



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 08:06 PM UTC

PDB ID : 5NB9 / pdb\_00005nb9  
BMRB ID : 34110  
Title : Structure of the N-terminal domain of the Escherichia Coli ProQ RNA binding protein  
Authors : Gonzales, G.; Hardwick, S.; Maslen, S.; Skehel, M.; Holmqvist, E.; Vogel, J.; Bateman, A.; Luisi, B.; Broadhurst, R.  
Deposited on : 2017-03-01

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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

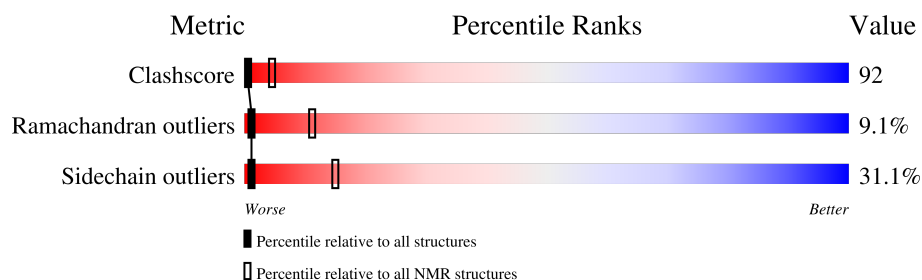
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 81%.

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     | 133    | <div> <div></div> <div>9%</div> <div>19%</div> <div>34%</div> <div>11%</div> <div>27%</div> </div> |

## 2 Ensemble composition and analysis

This entry contains 17 models. Model 13 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

| Well-defined (core) protein residues |                       |                   |              |
|--------------------------------------|-----------------------|-------------------|--------------|
| Well-defined core                    | Residue range (total) | Backbone RMSD (Å) | Medoid model |
| 1                                    | A:21-A:117 (97)       | 0.44              | 13           |

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

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

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

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2096 atoms, of which 1035 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called RNA chaperone ProQ.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|-------|
| 1   | A     | 133      | Total | C   | H    | N   | O   | S | 0     |
|     |       |          | 2096  | 653 | 1035 | 203 | 200 | 5 |       |

There are 14 discrepancies between the modelled and reference sequences:

