1,866)  | 1:4:A:MET:HE3   | 1:7:A:ILE:HD13  | 7        | 0.26          |
| (1,866)  | 1:4:A:MET:HE3   | 1:7:A:ILE:HD11  | 19       | 0.26          |
| (1,866)  | 1:4:A:MET:HE3   | 1:7:A:ILE:HD13  | 19       | 0.26          |
| (1,850)  | 1:31:A:LEU:HB3  | 1:76:A:VAL:HG23 | 19       | 0.26          |
| (1,731)  | 1:60:A:ILE:HA   | 1:60:A:ILE:HD12 | 17       | 0.26          |
| (1,731)  | 1:60:A:ILE:HA   | 1:60:A:ILE:HD12 | 18       | 0.26          |
| (1,695)  | 1:46:A:ILE:HD11 | 1:58:A:GLU:HB3  | 6        | 0.26          |
| (1,695)  | 1:46:A:ILE:HD11 | 1:58:A:GLU:HB3  | 8        | 0.26          |
| (1,611)  | 1:52:A:GLY:HA3  | 1:53:A:PHE:HD1  | 10       | 0.26          |
| (1,611)  | 1:52:A:GLY:HA2  | 1:53:A:PHE:HD1  | 10       | 0.26          |
| (1,365)  | 1:28:A:LEU:HA   | 1:28:A:LEU:HD21 | 3        | 0.26          |
| (1,365)  | 1:28:A:LEU:HA   | 1:28:A:LEU:HD21 | 7        | 0.26          |
| (1,337)  | 1:24:A:LEU:HD22 | 1:27:A:ALA:HB1  | 11       | 0.26          |
| (1,337)  | 1:24:A:LEU:HD22 | 1:27:A:ALA:HB1  | 14       | 0.26          |
| (1,337)  | 1:24:A:LEU:HD22 | 1:27:A:ALA:HB1  | 15       | 0.26          |
| (1,268)  | 1:19:A:ILE:HD11 | 1:59:A:PHE:HD2  | 16       | 0.26          |
| (1,1530) | 1:52:A:GLY:HA2  | 1:53:A:PHE:H    | 4        | 0.25          |
| (1,1530) | 1:52:A:GLY:HA3  | 1:53:A:PHE:H    | 4        | 0.25          |
| (1,1530) | 1:52:A:GLY:HA2  | 1:53:A:PHE:H    | 8        | 0.25          |
| (1,1530) | 1:52:A:GLY:HA3  | 1:53:A:PHE:H    | 8        | 0.25          |
| (1,1528) | 1:51:A:ASP:H    | 1:52:A:GLY:HA2  | 5        | 0.25          |
| (1,1528) | 1:51:A:ASP:H    | 1:52:A:GLY:HA3  | 5        | 0.25          |
| (1,1528) | 1:51:A:ASP:H    | 1:52:A:GLY:HA2  | 14       | 0.25          |
| (1,1528) | 1:51:A:ASP:H    | 1:52:A:GLY:HA3  | 14       | 0.25          |
| (1,1528) | 1:51:A:ASP:H    | 1:52:A:GLY:HA2  | 20       | 0.25          |
| (1,1528) | 1:51:A:ASP:H    | 1:52:A:GLY:HA3  | 20       | 0.25          |
| (1,1472) | 1:34:A:THR:HG23 | 1:35:A:SER:HB2  | 4        | 0.25          |
| (1,1472) | 1:34:A:THR:HG23 | 1:35:A:SER:HB3  | 4        | 0.25          |
| (1,1190) | 1:25:A:THR:HG22 | 1:40:A:GLN:H    | 11       | 0.25          |
| (1,1190) | 1:25:A:THR:HG22 | 1:40:A:GLN:H    | 12       | 0.25          |
| (1,1135) | 1:25:A:THR:H    | 1:43:A:MET:HE3  | 17       | 0.25          |
| (1,1125) | 1:21:A:LEU:HG   | 1:22:A:SER:H    | 7        | 0.25          |
| (1,999)  | 1:24:A:LEU:H    | 1:24:A:LEU:HD22 | 8        | 0.25          |
| (1,999)  | 1:24:A:LEU:H    | 1:24:A:LEU:HD22 | 9        | 0.25          |
| (1,999)  | 1:24:A:LEU:H    | 1:24:A:LEU:HD22 | 11       | 0.25          |
| (1,988)  | 1:34:A:THR:H    | 1:34:A:THR:HG23 | 1        | 0.25          |
| (1,988)  | 1:34:A:THR:H    | 1:34:A:THR:HG23 | 16       | 0.25          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,850)  | 1:31:A:LEU:HB3  | 1:76:A:VAL:HG23 | 10       | 0.25          |
| (1,693)  | 1:46:A:ILE:HG21 | 1:58:A:GLU:HB3  | 3        | 0.25          |
| (1,693)  | 1:46:A:ILE:HG21 | 1:58:A:GLU:HB3  | 19       | 0.25          |
| (1,611)  | 1:52:A:GLY:HA3  | 1:53:A:PHE:HD1  | 7        | 0.25          |
| (1,611)  | 1:52:A:GLY:HA2  | 1:53:A:PHE:HD1  | 7        | 0.25          |
| (1,611)  | 1:52:A:GLY:HA3  | 1:53:A:PHE:HD1  | 19       | 0.25          |
| (1,611)  | 1:52:A:GLY:HA2  | 1:53:A:PHE:HD1  | 19       | 0.25          |
| (1,417)  | 1:28:A:LEU:HD22 | 1:33:A:SER:HA   | 1        | 0.25          |
| (1,417)  | 1:28:A:LEU:HD22 | 1:33:A:SER:HA   | 9        | 0.25          |
| (1,417)  | 1:28:A:LEU:HD22 | 1:33:A:SER:HA   | 17       | 0.25          |
| (1,365)  | 1:28:A:LEU:HA   | 1:28:A:LEU:HD21 | 19       | 0.25          |
| (1,268)  | 1:19:A:ILE:HD11 | 1:59:A:PHE:HD2  | 3        | 0.25          |
| (1,1530) | 1:52:A:GLY:HA2  | 1:53:A:PHE:H    | 1        | 0.24          |
| (1,1530) | 1:52:A:GLY:HA3  | 1:53:A:PHE:H    | 1        | 0.24          |
| (1,1530) | 1:52:A:GLY:HA2  | 1:53:A:PHE:H    | 6        | 0.24          |
| (1,1530) | 1:52:A:GLY:HA3  | 1:53:A:PHE:H    | 6        | 0.24          |
| (1,1530) | 1:52:A:GLY:HA2  | 1:53:A:PHE:H    | 9        | 0.24          |
| (1,1530) | 1:52:A:GLY:HA3  | 1:53:A:PHE:H    | 9        | 0.24          |
| (1,1530) | 1:52:A:GLY:HA2  | 1:53:A:PHE:H    | 12       | 0.24          |
| (1,1530) | 1:52:A:GLY:HA3  | 1:53:A:PHE:H    | 12       | 0.24          |
| (1,1530) | 1:52:A:GLY:HA2  | 1:53:A:PHE:H    | 14       | 0.24          |
| (1,1530) | 1:52:A:GLY:HA3  | 1:53:A:PHE:H    | 14       | 0.24          |
| (1,1530) | 1:52:A:GLY:HA2  | 1:53:A:PHE:H    | 20       | 0.24          |
| (1,1530) | 1:52:A:GLY:HA3  | 1:53:A:PHE:H    | 20       | 0.24          |
| (1,1528) | 1:51:A:ASP:H    | 1:52:A:GLY:HA2  | 11       | 0.24          |
| (1,1528) | 1:51:A:ASP:H    | 1:52:A:GLY:HA3  | 11       | 0.24          |
| (1,1472) | 1:34:A:THR:HG23 | 1:35:A:SER:HB2  | 17       | 0.24          |
| (1,1472) | 1:34:A:THR:HG23 | 1:35:A:SER:HB3  | 17       | 0.24          |
| (1,1190) | 1:25:A:THR:HG22 | 1:40:A:GLN:H    | 18       | 0.24          |
| (1,1125) | 1:21:A:LEU:HG   | 1:22:A:SER:H    | 10       | 0.24          |
| (1,1125) | 1:21:A:LEU:HG   | 1:22:A:SER:H    | 15       | 0.24          |
| (1,1052) | 1:7:A:ILE:HD13  | 1:8:A:PHE:H     | 6        | 0.24          |
| (1,1010) | 1:42:A:MET:HG2  | 1:44:A:ALA:H    | 9        | 0.24          |
| (1,1010) | 1:42:A:MET:HG2  | 1:44:A:ALA:H    | 10       | 0.24          |
| (1,999)  | 1:24:A:LEU:H    | 1:24:A:LEU:HD22 | 16       | 0.24          |
| (1,999)  | 1:24:A:LEU:H    | 1:24:A:LEU:HD22 | 19       | 0.24          |
| (1,866)  | 1:4:A:MET:HE3   | 1:7:A:ILE:HD11  | 5        | 0.24          |
| (1,866)  | 1:4:A:MET:HE3   | 1:7:A:ILE:HD13  | 5        | 0.24          |
| (1,787)  | 1:69:A:LEU:HA   | 1:69:A:LEU:HG   | 2        | 0.24          |
| (1,787)  | 1:69:A:LEU:HA   | 1:69:A:LEU:HG   | 3        | 0.24          |
| (1,787)  | 1:69:A:LEU:HA   | 1:69:A:LEU:HG   | 9        | 0.24          |
| (1,739)  | 1:62:A:PHE:HB3  | 1:62:A:PHE:HD2  | 13       | 0.24          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,739)  | 1:62:A:PHE:HB2  | 1:62:A:PHE:HD1  | 13       | 0.24          |
| (1,739)  | 1:62:A:PHE:HB3  | 1:62:A:PHE:HD2  | 14       | 0.24          |
| (1,739)  | 1:62:A:PHE:HB2  | 1:62:A:PHE:HD1  | 14       | 0.24          |
| (1,731)  | 1:60:A:ILE:HA   | 1:60:A:ILE:HD12 | 12       | 0.24          |
| (1,693)  | 1:46:A:ILE:HG21 | 1:58:A:GLU:HB3  | 1        | 0.24          |
| (1,693)  | 1:46:A:ILE:HG21 | 1:58:A:GLU:HB3  | 2        | 0.24          |
| (1,693)  | 1:46:A:ILE:HG21 | 1:58:A:GLU:HB3  | 7        | 0.24          |
| (1,693)  | 1:46:A:ILE:HG21 | 1:58:A:GLU:HB3  | 8        | 0.24          |
| (1,693)  | 1:46:A:ILE:HG21 | 1:58:A:GLU:HB3  | 9        | 0.24          |
| (1,693)  | 1:46:A:ILE:HG21 | 1:58:A:GLU:HB3  | 14       | 0.24          |
| (1,693)  | 1:46:A:ILE:HG21 | 1:58:A:GLU:HB3  | 16       | 0.24          |
| (1,693)  | 1:46:A:ILE:HG21 | 1:58:A:GLU:HB3  | 17       | 0.24          |
| (1,611)  | 1:52:A:GLY:HA3  | 1:53:A:PHE:HD1  | 15       | 0.24          |
| (1,611)  | 1:52:A:GLY:HA2  | 1:53:A:PHE:HD1  | 15       | 0.24          |
| (1,433)  | 1:34:A:THR:HA   | 1:34:A:THR:HG23 | 4        | 0.24          |
| (1,433)  | 1:34:A:THR:HA   | 1:34:A:THR:HG23 | 9        | 0.24          |
| (1,433)  | 1:34:A:THR:HA   | 1:34:A:THR:HG23 | 17       | 0.24          |
| (1,365)  | 1:28:A:LEU:HA   | 1:28:A:LEU:HD21 | 15       | 0.24          |
| (1,365)  | 1:28:A:LEU:HA   | 1:28:A:LEU:HD21 | 20       | 0.24          |
| (1,337)  | 1:24:A:LEU:HD22 | 1:27:A:ALA:HB1  | 19       | 0.24          |
| (1,268)  | 1:19:A:ILE:HD11 | 1:59:A:PHE:HD2  | 17       | 0.24          |
| (1,268)  | 1:19:A:ILE:HD11 | 1:59:A:PHE:HD2  | 20       | 0.24          |
| (1,199)  | 1:8:A:PHE:HE1   | 1:18:A:LYS:HA   | 4        | 0.24          |
| (1,16)   | 1:42:A:MET:HG2  | 1:62:A:PHE:HE1  | 12       | 0.24          |
| (1,1537) | 1:55:A:ASP:HA   | 1:55:A:ASP:HB2  | 1        | 0.23          |
| (1,1537) | 1:55:A:ASP:HA   | 1:55:A:ASP:HB3  | 1        | 0.23          |
| (1,1537) | 1:55:A:ASP:HA   | 1:55:A:ASP:HB2  | 4        | 0.23          |
| (1,1537) | 1:55:A:ASP:HA   | 1:55:A:ASP:HB3  | 4        | 0.23          |
| (1,1537) | 1:55:A:ASP:HA   | 1:55:A:ASP:HB2  | 5        | 0.23          |
| (1,1537) | 1:55:A:ASP:HA   | 1:55:A:ASP:HB3  | 5        | 0.23          |
| (1,1537) | 1:55:A:ASP:HA   | 1:55:A:ASP:HB2  | 6        | 0.23          |
| (1,1537) | 1:55:A:ASP:HA   | 1:55:A:ASP:HB3  | 6        | 0.23          |
| (1,1530) | 1:52:A:GLY:HA2  | 1:53:A:PHE:H    | 16       | 0.23          |
| (1,1530) | 1:52:A:GLY:HA3  | 1:53:A:PHE:H    | 16       | 0.23          |
| (1,1530) | 1:52:A:GLY:HA2  | 1:53:A:PHE:H    | 17       | 0.23          |
| (1,1530) | 1:52:A:GLY:HA3  | 1:53:A:PHE:H    | 17       | 0.23          |
| (1,1528) | 1:51:A:ASP:H    | 1:52:A:GLY:HA2  | 12       | 0.23          |
| (1,1528) | 1:51:A:ASP:H    | 1:52:A:GLY:HA3  | 12       | 0.23          |
| (1,1262) | 1:53:A:PHE:HB2  | 1:54:A:ILE:H    | 4        | 0.23          |
| (1,1262) | 1:53:A:PHE:HB2  | 1:54:A:ILE:H    | 6        | 0.23          |
| (1,1238) | 1:48:A:THR:H    | 1:48:A:THR:HG22 | 5        | 0.23          |
| (1,1238) | 1:48:A:THR:H    | 1:48:A:THR:HG22 | 13       | 0.23          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1190) | 1:25:A:THR:HG22 | 1:40:A:GLN:H    | 1        | 0.23          |
| (1,1190) | 1:25:A:THR:HG22 | 1:40:A:GLN:H    | 6        | 0.23          |
| (1,1022) | 1:31:A:LEU:H    | 1:31:A:LEU:HD21 | 14       | 0.23          |
| (1,1010) | 1:42:A:MET:HG2  | 1:44:A:ALA:H    | 11       | 0.23          |
| (1,1010) | 1:42:A:MET:HG2  | 1:44:A:ALA:H    | 16       | 0.23          |
| (1,999)  | 1:24:A:LEU:H    | 1:24:A:LEU:HD22 | 1        | 0.23          |
| (1,999)  | 1:24:A:LEU:H    | 1:24:A:LEU:HD22 | 14       | 0.23          |
| (1,999)  | 1:24:A:LEU:H    | 1:24:A:LEU:HD22 | 15       | 0.23          |
| (1,988)  | 1:34:A:THR:H    | 1:34:A:THR:HG23 | 12       | 0.23          |
| (1,866)  | 1:4:A:MET:HE3   | 1:7:A:ILE:HD11  | 2        | 0.23          |
| (1,866)  | 1:4:A:MET:HE3   | 1:7:A:ILE:HD13  | 2        | 0.23          |
| (1,787)  | 1:69:A:LEU:HA   | 1:69:A:LEU:HG   | 4        | 0.23          |
| (1,787)  | 1:69:A:LEU:HA   | 1:69:A:LEU:HG   | 7        | 0.23          |
| (1,787)  | 1:69:A:LEU:HA   | 1:69:A:LEU:HG   | 8        | 0.23          |
| (1,739)  | 1:62:A:PHE:HB3  | 1:62:A:PHE:HD2  | 18       | 0.23          |
| (1,739)  | 1:62:A:PHE:HB2  | 1:62:A:PHE:HD1  | 18       | 0.23          |
| (1,734)  | 1:60:A:ILE:HB   | 1:60:A:ILE:HD12 | 14       | 0.23          |
| (1,734)  | 1:60:A:ILE:HB   | 1:60:A:ILE:HD12 | 15       | 0.23          |
| (1,734)  | 1:60:A:ILE:HB   | 1:60:A:ILE:HD12 | 20       | 0.23          |
| (1,695)  | 1:46:A:ILE:HD11 | 1:58:A:GLU:HB3  | 4        | 0.23          |
| (1,693)  | 1:46:A:ILE:HG21 | 1:58:A:GLU:HB3  | 4        | 0.23          |
| (1,693)  | 1:46:A:ILE:HG21 | 1:58:A:GLU:HB3  | 6        | 0.23          |
| (1,611)  | 1:52:A:GLY:HA3  | 1:53:A:PHE:HD1  | 18       | 0.23          |
| (1,611)  | 1:52:A:GLY:HA2  | 1:53:A:PHE:HD1  | 18       | 0.23          |
| (1,427)  | 1:28:A:LEU:HB2  | 1:33:A:SER:HB2  | 16       | 0.23          |
| (1,320)  | 1:11:A:PHE:HE1  | 1:24:A:LEU:HB2  | 6        | 0.23          |
| (1,170)  | 1:48:A:THR:HB   | 1:49:A:ASP:H    | 10       | 0.23          |
| (1,170)  | 1:48:A:THR:HB   | 1:49:A:ASP:H    | 18       | 0.23          |
| (1,1239) | 1:21:A:LEU:HD22 | 1:48:A:THR:H    | 20       | 0.22          |
| (1,1239) | 1:21:A:LEU:HD23 | 1:48:A:THR:H    | 20       | 0.22          |
| (1,1192) | 1:40:A:GLN:HE22 | 1:41:A:ARG:H    | 13       | 0.22          |
| (1,1192) | 1:40:A:GLN:HE22 | 1:41:A:ARG:H    | 14       | 0.22          |
| (1,1190) | 1:25:A:THR:HG22 | 1:40:A:GLN:H    | 17       | 0.22          |
| (1,1190) | 1:25:A:THR:HG22 | 1:40:A:GLN:H    | 19       | 0.22          |
| (1,1168) | 1:28:A:LEU:HD21 | 1:33:A:SER:H    | 1        | 0.22          |
| (1,1125) | 1:21:A:LEU:HG   | 1:22:A:SER:H    | 19       | 0.22          |
| (1,1052) | 1:7:A:ILE:HD13  | 1:8:A:PHE:H     | 15       | 0.22          |
| (1,1022) | 1:31:A:LEU:H    | 1:31:A:LEU:HD21 | 3        | 0.22          |
| (1,1010) | 1:42:A:MET:HG2  | 1:44:A:ALA:H    | 1        | 0.22          |
| (1,1010) | 1:42:A:MET:HG2  | 1:44:A:ALA:H    | 4        | 0.22          |
| (1,1010) | 1:42:A:MET:HG2  | 1:44:A:ALA:H    | 6        | 0.22          |
| (1,1010) | 1:42:A:MET:HG2  | 1:44:A:ALA:H    | 17       | 0.22          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1010) | 1:42:A:MET:HG2  | 1:44:A:ALA:H    | 18       | 0.22          |
| (1,1010) | 1:42:A:MET:HG2  | 1:44:A:ALA:H    | 19       | 0.22          |
| (1,989)  | 1:46:A:ILE:HD11 | 1:59:A:PHE:H    | 16       | 0.22          |
| (1,988)  | 1:34:A:THR:H    | 1:34:A:THR:HG23 | 3        | 0.22          |
| (1,866)  | 1:4:A:MET:HE3   | 1:7:A:ILE:HD11  | 1        | 0.22          |
| (1,866)  | 1:4:A:MET:HE3   | 1:7:A:ILE:HD13  | 1        | 0.22          |
| (1,787)  | 1:69:A:LEU:HA   | 1:69:A:LEU:HG   | 6        | 0.22          |
| (1,787)  | 1:69:A:LEU:HA   | 1:69:A:LEU:HG   | 11       | 0.22          |
| (1,787)  | 1:69:A:LEU:HA   | 1:69:A:LEU:HG   | 15       | 0.22          |
| (1,787)  | 1:69:A:LEU:HA   | 1:69:A:LEU:HG   | 17       | 0.22          |
| (1,787)  | 1:69:A:LEU:HA   | 1:69:A:LEU:HG   | 19       | 0.22          |
| (1,734)  | 1:60:A:ILE:HB   | 1:60:A:ILE:HD12 | 13       | 0.22          |
| (1,731)  | 1:60:A:ILE:HA   | 1:60:A:ILE:HD12 | 11       | 0.22          |
| (1,695)  | 1:46:A:ILE:HD11 | 1:58:A:GLU:HB3  | 17       | 0.22          |
| (1,693)  | 1:46:A:ILE:HG21 | 1:58:A:GLU:HB3  | 13       | 0.22          |
| (1,693)  | 1:46:A:ILE:HG21 | 1:58:A:GLU:HB3  | 20       | 0.22          |
| (1,320)  | 1:11:A:PHE:HE1  | 1:24:A:LEU:HB2  | 4        | 0.22          |
| (1,313)  | 1:69:A:LEU:HB2  | 1:69:A:LEU:HD21 | 18       | 0.22          |
| (1,268)  | 1:19:A:ILE:HD11 | 1:59:A:PHE:HD2  | 9        | 0.22          |
| (1,1530) | 1:52:A:GLY:HA2  | 1:53:A:PHE:H    | 11       | 0.21          |
| (1,1530) | 1:52:A:GLY:HA3  | 1:53:A:PHE:H    | 11       | 0.21          |
| (1,1472) | 1:34:A:THR:HG23 | 1:35:A:SER:HB2  | 9        | 0.21          |
| (1,1472) | 1:34:A:THR:HG23 | 1:35:A:SER:HB3  | 9        | 0.21          |
| (1,1472) | 1:34:A:THR:HG23 | 1:35:A:SER:HB2  | 16       | 0.21          |
| (1,1472) | 1:34:A:THR:HG23 | 1:35:A:SER:HB3  | 16       | 0.21          |
| (1,1262) | 1:53:A:PHE:HB2  | 1:54:A:ILE:H    | 8        | 0.21          |
| (1,1262) | 1:53:A:PHE:HB2  | 1:54:A:ILE:H    | 17       | 0.21          |
| (1,1192) | 1:40:A:GLN:HE22 | 1:41:A:ARG:H    | 5        | 0.21          |
| (1,1192) | 1:40:A:GLN:HE22 | 1:41:A:ARG:H    | 11       | 0.21          |
| (1,1192) | 1:40:A:GLN:HE22 | 1:41:A:ARG:H    | 17       | 0.21          |
| (1,1192) | 1:40:A:GLN:HE22 | 1:41:A:ARG:H    | 18       | 0.21          |
| (1,1190) | 1:25:A:THR:HG22 | 1:40:A:GLN:H    | 4        | 0.21          |
| (1,1173) | 1:34:A:THR:HG23 | 1:35:A:SER:H    | 9        | 0.21          |
| (1,1168) | 1:28:A:LEU:HD21 | 1:33:A:SER:H    | 15       | 0.21          |
| (1,1052) | 1:7:A:ILE:HD13  | 1:8:A:PHE:H     | 1        | 0.21          |
| (1,1052) | 1:7:A:ILE:HD13  | 1:8:A:PHE:H     | 7        | 0.21          |
| (1,1010) | 1:42:A:MET:HG2  | 1:44:A:ALA:H    | 2        | 0.21          |
| (1,1010) | 1:42:A:MET:HG2  | 1:44:A:ALA:H    | 3        | 0.21          |
| (1,1010) | 1:42:A:MET:HG2  | 1:44:A:ALA:H    | 7        | 0.21          |
| (1,1010) | 1:42:A:MET:HG2  | 1:44:A:ALA:H    | 8        | 0.21          |
| (1,1010) | 1:42:A:MET:HG2  | 1:44:A:ALA:H    | 14       | 0.21          |
| (1,787)  | 1:69:A:LEU:HA   | 1:69:A:LEU:HG   | 5        | 0.21          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,787)  | 1:69:A:LEU:HA   | 1:69:A:LEU:HG   | 10       | 0.21          |
| (1,787)  | 1:69:A:LEU:HA   | 1:69:A:LEU:HG   | 20       | 0.21          |
| (1,739)  | 1:62:A:PHE:HB3  | 1:62:A:PHE:HD2  | 1        | 0.21          |
| (1,739)  | 1:62:A:PHE:HB2  | 1:62:A:PHE:HD1  | 1        | 0.21          |
| (1,739)  | 1:62:A:PHE:HB3  | 1:62:A:PHE:HD2  | 12       | 0.21          |
| (1,739)  | 1:62:A:PHE:HB2  | 1:62:A:PHE:HD1  | 12       | 0.21          |
| (1,731)  | 1:60:A:ILE:HA   | 1:60:A:ILE:HD12 | 5        | 0.21          |
| (1,731)  | 1:60:A:ILE:HA   | 1:60:A:ILE:HD12 | 10       | 0.21          |
| (1,695)  | 1:46:A:ILE:HD11 | 1:58:A:GLU:HB3  | 1        | 0.21          |
| (1,693)  | 1:46:A:ILE:HG21 | 1:58:A:GLU:HB3  | 10       | 0.21          |
| (1,693)  | 1:46:A:ILE:HG21 | 1:58:A:GLU:HB3  | 15       | 0.21          |
| (1,611)  | 1:52:A:GLY:HA3  | 1:53:A:PHE:HD1  | 5        | 0.21          |
| (1,611)  | 1:52:A:GLY:HA2  | 1:53:A:PHE:HD1  | 5        | 0.21          |
| (1,479)  | 1:36:A:ALA:HA   | 1:39:A:VAL:HG23 | 2        | 0.21          |
| (1,479)  | 1:36:A:ALA:HA   | 1:39:A:VAL:HG23 | 4        | 0.21          |
| (1,479)  | 1:36:A:ALA:HA   | 1:39:A:VAL:HG23 | 11       | 0.21          |
| (1,479)  | 1:36:A:ALA:HA   | 1:39:A:VAL:HG23 | 17       | 0.21          |
| (1,411)  | 1:30:A:THR:HG22 | 1:31:A:LEU:HG   | 3        | 0.21          |
| (1,365)  | 1:28:A:LEU:HA   | 1:28:A:LEU:HD21 | 14       | 0.21          |
| (1,313)  | 1:69:A:LEU:HB2  | 1:69:A:LEU:HD21 | 14       | 0.21          |
| (1,307)  | 1:24:A:LEU:HA   | 1:24:A:LEU:HD21 | 2        | 0.21          |
| (1,307)  | 1:24:A:LEU:HA   | 1:24:A:LEU:HD21 | 3        | 0.21          |
| (1,307)  | 1:24:A:LEU:HA   | 1:24:A:LEU:HD21 | 4        | 0.21          |
| (1,307)  | 1:24:A:LEU:HA   | 1:24:A:LEU:HD21 | 5        | 0.21          |
| (1,307)  | 1:24:A:LEU:HA   | 1:24:A:LEU:HD21 | 6        | 0.21          |
| (1,307)  | 1:24:A:LEU:HA   | 1:24:A:LEU:HD21 | 7        | 0.21          |
| (1,307)  | 1:24:A:LEU:HA   | 1:24:A:LEU:HD21 | 10       | 0.21          |
| (1,307)  | 1:24:A:LEU:HA   | 1:24:A:LEU:HD21 | 12       | 0.21          |
| (1,307)  | 1:24:A:LEU:HA   | 1:24:A:LEU:HD21 | 13       | 0.21          |
| (1,307)  | 1:24:A:LEU:HA   | 1:24:A:LEU:HD21 | 20       | 0.21          |
| (1,268)  | 1:19:A:ILE:HD11 | 1:59:A:PHE:HD2  | 10       | 0.21          |
| (1,1530) | 1:52:A:GLY:HA2  | 1:53:A:PHE:H    | 5        | 0.2           |
| (1,1530) | 1:52:A:GLY:HA3  | 1:53:A:PHE:H    | 5        | 0.2           |
| (1,1453) | 1:23:A:GLU:HB2  | 1:27:A:ALA:HA   | 7        | 0.2           |
| (1,1453) | 1:23:A:GLU:HB3  | 1:27:A:ALA:HA   | 7        | 0.2           |
| (1,1453) | 1:23:A:GLU:HB2  | 1:27:A:ALA:HA   | 14       | 0.2           |
| (1,1453) | 1:23:A:GLU:HB3  | 1:27:A:ALA:HA   | 14       | 0.2           |
| (1,1365) | 1:4:A:MET:H     | 1:4:A:MET:HG2   | 14       | 0.2           |
| (1,1365) | 1:4:A:MET:H     | 1:4:A:MET:HG3   | 14       | 0.2           |
| (1,1262) | 1:53:A:PHE:HB2  | 1:54:A:ILE:H    | 9        | 0.2           |
| (1,1192) | 1:40:A:GLN:HE22 | 1:41:A:ARG:H    | 1        | 0.2           |
| (1,1192) | 1:40:A:GLN:HE22 | 1:41:A:ARG:H    | 9        | 0.2           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1192) | 1:40:A:GLN:HE22 | 1:41:A:ARG:H    | 10       | 0.2           |
| (1,1192) | 1:40:A:GLN:HE22 | 1:41:A:ARG:H    | 12       | 0.2           |
| (1,1192) | 1:40:A:GLN:HE22 | 1:41:A:ARG:H    | 15       | 0.2           |
| (1,1192) | 1:40:A:GLN:HE22 | 1:41:A:ARG:H    | 16       | 0.2           |
| (1,1190) | 1:25:A:THR:HG22 | 1:40:A:GLN:H    | 3        | 0.2           |
| (1,1190) | 1:25:A:THR:HG22 | 1:40:A:GLN:H    | 8        | 0.2           |
| (1,1125) | 1:21:A:LEU:HG   | 1:22:A:SER:H    | 13       | 0.2           |
| (1,1010) | 1:42:A:MET:HG2  | 1:44:A:ALA:H    | 5        | 0.2           |
| (1,1010) | 1:42:A:MET:HG2  | 1:44:A:ALA:H    | 20       | 0.2           |
| (1,952)  | 1:54:A:ILE:HG21 | 1:55:A:ASP:H    | 4        | 0.2           |
| (1,866)  | 1:4:A:MET:HE3   | 1:7:A:ILE:HD11  | 8        | 0.2           |
| (1,866)  | 1:4:A:MET:HE3   | 1:7:A:ILE:HD13  | 8        | 0.2           |
| (1,787)  | 1:69:A:LEU:HA   | 1:69:A:LEU:HG   | 12       | 0.2           |
| (1,787)  | 1:69:A:LEU:HA   | 1:69:A:LEU:HG   | 16       | 0.2           |
| (1,739)  | 1:62:A:PHE:HB3  | 1:62:A:PHE:HD2  | 16       | 0.2           |
| (1,739)  | 1:62:A:PHE:HB2  | 1:62:A:PHE:HD1  | 16       | 0.2           |
| (1,739)  | 1:62:A:PHE:HB3  | 1:62:A:PHE:HD2  | 17       | 0.2           |
| (1,739)  | 1:62:A:PHE:HB2  | 1:62:A:PHE:HD1  | 17       | 0.2           |
| (1,739)  | 1:62:A:PHE:HB3  | 1:62:A:PHE:HD2  | 20       | 0.2           |
| (1,739)  | 1:62:A:PHE:HB2  | 1:62:A:PHE:HD1  | 20       | 0.2           |
| (1,731)  | 1:60:A:ILE:HA   | 1:60:A:ILE:HD12 | 4        | 0.2           |
| (1,731)  | 1:60:A:ILE:HA   | 1:60:A:ILE:HD12 | 8        | 0.2           |
| (1,731)  | 1:60:A:ILE:HA   | 1:60:A:ILE:HD12 | 19       | 0.2           |
| (1,695)  | 1:46:A:ILE:HD11 | 1:58:A:GLU:HB3  | 14       | 0.2           |
| (1,693)  | 1:46:A:ILE:HG21 | 1:58:A:GLU:HB3  | 11       | 0.2           |
| (1,693)  | 1:46:A:ILE:HG21 | 1:58:A:GLU:HB3  | 12       | 0.2           |
| (1,693)  | 1:46:A:ILE:HG21 | 1:58:A:GLU:HB3  | 18       | 0.2           |
| (1,611)  | 1:52:A:GLY:HA3  | 1:53:A:PHE:HD1  | 1        | 0.2           |
| (1,611)  | 1:52:A:GLY:HA2  | 1:53:A:PHE:HD1  | 1        | 0.2           |
| (1,572)  | 1:46:A:ILE:HG22 | 1:62:A:PHE:HD1  | 12       | 0.2           |
| (1,572)  | 1:46:A:ILE:HG23 | 1:62:A:PHE:HD1  | 12       | 0.2           |
| (1,501)  | 1:42:A:MET:HB3  | 1:62:A:PHE:HD1  | 1        | 0.2           |
| (1,479)  | 1:36:A:ALA:HA   | 1:39:A:VAL:HG23 | 3        | 0.2           |
| (1,479)  | 1:36:A:ALA:HA   | 1:39:A:VAL:HG23 | 6        | 0.2           |
| (1,479)  | 1:36:A:ALA:HA   | 1:39:A:VAL:HG23 | 7        | 0.2           |
| (1,479)  | 1:36:A:ALA:HA   | 1:39:A:VAL:HG23 | 8        | 0.2           |
| (1,479)  | 1:36:A:ALA:HA   | 1:39:A:VAL:HG23 | 9        | 0.2           |
| (1,479)  | 1:36:A:ALA:HA   | 1:39:A:VAL:HG23 | 19       | 0.2           |
| (1,417)  | 1:28:A:LEU:HD22 | 1:33:A:SER:HA   | 18       | 0.2           |
| (1,320)  | 1:11:A:PHE:HE1  | 1:24:A:LEU:HB2  | 7        | 0.2           |
| (1,307)  | 1:24:A:LEU:HA   | 1:24:A:LEU:HD21 | 17       | 0.2           |
| (1,307)  | 1:24:A:LEU:HA   | 1:24:A:LEU:HD21 | 18       | 0.2           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,7)    | 1:3:A:ASP:HB2   | 1:4:A:MET:HE3   | 3        | 0.2           |
| (1,7)    | 1:3:A:ASP:HB3   | 1:4:A:MET:HE3   | 3        | 0.2           |
| (1,7)    | 1:3:A:ASP:HB2   | 1:4:A:MET:HE3   | 6        | 0.2           |
| (1,7)    | 1:3:A:ASP:HB3   | 1:4:A:MET:HE3   | 6        | 0.2           |
| (1,1472) | 1:34:A:THR:HG23 | 1:35:A:SER:HB2  | 8        | 0.19          |
| (1,1472) | 1:34:A:THR:HG23 | 1:35:A:SER:HB3  | 8        | 0.19          |
| (1,1453) | 1:23:A:GLU:HB2  | 1:27:A:ALA:HA   | 1        | 0.19          |
| (1,1453) | 1:23:A:GLU:HB3  | 1:27:A:ALA:HA   | 1        | 0.19          |
| (1,1453) | 1:23:A:GLU:HB2  | 1:27:A:ALA:HA   | 18       | 0.19          |
| (1,1453) | 1:23:A:GLU:HB3  | 1:27:A:ALA:HA   | 18       | 0.19          |
| (1,1365) | 1:4:A:MET:H     | 1:4:A:MET:HG2   | 20       | 0.19          |
| (1,1365) | 1:4:A:MET:H     | 1:4:A:MET:HG3   | 20       | 0.19          |
| (1,1262) | 1:53:A:PHE:HB2  | 1:54:A:ILE:H    | 14       | 0.19          |
| (1,1262) | 1:53:A:PHE:HB2  | 1:54:A:ILE:H    | 16       | 0.19          |
| (1,1192) | 1:40:A:GLN:HE22 | 1:41:A:ARG:H    | 6        | 0.19          |
| (1,1192) | 1:40:A:GLN:HE22 | 1:41:A:ARG:H    | 20       | 0.19          |
| (1,1190) | 1:25:A:THR:HG22 | 1:40:A:GLN:H    | 10       | 0.19          |
| (1,1173) | 1:34:A:THR:HG23 | 1:35:A:SER:H    | 13       | 0.19          |
| (1,1052) | 1:7:A:ILE:HD13  | 1:8:A:PHE:H     | 5        | 0.19          |
| (1,1052) | 1:7:A:ILE:HD13  | 1:8:A:PHE:H     | 18       | 0.19          |
| (1,1052) | 1:7:A:ILE:HD13  | 1:8:A:PHE:H     | 19       | 0.19          |
| (1,1010) | 1:42:A:MET:HG2  | 1:44:A:ALA:H    | 12       | 0.19          |
| (1,952)  | 1:54:A:ILE:HG21 | 1:55:A:ASP:H    | 1        | 0.19          |
| (1,787)  | 1:69:A:LEU:HA   | 1:69:A:LEU:HG   | 1        | 0.19          |
| (1,787)  | 1:69:A:LEU:HA   | 1:69:A:LEU:HG   | 13       | 0.19          |
| (1,739)  | 1:62:A:PHE:HB3  | 1:62:A:PHE:HD2  | 5        | 0.19          |
| (1,739)  | 1:62:A:PHE:HB2  | 1:62:A:PHE:HD1  | 5        | 0.19          |
| (1,739)  | 1:62:A:PHE:HB3  | 1:62:A:PHE:HD2  | 6        | 0.19          |
| (1,739)  | 1:62:A:PHE:HB2  | 1:62:A:PHE:HD1  | 6        | 0.19          |
| (1,739)  | 1:62:A:PHE:HB3  | 1:62:A:PHE:HD2  | 9        | 0.19          |
| (1,739)  | 1:62:A:PHE:HB2  | 1:62:A:PHE:HD1  | 9        | 0.19          |
| (1,739)  | 1:62:A:PHE:HB3  | 1:62:A:PHE:HD2  | 11       | 0.19          |
| (1,739)  | 1:62:A:PHE:HB2  | 1:62:A:PHE:HD1  | 11       | 0.19          |
| (1,731)  | 1:60:A:ILE:HA   | 1:60:A:ILE:HD12 | 2        | 0.19          |
| (1,731)  | 1:60:A:ILE:HA   | 1:60:A:ILE:HD12 | 3        | 0.19          |
| (1,731)  | 1:60:A:ILE:HA   | 1:60:A:ILE:HD12 | 6        | 0.19          |
| (1,695)  | 1:46:A:ILE:HD11 | 1:58:A:GLU:HB3  | 2        | 0.19          |
| (1,695)  | 1:46:A:ILE:HD11 | 1:58:A:GLU:HB3  | 16       | 0.19          |
| (1,611)  | 1:52:A:GLY:HA3  | 1:53:A:PHE:HD1  | 4        | 0.19          |
| (1,611)  | 1:52:A:GLY:HA2  | 1:53:A:PHE:HD1  | 4        | 0.19          |
| (1,611)  | 1:52:A:GLY:HA3  | 1:53:A:PHE:HD1  | 6        | 0.19          |
| (1,611)  | 1:52:A:GLY:HA2  | 1:53:A:PHE:HD1  | 6        | 0.19          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,572)  | 1:46:A:ILE:HG22 | 1:62:A:PHE:HD1  | 11       | 0.19          |
| (1,572)  | 1:46:A:ILE:HG23 | 1:62:A:PHE:HD1  | 11       | 0.19          |
| (1,479)  | 1:36:A:ALA:HA   | 1:39:A:VAL:HG23 | 5        | 0.19          |
| (1,479)  | 1:36:A:ALA:HA   | 1:39:A:VAL:HG23 | 10       | 0.19          |
| (1,479)  | 1:36:A:ALA:HA   | 1:39:A:VAL:HG23 | 15       | 0.19          |
| (1,479)  | 1:36:A:ALA:HA   | 1:39:A:VAL:HG23 | 16       | 0.19          |
| (1,417)  | 1:28:A:LEU:HD22 | 1:33:A:SER:HA   | 19       | 0.19          |
| (1,338)  | 1:24:A:LEU:HB3  | 1:24:A:LEU:HD21 | 2        | 0.19          |
| (1,338)  | 1:24:A:LEU:HB3  | 1:24:A:LEU:HD21 | 3        | 0.19          |
| (1,338)  | 1:24:A:LEU:HB3  | 1:24:A:LEU:HD21 | 4        | 0.19          |
| (1,338)  | 1:24:A:LEU:HB3  | 1:24:A:LEU:HD21 | 5        | 0.19          |
| (1,338)  | 1:24:A:LEU:HB3  | 1:24:A:LEU:HD21 | 6        | 0.19          |
| (1,338)  | 1:24:A:LEU:HB3  | 1:24:A:LEU:HD21 | 7        | 0.19          |
| (1,338)  | 1:24:A:LEU:HB3  | 1:24:A:LEU:HD21 | 10       | 0.19          |
| (1,338)  | 1:24:A:LEU:HB3  | 1:24:A:LEU:HD21 | 12       | 0.19          |
| (1,338)  | 1:24:A:LEU:HB3  | 1:24:A:LEU:HD21 | 13       | 0.19          |
| (1,338)  | 1:24:A:LEU:HB3  | 1:24:A:LEU:HD21 | 17       | 0.19          |
| (1,338)  | 1:24:A:LEU:HB3  | 1:24:A:LEU:HD21 | 18       | 0.19          |
| (1,338)  | 1:24:A:LEU:HB3  | 1:24:A:LEU:HD21 | 20       | 0.19          |
| (1,321)  | 1:24:A:LEU:HB2  | 1:24:A:LEU:HD21 | 1        | 0.19          |
| (1,321)  | 1:24:A:LEU:HB2  | 1:24:A:LEU:HD21 | 14       | 0.19          |
| (1,321)  | 1:24:A:LEU:HB2  | 1:24:A:LEU:HD21 | 15       | 0.19          |
| (1,16)   | 1:42:A:MET:HG2  | 1:62:A:PHE:HE1  | 16       | 0.19          |
| (1,1262) | 1:53:A:PHE:HB2  | 1:54:A:ILE:H    | 2        | 0.18          |
| (1,1262) | 1:53:A:PHE:HB2  | 1:54:A:ILE:H    | 11       | 0.18          |
| (1,1262) | 1:53:A:PHE:HB2  | 1:54:A:ILE:H    | 20       | 0.18          |
| (1,1192) | 1:40:A:GLN:HE22 | 1:41:A:ARG:H    | 2        | 0.18          |
| (1,1190) | 1:25:A:THR:HG22 | 1:40:A:GLN:H    | 9        | 0.18          |
| (1,1190) | 1:25:A:THR:HG22 | 1:40:A:GLN:H    | 15       | 0.18          |
| (1,1125) | 1:21:A:LEU:HG   | 1:22:A:SER:H    | 11       | 0.18          |
| (1,1125) | 1:21:A:LEU:HG   | 1:22:A:SER:H    | 12       | 0.18          |
| (1,1052) | 1:7:A:ILE:HD13  | 1:8:A:PHE:H     | 3        | 0.18          |
| (1,1052) | 1:7:A:ILE:HD13  | 1:8:A:PHE:H     | 12       | 0.18          |
| (1,1010) | 1:42:A:MET:HG2  | 1:44:A:ALA:H    | 13       | 0.18          |
| (1,988)  | 1:34:A:THR:H    | 1:34:A:THR:HG23 | 2        | 0.18          |
| (1,988)  | 1:34:A:THR:H    | 1:34:A:THR:HG23 | 6        | 0.18          |
| (1,952)  | 1:54:A:ILE:HG21 | 1:55:A:ASP:H    | 3        | 0.18          |
| (1,850)  | 1:31:A:LEU:HB3  | 1:76:A:VAL:HG23 | 11       | 0.18          |
| (1,762)  | 1:60:A:ILE:HG12 | 1:63:A:CYS:HB3  | 17       | 0.18          |
| (1,739)  | 1:62:A:PHE:HB3  | 1:62:A:PHE:HD2  | 4        | 0.18          |
| (1,739)  | 1:62:A:PHE:HB2  | 1:62:A:PHE:HD1  | 4        | 0.18          |
| (1,739)  | 1:62:A:PHE:HB3  | 1:62:A:PHE:HD2  | 15       | 0.18          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,739)  | 1:62:A:PHE:HB2  | 1:62:A:PHE:HD1  | 15       | 0.18          |
| (1,734)  | 1:60:A:ILE:HB   | 1:60:A:ILE:HD12 | 9        | 0.18          |
| (1,731)  | 1:60:A:ILE:HA   | 1:60:A:ILE:HD12 | 1        | 0.18          |
| (1,731)  | 1:60:A:ILE:HA   | 1:60:A:ILE:HD12 | 7        | 0.18          |
| (1,483)  | 1:37:A:ASP:HA   | 1:40:A:GLN:HA   | 11       | 0.18          |
| (1,483)  | 1:37:A:ASP:HA   | 1:40:A:GLN:HA   | 14       | 0.18          |
| (1,483)  | 1:37:A:ASP:HA   | 1:40:A:GLN:HA   | 20       | 0.18          |
| (1,479)  | 1:36:A:ALA:HA   | 1:39:A:VAL:HG23 | 12       | 0.18          |
| (1,479)  | 1:36:A:ALA:HA   | 1:39:A:VAL:HG23 | 20       | 0.18          |
| (1,433)  | 1:34:A:THR:HA   | 1:34:A:THR:HG23 | 13       | 0.18          |
| (1,417)  | 1:28:A:LEU:HD22 | 1:33:A:SER:HA   | 5        | 0.18          |
| (1,417)  | 1:28:A:LEU:HD22 | 1:33:A:SER:HA   | 16       | 0.18          |
| (1,377)  | 1:28:A:LEU:HB3  | 1:36:A:ALA:H    | 16       | 0.18          |
| (1,326)  | 1:24:A:LEU:HA   | 1:24:A:LEU:HG   | 2        | 0.18          |
| (1,326)  | 1:24:A:LEU:HA   | 1:24:A:LEU:HG   | 6        | 0.18          |
| (1,326)  | 1:24:A:LEU:HA   | 1:24:A:LEU:HG   | 12       | 0.18          |
| (1,326)  | 1:24:A:LEU:HA   | 1:24:A:LEU:HG   | 13       | 0.18          |
| (1,326)  | 1:24:A:LEU:HA   | 1:24:A:LEU:HG   | 20       | 0.18          |
| (1,321)  | 1:24:A:LEU:HB2  | 1:24:A:LEU:HD21 | 16       | 0.18          |
| (1,321)  | 1:24:A:LEU:HB2  | 1:24:A:LEU:HD21 | 19       | 0.18          |
| (1,1510) | 1:46:A:ILE:HG21 | 1:58:A:GLU:HG2  | 10       | 0.17          |
| (1,1510) | 1:46:A:ILE:HG21 | 1:58:A:GLU:HG3  | 10       | 0.17          |
| (1,1262) | 1:53:A:PHE:HB2  | 1:54:A:ILE:H    | 1        | 0.17          |
| (1,1262) | 1:53:A:PHE:HB2  | 1:54:A:ILE:H    | 5        | 0.17          |
| (1,1192) | 1:40:A:GLN:HE22 | 1:41:A:ARG:H    | 4        | 0.17          |
| (1,1125) | 1:21:A:LEU:HG   | 1:22:A:SER:H    | 5        | 0.17          |
| (1,1052) | 1:7:A:ILE:HD13  | 1:8:A:PHE:H     | 11       | 0.17          |
| (1,952)  | 1:54:A:ILE:HG21 | 1:55:A:ASP:H    | 2        | 0.17          |
| (1,952)  | 1:54:A:ILE:HG21 | 1:55:A:ASP:H    | 6        | 0.17          |
| (1,880)  | 1:77:A:PHE:H    | 1:77:A:PHE:HB3  | 9        | 0.17          |
| (1,841)  | 1:72:A:ASP:H    | 1:74:A:ALA:HB3  | 9        | 0.17          |
| (1,762)  | 1:60:A:ILE:HG12 | 1:63:A:CYS:HB3  | 16       | 0.17          |
| (1,739)  | 1:62:A:PHE:HB3  | 1:62:A:PHE:HD2  | 8        | 0.17          |
| (1,739)  | 1:62:A:PHE:HB2  | 1:62:A:PHE:HD1  | 8        | 0.17          |
| (1,739)  | 1:62:A:PHE:HB3  | 1:62:A:PHE:HD2  | 10       | 0.17          |
| (1,739)  | 1:62:A:PHE:HB2  | 1:62:A:PHE:HD1  | 10       | 0.17          |
| (1,734)  | 1:60:A:ILE:HB   | 1:60:A:ILE:HD12 | 12       | 0.17          |
| (1,734)  | 1:60:A:ILE:HB   | 1:60:A:ILE:HD12 | 16       | 0.17          |
| (1,665)  | 1:55:A:ASP:HB2  | 1:56:A:PHE:H    | 4        | 0.17          |
| (1,611)  | 1:52:A:GLY:HA3  | 1:53:A:PHE:HD1  | 2        | 0.17          |
| (1,611)  | 1:52:A:GLY:HA2  | 1:53:A:PHE:HD1  | 2        | 0.17          |
| (1,611)  | 1:52:A:GLY:HA3  | 1:53:A:PHE:HD1  | 8        | 0.17          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,611)  | 1:52:A:GLY:HA2  | 1:53:A:PHE:HD1  | 8        | 0.17          |
| (1,611)  | 1:52:A:GLY:HA3  | 1:53:A:PHE:HD1  | 17       | 0.17          |
| (1,611)  | 1:52:A:GLY:HA2  | 1:53:A:PHE:HD1  | 17       | 0.17          |
| (1,572)  | 1:46:A:ILE:HG22 | 1:62:A:PHE:HD1  | 18       | 0.17          |
| (1,572)  | 1:46:A:ILE:HG23 | 1:62:A:PHE:HD1  | 18       | 0.17          |
| (1,483)  | 1:37:A:ASP:HA   | 1:40:A:GLN:HA   | 2        | 0.17          |
| (1,483)  | 1:37:A:ASP:HA   | 1:40:A:GLN:HA   | 12       | 0.17          |
| (1,483)  | 1:37:A:ASP:HA   | 1:40:A:GLN:HA   | 18       | 0.17          |
| (1,479)  | 1:36:A:ALA:HA   | 1:39:A:VAL:HG23 | 1        | 0.17          |
| (1,479)  | 1:36:A:ALA:HA   | 1:39:A:VAL:HG23 | 13       | 0.17          |
| (1,479)  | 1:36:A:ALA:HA   | 1:39:A:VAL:HG23 | 14       | 0.17          |
| (1,401)  | 1:30:A:THR:HB   | 1:31:A:LEU:HD21 | 14       | 0.17          |
| (1,326)  | 1:24:A:LEU:HA   | 1:24:A:LEU:HG   | 3        | 0.17          |
| (1,326)  | 1:24:A:LEU:HA   | 1:24:A:LEU:HG   | 4        | 0.17          |
| (1,326)  | 1:24:A:LEU:HA   | 1:24:A:LEU:HG   | 5        | 0.17          |
| (1,326)  | 1:24:A:LEU:HA   | 1:24:A:LEU:HG   | 7        | 0.17          |
| (1,326)  | 1:24:A:LEU:HA   | 1:24:A:LEU:HG   | 10       | 0.17          |
| (1,326)  | 1:24:A:LEU:HA   | 1:24:A:LEU:HG   | 11       | 0.17          |
| (1,326)  | 1:24:A:LEU:HA   | 1:24:A:LEU:HG   | 17       | 0.17          |
| (1,326)  | 1:24:A:LEU:HA   | 1:24:A:LEU:HG   | 18       | 0.17          |
| (1,326)  | 1:24:A:LEU:HA   | 1:24:A:LEU:HG   | 19       | 0.17          |
| (1,321)  | 1:24:A:LEU:HB2  | 1:24:A:LEU:HD21 | 9        | 0.17          |
| (1,321)  | 1:24:A:LEU:HB2  | 1:24:A:LEU:HD21 | 11       | 0.17          |
| (1,320)  | 1:11:A:PHE:HE1  | 1:24:A:LEU:HB2  | 2        | 0.17          |
| (1,320)  | 1:11:A:PHE:HE1  | 1:24:A:LEU:HB2  | 9        | 0.17          |
| (1,82)   | 1:8:A:PHE:HA    | 1:19:A:ILE:HD13 | 19       | 0.17          |
| (1,16)   | 1:42:A:MET:HG2  | 1:62:A:PHE:HE1  | 6        | 0.17          |
| (1,1519) | 1:49:A:ASP:H    | 1:49:A:ASP:HB2  | 10       | 0.16          |
| (1,1519) | 1:49:A:ASP:H    | 1:49:A:ASP:HB3  | 10       | 0.16          |
| (1,1519) | 1:49:A:ASP:H    | 1:49:A:ASP:HB2  | 18       | 0.16          |
| (1,1519) | 1:49:A:ASP:H    | 1:49:A:ASP:HB3  | 18       | 0.16          |
| (1,1510) | 1:46:A:ILE:HG21 | 1:58:A:GLU:HG2  | 15       | 0.16          |
| (1,1510) | 1:46:A:ILE:HG21 | 1:58:A:GLU:HG3  | 15       | 0.16          |
| (1,1472) | 1:34:A:THR:HG23 | 1:35:A:SER:HB2  | 13       | 0.16          |
| (1,1472) | 1:34:A:THR:HG23 | 1:35:A:SER:HB3  | 13       | 0.16          |
| (1,1453) | 1:23:A:GLU:HB2  | 1:27:A:ALA:HA   | 2        | 0.16          |
| (1,1453) | 1:23:A:GLU:HB3  | 1:27:A:ALA:HA   | 2        | 0.16          |
| (1,1453) | 1:23:A:GLU:HB2  | 1:27:A:ALA:HA   | 6        | 0.16          |
| (1,1453) | 1:23:A:GLU:HB3  | 1:27:A:ALA:HA   | 6        | 0.16          |
| (1,1453) | 1:23:A:GLU:HB2  | 1:27:A:ALA:HA   | 20       | 0.16          |
| (1,1453) | 1:23:A:GLU:HB3  | 1:27:A:ALA:HA   | 20       | 0.16          |
| (1,1285) | 1:46:A:ILE:HD12 | 1:61:A:SER:H    | 5        | 0.16          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1262) | 1:53:A:PHE:HB2  | 1:54:A:ILE:H    | 3        | 0.16          |
| (1,1262) | 1:53:A:PHE:HB2  | 1:54:A:ILE:H    | 10       | 0.16          |
| (1,1262) | 1:53:A:PHE:HB2  | 1:54:A:ILE:H    | 15       | 0.16          |
| (1,1262) | 1:53:A:PHE:HB2  | 1:54:A:ILE:H    | 18       | 0.16          |
| (1,1262) | 1:53:A:PHE:HB2  | 1:54:A:ILE:H    | 19       | 0.16          |
| (1,1192) | 1:40:A:GLN:HE22 | 1:41:A:ARG:H    | 3        | 0.16          |
| (1,1192) | 1:40:A:GLN:HE22 | 1:41:A:ARG:H    | 8        | 0.16          |
| (1,1052) | 1:7:A:ILE:HD13  | 1:8:A:PHE:H     | 8        | 0.16          |
| (1,1052) | 1:7:A:ILE:HD13  | 1:8:A:PHE:H     | 20       | 0.16          |
| (1,988)  | 1:34:A:THR:H    | 1:34:A:THR:HG23 | 18       | 0.16          |
| (1,952)  | 1:54:A:ILE:HG21 | 1:55:A:ASP:H    | 8        | 0.16          |
| (1,880)  | 1:77:A:PHE:H    | 1:77:A:PHE:HB3  | 15       | 0.16          |
| (1,762)  | 1:60:A:ILE:HG12 | 1:63:A:CYS:HB3  | 9        | 0.16          |
| (1,762)  | 1:60:A:ILE:HG12 | 1:63:A:CYS:HB3  | 15       | 0.16          |
| (1,739)  | 1:62:A:PHE:HB3  | 1:62:A:PHE:HD2  | 2        | 0.16          |
| (1,739)  | 1:62:A:PHE:HB2  | 1:62:A:PHE:HD1  | 2        | 0.16          |
| (1,739)  | 1:62:A:PHE:HB3  | 1:62:A:PHE:HD2  | 3        | 0.16          |
| (1,739)  | 1:62:A:PHE:HB2  | 1:62:A:PHE:HD1  | 3        | 0.16          |
| (1,739)  | 1:62:A:PHE:HB3  | 1:62:A:PHE:HD2  | 7        | 0.16          |
| (1,739)  | 1:62:A:PHE:HB2  | 1:62:A:PHE:HD1  | 7        | 0.16          |
| (1,665)  | 1:55:A:ASP:HB2  | 1:56:A:PHE:H    | 5        | 0.16          |
| (1,665)  | 1:55:A:ASP:HB2  | 1:56:A:PHE:H    | 6        | 0.16          |
| (1,654)  | 1:19:A:ILE:HD11 | 1:54:A:ILE:HD12 | 7        | 0.16          |
| (1,611)  | 1:52:A:GLY:HA3  | 1:53:A:PHE:HD1  | 9        | 0.16          |
| (1,611)  | 1:52:A:GLY:HA2  | 1:53:A:PHE:HD1  | 9        | 0.16          |
| (1,611)  | 1:52:A:GLY:HA3  | 1:53:A:PHE:HD1  | 14       | 0.16          |
| (1,611)  | 1:52:A:GLY:HA2  | 1:53:A:PHE:HD1  | 14       | 0.16          |
| (1,611)  | 1:52:A:GLY:HA3  | 1:53:A:PHE:HD1  | 16       | 0.16          |
| (1,611)  | 1:52:A:GLY:HA2  | 1:53:A:PHE:HD1  | 16       | 0.16          |
| (1,572)  | 1:46:A:ILE:HG22 | 1:62:A:PHE:HD1  | 14       | 0.16          |
| (1,572)  | 1:46:A:ILE:HG23 | 1:62:A:PHE:HD1  | 14       | 0.16          |
| (1,501)  | 1:42:A:MET:HB3  | 1:62:A:PHE:HD1  | 12       | 0.16          |
| (1,483)  | 1:37:A:ASP:HA   | 1:40:A:GLN:HA   | 1        | 0.16          |
| (1,483)  | 1:37:A:ASP:HA   | 1:40:A:GLN:HA   | 3        | 0.16          |
| (1,483)  | 1:37:A:ASP:HA   | 1:40:A:GLN:HA   | 5        | 0.16          |
| (1,483)  | 1:37:A:ASP:HA   | 1:40:A:GLN:HA   | 8        | 0.16          |
| (1,483)  | 1:37:A:ASP:HA   | 1:40:A:GLN:HA   | 13       | 0.16          |
| (1,483)  | 1:37:A:ASP:HA   | 1:40:A:GLN:HA   | 17       | 0.16          |
| (1,479)  | 1:36:A:ALA:HA   | 1:39:A:VAL:HG23 | 18       | 0.16          |
| (1,472)  | 1:62:A:PHE:HE2  | 1:69:A:LEU:HD21 | 16       | 0.16          |
| (1,417)  | 1:28:A:LEU:HD22 | 1:33:A:SER:HA   | 15       | 0.16          |
| (1,329)  | 1:21:A:LEU:HA   | 1:24:A:LEU:HD12 | 1        | 0.16          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,329)  | 1:21:A:LEU:HA   | 1:24:A:LEU:HD12 | 18       | 0.16          |
| (1,326)  | 1:24:A:LEU:HA   | 1:24:A:LEU:HG   | 1        | 0.16          |
| (1,326)  | 1:24:A:LEU:HA   | 1:24:A:LEU:HG   | 8        | 0.16          |
| (1,326)  | 1:24:A:LEU:HA   | 1:24:A:LEU:HG   | 9        | 0.16          |
| (1,326)  | 1:24:A:LEU:HA   | 1:24:A:LEU:HG   | 14       | 0.16          |
| (1,326)  | 1:24:A:LEU:HA   | 1:24:A:LEU:HG   | 15       | 0.16          |
| (1,326)  | 1:24:A:LEU:HA   | 1:24:A:LEU:HG   | 16       | 0.16          |
| (1,321)  | 1:24:A:LEU:HB2  | 1:24:A:LEU:HD21 | 8        | 0.16          |
| (1,320)  | 1:11:A:PHE:HE1  | 1:24:A:LEU:HB2  | 16       | 0.16          |
| (1,285)  | 1:31:A:LEU:HB2  | 1:31:A:LEU:HD21 | 20       | 0.16          |
| (1,89)   | 1:8:A:PHE:HB2   | 1:8:A:PHE:HD1   | 4        | 0.16          |
| (1,89)   | 1:8:A:PHE:HB3   | 1:8:A:PHE:HD2   | 4        | 0.16          |
| (1,89)   | 1:8:A:PHE:HB2   | 1:8:A:PHE:HD1   | 6        | 0.16          |
| (1,89)   | 1:8:A:PHE:HB3   | 1:8:A:PHE:HD2   | 6        | 0.16          |
| (1,16)   | 1:42:A:MET:HG2  | 1:62:A:PHE:HE1  | 17       | 0.16          |
| (1,7)    | 1:3:A:ASP:HB2   | 1:4:A:MET:HE3   | 4        | 0.16          |
| (1,7)    | 1:3:A:ASP:HB3   | 1:4:A:MET:HE3   | 4        | 0.16          |
| (1,1519) | 1:49:A:ASP:H    | 1:49:A:ASP:HB2  | 7        | 0.15          |
| (1,1519) | 1:49:A:ASP:H    | 1:49:A:ASP:HB3  | 7        | 0.15          |
| (1,1519) | 1:49:A:ASP:H    | 1:49:A:ASP:HB2  | 19       | 0.15          |
| (1,1519) | 1:49:A:ASP:H    | 1:49:A:ASP:HB3  | 19       | 0.15          |
| (1,1510) | 1:46:A:ILE:HG21 | 1:58:A:GLU:HG2  | 7        | 0.15          |
| (1,1510) | 1:46:A:ILE:HG21 | 1:58:A:GLU:HG3  | 7        | 0.15          |
| (1,1510) | 1:46:A:ILE:HG21 | 1:58:A:GLU:HG2  | 18       | 0.15          |
| (1,1510) | 1:46:A:ILE:HG21 | 1:58:A:GLU:HG3  | 18       | 0.15          |
| (1,1453) | 1:23:A:GLU:HB2  | 1:27:A:ALA:HA   | 3        | 0.15          |
| (1,1453) | 1:23:A:GLU:HB3  | 1:27:A:ALA:HA   | 3        | 0.15          |
| (1,1453) | 1:23:A:GLU:HB2  | 1:27:A:ALA:HA   | 4        | 0.15          |
| (1,1453) | 1:23:A:GLU:HB3  | 1:27:A:ALA:HA   | 4        | 0.15          |
| (1,1453) | 1:23:A:GLU:HB2  | 1:27:A:ALA:HA   | 10       | 0.15          |
| (1,1453) | 1:23:A:GLU:HB3  | 1:27:A:ALA:HA   | 10       | 0.15          |
| (1,1453) | 1:23:A:GLU:HB2  | 1:27:A:ALA:HA   | 13       | 0.15          |
| (1,1453) | 1:23:A:GLU:HB3  | 1:27:A:ALA:HA   | 13       | 0.15          |
| (1,1417) | 1:18:A:LYS:HA   | 1:55:A:ASP:HB2  | 4        | 0.15          |
| (1,1417) | 1:18:A:LYS:HA   | 1:55:A:ASP:HB3  | 4        | 0.15          |
| (1,1262) | 1:53:A:PHE:HB2  | 1:54:A:ILE:H    | 7        | 0.15          |
| (1,1192) | 1:40:A:GLN:HE22 | 1:41:A:ARG:H    | 7        | 0.15          |
| (1,1190) | 1:25:A:THR:HG22 | 1:40:A:GLN:H    | 16       | 0.15          |
| (1,1052) | 1:7:A:ILE:HD13  | 1:8:A:PHE:H     | 2        | 0.15          |
| (1,1052) | 1:7:A:ILE:HD13  | 1:8:A:PHE:H     | 4        | 0.15          |
| (1,866)  | 1:4:A:MET:HE3   | 1:7:A:ILE:HD11  | 3        | 0.15          |
| (1,866)  | 1:4:A:MET:HE3   | 1:7:A:ILE:HD13  | 3        | 0.15          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,866)  | 1:4:A:MET:HE3   | 1:7:A:ILE:HD11  | 4        | 0.15          |
| (1,866)  | 1:4:A:MET:HE3   | 1:7:A:ILE:HD13  | 4        | 0.15          |
| (1,848)  | 1:31:A:LEU:HB2  | 1:76:A:VAL:HG23 | 9        | 0.15          |
| (1,847)  | 1:76:A:VAL:HA   | 1:76:A:VAL:HG21 | 1        | 0.15          |
| (1,847)  | 1:76:A:VAL:HA   | 1:76:A:VAL:HG21 | 4        | 0.15          |
| (1,847)  | 1:76:A:VAL:HA   | 1:76:A:VAL:HG21 | 5        | 0.15          |
| (1,847)  | 1:76:A:VAL:HA   | 1:76:A:VAL:HG21 | 6        | 0.15          |
| (1,847)  | 1:76:A:VAL:HA   | 1:76:A:VAL:HG21 | 7        | 0.15          |
| (1,847)  | 1:76:A:VAL:HA   | 1:76:A:VAL:HG21 | 8        | 0.15          |
| (1,847)  | 1:76:A:VAL:HA   | 1:76:A:VAL:HG21 | 10       | 0.15          |
| (1,847)  | 1:76:A:VAL:HA   | 1:76:A:VAL:HG21 | 13       | 0.15          |
| (1,847)  | 1:76:A:VAL:HA   | 1:76:A:VAL:HG21 | 14       | 0.15          |
| (1,847)  | 1:76:A:VAL:HA   | 1:76:A:VAL:HG21 | 16       | 0.15          |
| (1,847)  | 1:76:A:VAL:HA   | 1:76:A:VAL:HG21 | 17       | 0.15          |
| (1,847)  | 1:76:A:VAL:HA   | 1:76:A:VAL:HG21 | 19       | 0.15          |
| (1,847)  | 1:76:A:VAL:HA   | 1:76:A:VAL:HG21 | 20       | 0.15          |
| (1,739)  | 1:62:A:PHE:HB3  | 1:62:A:PHE:HD2  | 19       | 0.15          |
| (1,739)  | 1:62:A:PHE:HB2  | 1:62:A:PHE:HD1  | 19       | 0.15          |
| (1,665)  | 1:55:A:ASP:HB2  | 1:56:A:PHE:H    | 1        | 0.15          |
| (1,611)  | 1:52:A:GLY:HA3  | 1:53:A:PHE:HD1  | 20       | 0.15          |
| (1,611)  | 1:52:A:GLY:HA2  | 1:53:A:PHE:HD1  | 20       | 0.15          |
| (1,483)  | 1:37:A:ASP:HA   | 1:40:A:GLN:HA   | 4        | 0.15          |
| (1,483)  | 1:37:A:ASP:HA   | 1:40:A:GLN:HA   | 6        | 0.15          |
| (1,483)  | 1:37:A:ASP:HA   | 1:40:A:GLN:HA   | 7        | 0.15          |
| (1,483)  | 1:37:A:ASP:HA   | 1:40:A:GLN:HA   | 9        | 0.15          |
| (1,483)  | 1:37:A:ASP:HA   | 1:40:A:GLN:HA   | 10       | 0.15          |
| (1,483)  | 1:37:A:ASP:HA   | 1:40:A:GLN:HA   | 15       | 0.15          |
| (1,483)  | 1:37:A:ASP:HA   | 1:40:A:GLN:HA   | 16       | 0.15          |
| (1,483)  | 1:37:A:ASP:HA   | 1:40:A:GLN:HA   | 19       | 0.15          |
| (1,418)  | 1:33:A:SER:H    | 1:33:A:SER:HB2  | 16       | 0.15          |
| (1,411)  | 1:30:A:THR:HG22 | 1:31:A:LEU:HG   | 16       | 0.15          |
| (1,376)  | 1:68:A:GLY:H    | 1:69:A:LEU:HB2  | 18       | 0.15          |
| (1,320)  | 1:11:A:PHE:HE1  | 1:24:A:LEU:HB2  | 19       | 0.15          |
| (1,113)  | 1:29:A:ARG:H    | 1:29:A:ARG:HG3  | 3        | 0.15          |
| (1,1519) | 1:49:A:ASP:H    | 1:49:A:ASP:HB2  | 2        | 0.14          |
| (1,1519) | 1:49:A:ASP:H    | 1:49:A:ASP:HB3  | 2        | 0.14          |
| (1,1519) | 1:49:A:ASP:H    | 1:49:A:ASP:HB2  | 5        | 0.14          |
| (1,1519) | 1:49:A:ASP:H    | 1:49:A:ASP:HB3  | 5        | 0.14          |
| (1,1510) | 1:46:A:ILE:HG21 | 1:58:A:GLU:HG2  | 6        | 0.14          |
| (1,1510) | 1:46:A:ILE:HG21 | 1:58:A:GLU:HG3  | 6        | 0.14          |
| (1,1510) | 1:46:A:ILE:HG21 | 1:58:A:GLU:HG2  | 19       | 0.14          |
| (1,1510) | 1:46:A:ILE:HG21 | 1:58:A:GLU:HG3  | 19       | 0.14          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1453) | 1:23:A:GLU:HB2  | 1:27:A:ALA:HA   | 5        | 0.14          |
| (1,1453) | 1:23:A:GLU:HB3  | 1:27:A:ALA:HA   | 5        | 0.14          |
| (1,1453) | 1:23:A:GLU:HB2  | 1:27:A:ALA:HA   | 8        | 0.14          |
| (1,1453) | 1:23:A:GLU:HB3  | 1:27:A:ALA:HA   | 8        | 0.14          |
| (1,1453) | 1:23:A:GLU:HB2  | 1:27:A:ALA:HA   | 9        | 0.14          |
| (1,1453) | 1:23:A:GLU:HB3  | 1:27:A:ALA:HA   | 9        | 0.14          |
| (1,1453) | 1:23:A:GLU:HB2  | 1:27:A:ALA:HA   | 17       | 0.14          |
| (1,1453) | 1:23:A:GLU:HB3  | 1:27:A:ALA:HA   | 17       | 0.14          |
| (1,1453) | 1:23:A:GLU:HB2  | 1:27:A:ALA:HA   | 19       | 0.14          |
| (1,1453) | 1:23:A:GLU:HB3  | 1:27:A:ALA:HA   | 19       | 0.14          |
| (1,1285) | 1:46:A:ILE:HD12 | 1:61:A:SER:H    | 11       | 0.14          |
| (1,1192) | 1:40:A:GLN:HE22 | 1:41:A:ARG:H    | 19       | 0.14          |
| (1,1168) | 1:28:A:LEU:HD21 | 1:33:A:SER:H    | 17       | 0.14          |
| (1,1052) | 1:7:A:ILE:HD13  | 1:8:A:PHE:H     | 9        | 0.14          |
| (1,1022) | 1:31:A:LEU:H    | 1:31:A:LEU:HD21 | 16       | 0.14          |
| (1,988)  | 1:34:A:THR:H    | 1:34:A:THR:HG23 | 14       | 0.14          |
| (1,880)  | 1:77:A:PHE:H    | 1:77:A:PHE:HB3  | 6        | 0.14          |
| (1,866)  | 1:4:A:MET:HE3   | 1:7:A:ILE:HD11  | 15       | 0.14          |
| (1,866)  | 1:4:A:MET:HE3   | 1:7:A:ILE:HD13  | 15       | 0.14          |
| (1,833)  | 1:71:A:LYS:HA   | 1:73:A:VAL:HB   | 12       | 0.14          |
| (1,762)  | 1:60:A:ILE:HG12 | 1:63:A:CYS:HB3  | 3        | 0.14          |
| (1,734)  | 1:60:A:ILE:HB   | 1:60:A:ILE:HD12 | 11       | 0.14          |
| (1,734)  | 1:60:A:ILE:HB   | 1:60:A:ILE:HD12 | 17       | 0.14          |
| (1,575)  | 1:46:A:ILE:HD11 | 1:62:A:PHE:H    | 13       | 0.14          |
| (1,572)  | 1:46:A:ILE:HG22 | 1:62:A:PHE:HD1  | 19       | 0.14          |
| (1,572)  | 1:46:A:ILE:HG23 | 1:62:A:PHE:HD1  | 19       | 0.14          |
| (1,548)  | 1:43:A:MET:HG2  | 1:44:A:ALA:HA   | 16       | 0.14          |
| (1,548)  | 1:43:A:MET:HG2  | 1:44:A:ALA:HA   | 17       | 0.14          |
| (1,376)  | 1:68:A:GLY:H    | 1:69:A:LEU:HB2  | 14       | 0.14          |
| (1,329)  | 1:21:A:LEU:HA   | 1:24:A:LEU:HD12 | 14       | 0.14          |
| (1,320)  | 1:11:A:PHE:HE1  | 1:24:A:LEU:HB2  | 3        | 0.14          |
| (1,320)  | 1:11:A:PHE:HE1  | 1:24:A:LEU:HB2  | 17       | 0.14          |
| (1,1552) | 1:63:A:CYS:HA   | 1:71:A:LYS:HG2  | 8        | 0.13          |
| (1,1552) | 1:63:A:CYS:HA   | 1:71:A:LYS:HG3  | 8        | 0.13          |
| (1,1519) | 1:49:A:ASP:H    | 1:49:A:ASP:HB2  | 3        | 0.13          |
| (1,1519) | 1:49:A:ASP:H    | 1:49:A:ASP:HB3  | 3        | 0.13          |
| (1,1519) | 1:49:A:ASP:H    | 1:49:A:ASP:HB2  | 15       | 0.13          |
| (1,1519) | 1:49:A:ASP:H    | 1:49:A:ASP:HB3  | 15       | 0.13          |
| (1,1510) | 1:46:A:ILE:HG21 | 1:58:A:GLU:HG2  | 1        | 0.13          |
| (1,1510) | 1:46:A:ILE:HG21 | 1:58:A:GLU:HG3  | 1        | 0.13          |
| (1,1510) | 1:46:A:ILE:HG21 | 1:58:A:GLU:HG2  | 4        | 0.13          |
| (1,1510) | 1:46:A:ILE:HG21 | 1:58:A:GLU:HG3  | 4        | 0.13          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1490) | 1:39:A:VAL:H    | 1:41:A:ARG:HD2  | 3        | 0.13          |
| (1,1490) | 1:39:A:VAL:H    | 1:41:A:ARG:HD3  | 3        | 0.13          |
| (1,1490) | 1:39:A:VAL:H    | 1:41:A:ARG:HD2  | 8        | 0.13          |
| (1,1490) | 1:39:A:VAL:H    | 1:41:A:ARG:HD3  | 8        | 0.13          |
| (1,1453) | 1:23:A:GLU:HB2  | 1:27:A:ALA:HA   | 11       | 0.13          |
| (1,1453) | 1:23:A:GLU:HB3  | 1:27:A:ALA:HA   | 11       | 0.13          |
| (1,1453) | 1:23:A:GLU:HB2  | 1:27:A:ALA:HA   | 12       | 0.13          |
| (1,1453) | 1:23:A:GLU:HB3  | 1:27:A:ALA:HA   | 12       | 0.13          |
| (1,1453) | 1:23:A:GLU:HB2  | 1:27:A:ALA:HA   | 15       | 0.13          |
| (1,1453) | 1:23:A:GLU:HB3  | 1:27:A:ALA:HA   | 15       | 0.13          |
| (1,1453) | 1:23:A:GLU:HB2  | 1:27:A:ALA:HA   | 16       | 0.13          |
| (1,1453) | 1:23:A:GLU:HB3  | 1:27:A:ALA:HA   | 16       | 0.13          |
| (1,1280) | 1:57:A:ASN:HD21 | 1:58:A:GLU:H    | 19       | 0.13          |
| (1,1114) | 1:20:A:SER:H    | 1:22:A:SER:H    | 4        | 0.13          |
| (1,1114) | 1:20:A:SER:H    | 1:22:A:SER:H    | 5        | 0.13          |
| (1,1114) | 1:20:A:SER:H    | 1:22:A:SER:H    | 12       | 0.13          |
| (1,952)  | 1:54:A:ILE:HG21 | 1:55:A:ASP:H    | 17       | 0.13          |
| (1,875)  | 1:7:A:ILE:HD12  | 1:77:A:PHE:H    | 8        | 0.13          |
| (1,833)  | 1:71:A:LYS:HA   | 1:73:A:VAL:HB   | 4        | 0.13          |
| (1,833)  | 1:71:A:LYS:HA   | 1:73:A:VAL:HB   | 6        | 0.13          |
| (1,762)  | 1:60:A:ILE:HG12 | 1:63:A:CYS:HB3  | 8        | 0.13          |
| (1,654)  | 1:19:A:ILE:HD11 | 1:54:A:ILE:HD12 | 10       | 0.13          |
| (1,548)  | 1:43:A:MET:HG2  | 1:44:A:ALA:HA   | 10       | 0.13          |
| (1,501)  | 1:42:A:MET:HB3  | 1:62:A:PHE:HD1  | 16       | 0.13          |
| (1,329)  | 1:21:A:LEU:HA   | 1:24:A:LEU:HD12 | 7        | 0.13          |
| (1,329)  | 1:21:A:LEU:HA   | 1:24:A:LEU:HD12 | 10       | 0.13          |
| (1,329)  | 1:21:A:LEU:HA   | 1:24:A:LEU:HD12 | 17       | 0.13          |
| (1,285)  | 1:31:A:LEU:HB2  | 1:31:A:LEU:HD21 | 9        | 0.13          |
| (1,285)  | 1:31:A:LEU:HB2  | 1:31:A:LEU:HD21 | 11       | 0.13          |
| (1,285)  | 1:31:A:LEU:HB2  | 1:31:A:LEU:HD21 | 17       | 0.13          |
| (1,1519) | 1:49:A:ASP:H    | 1:49:A:ASP:HB2  | 1        | 0.12          |
| (1,1519) | 1:49:A:ASP:H    | 1:49:A:ASP:HB3  | 1        | 0.12          |
| (1,1519) | 1:49:A:ASP:H    | 1:49:A:ASP:HB2  | 4        | 0.12          |
| (1,1519) | 1:49:A:ASP:H    | 1:49:A:ASP:HB3  | 4        | 0.12          |
| (1,1519) | 1:49:A:ASP:H    | 1:49:A:ASP:HB2  | 6        | 0.12          |
| (1,1519) | 1:49:A:ASP:H    | 1:49:A:ASP:HB3  | 6        | 0.12          |
| (1,1519) | 1:49:A:ASP:H    | 1:49:A:ASP:HB2  | 8        | 0.12          |
| (1,1519) | 1:49:A:ASP:H    | 1:49:A:ASP:HB3  | 8        | 0.12          |
| (1,1510) | 1:46:A:ILE:HG21 | 1:58:A:GLU:HG2  | 14       | 0.12          |
| (1,1510) | 1:46:A:ILE:HG21 | 1:58:A:GLU:HG3  | 14       | 0.12          |
| (1,1510) | 1:46:A:ILE:HG21 | 1:58:A:GLU:HG2  | 17       | 0.12          |
| (1,1510) | 1:46:A:ILE:HG21 | 1:58:A:GLU:HG3  | 17       | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1510) | 1:46:A:ILE:HG21 | 1:58:A:GLU:HG2  | 20       | 0.12          |
| (1,1510) | 1:46:A:ILE:HG21 | 1:58:A:GLU:HG3  | 20       | 0.12          |
| (1,1423) | 1:19:A:ILE:HG13 | 1:20:A:SER:HB2  | 3        | 0.12          |
| (1,1423) | 1:19:A:ILE:HG13 | 1:20:A:SER:HB3  | 3        | 0.12          |
| (1,1385) | 1:6:A:ARG:HB3   | 1:6:A:ARG:HD2   | 4        | 0.12          |
| (1,1385) | 1:6:A:ARG:HB3   | 1:6:A:ARG:HD3   | 4        | 0.12          |
| (1,1385) | 1:6:A:ARG:HB3   | 1:6:A:ARG:HD2   | 14       | 0.12          |
| (1,1385) | 1:6:A:ARG:HB3   | 1:6:A:ARG:HD3   | 14       | 0.12          |
| (1,1385) | 1:6:A:ARG:HB3   | 1:6:A:ARG:HD2   | 19       | 0.12          |
| (1,1385) | 1:6:A:ARG:HB3   | 1:6:A:ARG:HD3   | 19       | 0.12          |
| (1,1280) | 1:57:A:ASN:HD21 | 1:58:A:GLU:H    | 6        | 0.12          |
| (1,1280) | 1:57:A:ASN:HD21 | 1:58:A:GLU:H    | 7        | 0.12          |
| (1,1280) | 1:57:A:ASN:HD21 | 1:58:A:GLU:H    | 9        | 0.12          |
| (1,1280) | 1:57:A:ASN:HD21 | 1:58:A:GLU:H    | 11       | 0.12          |
| (1,1239) | 1:21:A:LEU:HD22 | 1:48:A:THR:H    | 13       | 0.12          |
| (1,1239) | 1:21:A:LEU:HD23 | 1:48:A:THR:H    | 13       | 0.12          |
| (1,1193) | 1:37:A:ASP:H    | 1:40:A:GLN:HE21 | 4        | 0.12          |
| (1,1193) | 1:37:A:ASP:H    | 1:40:A:GLN:HE21 | 6        | 0.12          |
| (1,1193) | 1:37:A:ASP:H    | 1:40:A:GLN:HE21 | 7        | 0.12          |
| (1,1193) | 1:37:A:ASP:H    | 1:40:A:GLN:HE21 | 13       | 0.12          |
| (1,1193) | 1:37:A:ASP:H    | 1:40:A:GLN:HE21 | 15       | 0.12          |
| (1,1193) | 1:37:A:ASP:H    | 1:40:A:GLN:HE21 | 16       | 0.12          |
| (1,1193) | 1:37:A:ASP:H    | 1:40:A:GLN:HE21 | 19       | 0.12          |
| (1,1114) | 1:20:A:SER:H    | 1:22:A:SER:H    | 3        | 0.12          |
| (1,1114) | 1:20:A:SER:H    | 1:22:A:SER:H    | 8        | 0.12          |
| (1,1114) | 1:20:A:SER:H    | 1:22:A:SER:H    | 13       | 0.12          |
| (1,1114) | 1:20:A:SER:H    | 1:22:A:SER:H    | 16       | 0.12          |
| (1,1052) | 1:7:A:ILE:HD13  | 1:8:A:PHE:H     | 13       | 0.12          |
| (1,988)  | 1:34:A:THR:H    | 1:34:A:THR:HG23 | 7        | 0.12          |
| (1,988)  | 1:34:A:THR:H    | 1:34:A:THR:HG23 | 19       | 0.12          |
| (1,952)  | 1:54:A:ILE:HG21 | 1:55:A:ASP:H    | 5        | 0.12          |
| (1,952)  | 1:54:A:ILE:HG21 | 1:55:A:ASP:H    | 13       | 0.12          |
| (1,904)  | 1:25:A:THR:HA   | 1:27:A:ALA:H    | 13       | 0.12          |
| (1,841)  | 1:72:A:ASP:H    | 1:74:A:ALA:HB3  | 10       | 0.12          |
| (1,787)  | 1:69:A:LEU:HA   | 1:69:A:LEU:HG   | 18       | 0.12          |
| (1,762)  | 1:60:A:ILE:HG12 | 1:63:A:CYS:HB3  | 7        | 0.12          |
| (1,762)  | 1:60:A:ILE:HG12 | 1:63:A:CYS:HB3  | 10       | 0.12          |
| (1,762)  | 1:60:A:ILE:HG12 | 1:63:A:CYS:HB3  | 13       | 0.12          |
| (1,762)  | 1:60:A:ILE:HG12 | 1:63:A:CYS:HB3  | 20       | 0.12          |
| (1,734)  | 1:60:A:ILE:HB   | 1:60:A:ILE:HD12 | 2        | 0.12          |
| (1,654)  | 1:19:A:ILE:HD11 | 1:54:A:ILE:HD12 | 19       | 0.12          |
| (1,575)  | 1:46:A:ILE:HD11 | 1:62:A:PHE:H    | 5        | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,575)  | 1:46:A:ILE:HD11 | 1:62:A:PHE:H    | 11       | 0.12          |
| (1,572)  | 1:46:A:ILE:HG22 | 1:62:A:PHE:HD1  | 7        | 0.12          |
| (1,572)  | 1:46:A:ILE:HG23 | 1:62:A:PHE:HD1  | 7        | 0.12          |
| (1,548)  | 1:43:A:MET:HG2  | 1:44:A:ALA:HA   | 9        | 0.12          |
| (1,548)  | 1:43:A:MET:HG2  | 1:44:A:ALA:HA   | 15       | 0.12          |
| (1,539)  | 1:43:A:MET:HB3  | 1:45:A:GLU:H    | 19       | 0.12          |
| (1,501)  | 1:42:A:MET:HB3  | 1:62:A:PHE:HD1  | 20       | 0.12          |
| (1,329)  | 1:21:A:LEU:HA   | 1:24:A:LEU:HD12 | 2        | 0.12          |
| (1,329)  | 1:21:A:LEU:HA   | 1:24:A:LEU:HD12 | 4        | 0.12          |
| (1,329)  | 1:21:A:LEU:HA   | 1:24:A:LEU:HD12 | 5        | 0.12          |
| (1,329)  | 1:21:A:LEU:HA   | 1:24:A:LEU:HD12 | 6        | 0.12          |
| (1,329)  | 1:21:A:LEU:HA   | 1:24:A:LEU:HD12 | 15       | 0.12          |
| (1,329)  | 1:21:A:LEU:HA   | 1:24:A:LEU:HD12 | 20       | 0.12          |
| (1,285)  | 1:31:A:LEU:HB2  | 1:31:A:LEU:HD21 | 7        | 0.12          |
| (1,285)  | 1:31:A:LEU:HB2  | 1:31:A:LEU:HD21 | 10       | 0.12          |
| (1,285)  | 1:31:A:LEU:HB2  | 1:31:A:LEU:HD21 | 12       | 0.12          |
| (1,285)  | 1:31:A:LEU:HB2  | 1:31:A:LEU:HD21 | 13       | 0.12          |
| (1,285)  | 1:31:A:LEU:HB2  | 1:31:A:LEU:HD21 | 15       | 0.12          |
| (1,257)  | 1:8:A:PHE:HE1   | 1:19:A:ILE:HG23 | 4        | 0.12          |
| (1,244)  | 1:35:A:SER:HA   | 1:39:A:VAL:HG13 | 14       | 0.12          |
| (1,170)  | 1:48:A:THR:HB   | 1:49:A:ASP:H    | 2        | 0.12          |
| (1,170)  | 1:48:A:THR:HB   | 1:49:A:ASP:H    | 5        | 0.12          |
| (1,170)  | 1:48:A:THR:HB   | 1:49:A:ASP:H    | 15       | 0.12          |
| (1,170)  | 1:48:A:THR:HB   | 1:49:A:ASP:H    | 19       | 0.12          |
| (1,170)  | 1:48:A:THR:HB   | 1:49:A:ASP:H    | 20       | 0.12          |
| (1,125)  | 1:21:A:LEU:HA   | 1:24:A:LEU:HB2  | 2        | 0.12          |
| (1,125)  | 1:21:A:LEU:HA   | 1:24:A:LEU:HB2  | 4        | 0.12          |
| (1,125)  | 1:21:A:LEU:HA   | 1:24:A:LEU:HB2  | 8        | 0.12          |
| (1,113)  | 1:29:A:ARG:H    | 1:29:A:ARG:HG3  | 16       | 0.12          |
| (1,16)   | 1:42:A:MET:HG2  | 1:62:A:PHE:HE1  | 20       | 0.12          |
| (1,1519) | 1:49:A:ASP:H    | 1:49:A:ASP:HB2  | 9        | 0.11          |
| (1,1519) | 1:49:A:ASP:H    | 1:49:A:ASP:HB3  | 9        | 0.11          |
| (1,1519) | 1:49:A:ASP:H    | 1:49:A:ASP:HB2  | 14       | 0.11          |
| (1,1519) | 1:49:A:ASP:H    | 1:49:A:ASP:HB3  | 14       | 0.11          |
| (1,1519) | 1:49:A:ASP:H    | 1:49:A:ASP:HB2  | 16       | 0.11          |
| (1,1519) | 1:49:A:ASP:H    | 1:49:A:ASP:HB3  | 16       | 0.11          |
| (1,1519) | 1:49:A:ASP:H    | 1:49:A:ASP:HB2  | 20       | 0.11          |
| (1,1519) | 1:49:A:ASP:H    | 1:49:A:ASP:HB3  | 20       | 0.11          |
| (1,1510) | 1:46:A:ILE:HG21 | 1:58:A:GLU:HG2  | 2        | 0.11          |
| (1,1510) | 1:46:A:ILE:HG21 | 1:58:A:GLU:HG3  | 2        | 0.11          |
| (1,1510) | 1:46:A:ILE:HG21 | 1:58:A:GLU:HG2  | 9        | 0.11          |
| (1,1510) | 1:46:A:ILE:HG21 | 1:58:A:GLU:HG3  | 9        | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1490) | 1:39:A:VAL:H    | 1:41:A:ARG:HD2  | 2        | 0.11          |
| (1,1490) | 1:39:A:VAL:H    | 1:41:A:ARG:HD3  | 2        | 0.11          |
| (1,1490) | 1:39:A:VAL:H    | 1:41:A:ARG:HD2  | 16       | 0.11          |
| (1,1490) | 1:39:A:VAL:H    | 1:41:A:ARG:HD3  | 16       | 0.11          |
| (1,1417) | 1:18:A:LYS:HA   | 1:55:A:ASP:HB2  | 17       | 0.11          |
| (1,1417) | 1:18:A:LYS:HA   | 1:55:A:ASP:HB3  | 17       | 0.11          |
| (1,1280) | 1:57:A:ASN:HD21 | 1:58:A:GLU:H    | 3        | 0.11          |
| (1,1280) | 1:57:A:ASN:HD21 | 1:58:A:GLU:H    | 15       | 0.11          |
| (1,1240) | 1:49:A:ASP:H    | 1:49:A:ASP:HB3  | 2        | 0.11          |
| (1,1239) | 1:21:A:LEU:HD22 | 1:48:A:THR:H    | 11       | 0.11          |
| (1,1239) | 1:21:A:LEU:HD23 | 1:48:A:THR:H    | 11       | 0.11          |
| (1,1193) | 1:37:A:ASP:H    | 1:40:A:GLN:HE21 | 1        | 0.11          |
| (1,1193) | 1:37:A:ASP:H    | 1:40:A:GLN:HE21 | 3        | 0.11          |
| (1,1193) | 1:37:A:ASP:H    | 1:40:A:GLN:HE21 | 8        | 0.11          |
| (1,1193) | 1:37:A:ASP:H    | 1:40:A:GLN:HE21 | 9        | 0.11          |
| (1,1193) | 1:37:A:ASP:H    | 1:40:A:GLN:HE21 | 10       | 0.11          |
| (1,1193) | 1:37:A:ASP:H    | 1:40:A:GLN:HE21 | 11       | 0.11          |
| (1,1193) | 1:37:A:ASP:H    | 1:40:A:GLN:HE21 | 12       | 0.11          |
| (1,1193) | 1:37:A:ASP:H    | 1:40:A:GLN:HE21 | 17       | 0.11          |
| (1,1168) | 1:28:A:LEU:HD21 | 1:33:A:SER:H    | 4        | 0.11          |
| (1,1121) | 1:19:A:ILE:HG22 | 1:20:A:SER:H    | 3        | 0.11          |
| (1,1114) | 1:20:A:SER:H    | 1:22:A:SER:H    | 2        | 0.11          |
| (1,1114) | 1:20:A:SER:H    | 1:22:A:SER:H    | 6        | 0.11          |
| (1,1114) | 1:20:A:SER:H    | 1:22:A:SER:H    | 9        | 0.11          |
| (1,1114) | 1:20:A:SER:H    | 1:22:A:SER:H    | 17       | 0.11          |
| (1,1114) | 1:20:A:SER:H    | 1:22:A:SER:H    | 20       | 0.11          |
| (1,1052) | 1:7:A:ILE:HD13  | 1:8:A:PHE:H     | 14       | 0.11          |
| (1,952)  | 1:54:A:ILE:HG21 | 1:55:A:ASP:H    | 14       | 0.11          |
| (1,904)  | 1:25:A:THR:HA   | 1:27:A:ALA:H    | 2        | 0.11          |
| (1,904)  | 1:25:A:THR:HA   | 1:27:A:ALA:H    | 12       | 0.11          |
| (1,875)  | 1:7:A:ILE:HD12  | 1:77:A:PHE:H    | 17       | 0.11          |
| (1,841)  | 1:72:A:ASP:H    | 1:74:A:ALA:HB3  | 2        | 0.11          |
| (1,841)  | 1:72:A:ASP:H    | 1:74:A:ALA:HB3  | 7        | 0.11          |
| (1,841)  | 1:72:A:ASP:H    | 1:74:A:ALA:HB3  | 8        | 0.11          |
| (1,841)  | 1:72:A:ASP:H    | 1:74:A:ALA:HB3  | 17       | 0.11          |
| (1,833)  | 1:71:A:LYS:HA   | 1:73:A:VAL:HB   | 3        | 0.11          |
| (1,833)  | 1:71:A:LYS:HA   | 1:73:A:VAL:HB   | 10       | 0.11          |
| (1,787)  | 1:69:A:LEU:HA   | 1:69:A:LEU:HG   | 14       | 0.11          |
| (1,762)  | 1:60:A:ILE:HG12 | 1:63:A:CYS:HB3  | 2        | 0.11          |
| (1,762)  | 1:60:A:ILE:HG12 | 1:63:A:CYS:HB3  | 4        | 0.11          |
| (1,762)  | 1:60:A:ILE:HG12 | 1:63:A:CYS:HB3  | 6        | 0.11          |
| (1,762)  | 1:60:A:ILE:HG12 | 1:63:A:CYS:HB3  | 19       | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,734)  | 1:60:A:ILE:HB   | 1:60:A:ILE:HD12 | 5        | 0.11          |
| (1,661)  | 1:18:A:LYS:HB3  | 1:55:A:ASP:HA   | 17       | 0.11          |
| (1,640)  | 1:20:A:SER:HA   | 1:54:A:ILE:HG22 | 13       | 0.11          |
| (1,575)  | 1:46:A:ILE:HD11 | 1:62:A:PHE:H    | 12       | 0.11          |
| (1,548)  | 1:43:A:MET:HG2  | 1:44:A:ALA:HA   | 1        | 0.11          |
| (1,539)  | 1:43:A:MET:HB3  | 1:45:A:GLU:H    | 2        | 0.11          |
| (1,539)  | 1:43:A:MET:HB3  | 1:45:A:GLU:H    | 3        | 0.11          |
| (1,539)  | 1:43:A:MET:HB3  | 1:45:A:GLU:H    | 7        | 0.11          |
| (1,539)  | 1:43:A:MET:HB3  | 1:45:A:GLU:H    | 10       | 0.11          |
| (1,539)  | 1:43:A:MET:HB3  | 1:45:A:GLU:H    | 18       | 0.11          |
| (1,487)  | 1:40:A:GLN:HA   | 1:44:A:ALA:HB2  | 11       | 0.11          |
| (1,487)  | 1:40:A:GLN:HA   | 1:44:A:ALA:HB2  | 12       | 0.11          |
| (1,487)  | 1:40:A:GLN:HA   | 1:44:A:ALA:HB2  | 13       | 0.11          |
| (1,431)  | 1:34:A:THR:HA   | 1:37:A:ASP:H    | 16       | 0.11          |
| (1,377)  | 1:28:A:LEU:HB3  | 1:36:A:ALA:H    | 2        | 0.11          |
| (1,377)  | 1:28:A:LEU:HB3  | 1:36:A:ALA:H    | 6        | 0.11          |
| (1,377)  | 1:28:A:LEU:HB3  | 1:36:A:ALA:H    | 18       | 0.11          |
| (1,376)  | 1:68:A:GLY:H    | 1:69:A:LEU:HB2  | 1        | 0.11          |
| (1,376)  | 1:68:A:GLY:H    | 1:69:A:LEU:HB2  | 12       | 0.11          |
| (1,376)  | 1:68:A:GLY:H    | 1:69:A:LEU:HB2  | 13       | 0.11          |
| (1,329)  | 1:21:A:LEU:HA   | 1:24:A:LEU:HD12 | 3        | 0.11          |
| (1,329)  | 1:21:A:LEU:HA   | 1:24:A:LEU:HD12 | 16       | 0.11          |
| (1,285)  | 1:31:A:LEU:HB2  | 1:31:A:LEU:HD21 | 1        | 0.11          |
| (1,285)  | 1:31:A:LEU:HB2  | 1:31:A:LEU:HD21 | 4        | 0.11          |
| (1,285)  | 1:31:A:LEU:HB2  | 1:31:A:LEU:HD21 | 5        | 0.11          |
| (1,285)  | 1:31:A:LEU:HB2  | 1:31:A:LEU:HD21 | 8        | 0.11          |
| (1,285)  | 1:31:A:LEU:HB2  | 1:31:A:LEU:HD21 | 16       | 0.11          |
| (1,285)  | 1:31:A:LEU:HB2  | 1:31:A:LEU:HD21 | 18       | 0.11          |
| (1,244)  | 1:35:A:SER:HA   | 1:39:A:VAL:HG13 | 2        | 0.11          |
| (1,170)  | 1:48:A:THR:HB   | 1:49:A:ASP:H    | 1        | 0.11          |
| (1,170)  | 1:48:A:THR:HB   | 1:49:A:ASP:H    | 4        | 0.11          |
| (1,170)  | 1:48:A:THR:HB   | 1:49:A:ASP:H    | 6        | 0.11          |
| (1,170)  | 1:48:A:THR:HB   | 1:49:A:ASP:H    | 7        | 0.11          |
| (1,170)  | 1:48:A:THR:HB   | 1:49:A:ASP:H    | 8        | 0.11          |
| (1,170)  | 1:48:A:THR:HB   | 1:49:A:ASP:H    | 9        | 0.11          |
| (1,125)  | 1:21:A:LEU:HA   | 1:24:A:LEU:HB2  | 6        | 0.11          |
| (1,125)  | 1:21:A:LEU:HA   | 1:24:A:LEU:HB2  | 15       | 0.11          |
| (1,125)  | 1:21:A:LEU:HA   | 1:24:A:LEU:HB2  | 16       | 0.11          |
| (1,125)  | 1:21:A:LEU:HA   | 1:24:A:LEU:HB2  | 17       | 0.11          |
| (1,125)  | 1:21:A:LEU:HA   | 1:24:A:LEU:HB2  | 19       | 0.11          |
| (1,1519) | 1:49:A:ASP:H    | 1:49:A:ASP:HB2  | 17       | 0.1           |
| (1,1519) | 1:49:A:ASP:H    | 1:49:A:ASP:HB3  | 17       | 0.1           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1510) | 1:46:A:ILE:HG21 | 1:58:A:GLU:HG2  | 3        | 0.1           |
| (1,1510) | 1:46:A:ILE:HG21 | 1:58:A:GLU:HG3  | 3        | 0.1           |
| (1,1510) | 1:46:A:ILE:HG21 | 1:58:A:GLU:HG2  | 16       | 0.1           |
| (1,1510) | 1:46:A:ILE:HG21 | 1:58:A:GLU:HG3  | 16       | 0.1           |
| (1,1445) | 1:22:A:SER:HB2  | 1:26:A:ASP:HB2  | 5        | 0.1           |
| (1,1445) | 1:22:A:SER:HB2  | 1:26:A:ASP:HB3  | 5        | 0.1           |
| (1,1445) | 1:22:A:SER:HB3  | 1:26:A:ASP:HB2  | 5        | 0.1           |
| (1,1445) | 1:22:A:SER:HB3  | 1:26:A:ASP:HB3  | 5        | 0.1           |
| (1,1445) | 1:22:A:SER:HB2  | 1:26:A:ASP:HB2  | 18       | 0.1           |
| (1,1445) | 1:22:A:SER:HB2  | 1:26:A:ASP:HB3  | 18       | 0.1           |
| (1,1445) | 1:22:A:SER:HB3  | 1:26:A:ASP:HB2  | 18       | 0.1           |
| (1,1445) | 1:22:A:SER:HB3  | 1:26:A:ASP:HB3  | 18       | 0.1           |
| (1,1417) | 1:18:A:LYS:HA   | 1:55:A:ASP:HB2  | 1        | 0.1           |
| (1,1417) | 1:18:A:LYS:HA   | 1:55:A:ASP:HB3  | 1        | 0.1           |
| (1,1417) | 1:18:A:LYS:HA   | 1:55:A:ASP:HB2  | 6        | 0.1           |
| (1,1417) | 1:18:A:LYS:HA   | 1:55:A:ASP:HB3  | 6        | 0.1           |
| (1,1285) | 1:46:A:ILE:HD12 | 1:61:A:SER:H    | 13       | 0.1           |
| (1,1262) | 1:53:A:PHE:HB2  | 1:54:A:ILE:H    | 12       | 0.1           |
| (1,1240) | 1:49:A:ASP:H    | 1:49:A:ASP:HB3  | 19       | 0.1           |
| (1,1193) | 1:37:A:ASP:H    | 1:40:A:GLN:HE21 | 2        | 0.1           |
| (1,1114) | 1:20:A:SER:H    | 1:22:A:SER:H    | 11       | 0.1           |
| (1,994)  | 1:21:A:LEU:HA   | 1:24:A:LEU:H    | 10       | 0.1           |
| (1,988)  | 1:34:A:THR:H    | 1:34:A:THR:HG23 | 15       | 0.1           |
| (1,952)  | 1:54:A:ILE:HG21 | 1:55:A:ASP:H    | 16       | 0.1           |
| (1,904)  | 1:25:A:THR:HA   | 1:27:A:ALA:H    | 4        | 0.1           |
| (1,904)  | 1:25:A:THR:HA   | 1:27:A:ALA:H    | 11       | 0.1           |
| (1,904)  | 1:25:A:THR:HA   | 1:27:A:ALA:H    | 20       | 0.1           |
| (1,762)  | 1:60:A:ILE:HG12 | 1:63:A:CYS:HB3  | 14       | 0.1           |
| (1,762)  | 1:60:A:ILE:HG12 | 1:63:A:CYS:HB3  | 18       | 0.1           |
| (1,734)  | 1:60:A:ILE:HB   | 1:60:A:ILE:HD12 | 18       | 0.1           |
| (1,575)  | 1:46:A:ILE:HD11 | 1:62:A:PHE:H    | 20       | 0.1           |
| (1,539)  | 1:43:A:MET:HB3  | 1:45:A:GLU:H    | 1        | 0.1           |
| (1,539)  | 1:43:A:MET:HB3  | 1:45:A:GLU:H    | 4        | 0.1           |
| (1,539)  | 1:43:A:MET:HB3  | 1:45:A:GLU:H    | 8        | 0.1           |
| (1,539)  | 1:43:A:MET:HB3  | 1:45:A:GLU:H    | 14       | 0.1           |
| (1,501)  | 1:42:A:MET:HB3  | 1:62:A:PHE:HD1  | 6        | 0.1           |
| (1,501)  | 1:42:A:MET:HB3  | 1:62:A:PHE:HD1  | 17       | 0.1           |
| (1,377)  | 1:28:A:LEU:HB3  | 1:36:A:ALA:H    | 1        | 0.1           |
| (1,377)  | 1:28:A:LEU:HB3  | 1:36:A:ALA:H    | 10       | 0.1           |
| (1,377)  | 1:28:A:LEU:HB3  | 1:36:A:ALA:H    | 15       | 0.1           |
| (1,329)  | 1:21:A:LEU:HA   | 1:24:A:LEU:HD12 | 9        | 0.1           |
| (1,329)  | 1:21:A:LEU:HA   | 1:24:A:LEU:HD12 | 12       | 0.1           |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,329) | 1:21:A:LEU:HA  | 1:24:A:LEU:HD12 | 19       | 0.1           |
| (1,285) | 1:31:A:LEU:HB2 | 1:31:A:LEU:HD21 | 3        | 0.1           |
| (1,285) | 1:31:A:LEU:HB2 | 1:31:A:LEU:HD21 | 19       | 0.1           |
| (1,170) | 1:48:A:THR:HB  | 1:49:A:ASP:H    | 3        | 0.1           |
| (1,170) | 1:48:A:THR:HB  | 1:49:A:ASP:H    | 14       | 0.1           |
| (1,170) | 1:48:A:THR:HB  | 1:49:A:ASP:H    | 16       | 0.1           |
| (1,125) | 1:21:A:LEU:HA  | 1:24:A:LEU:HB2  | 9        | 0.1           |
| (1,16)  | 1:42:A:MET:HG2 | 1:62:A:PHE:HE1  | 5        | 0.1           |

## 10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found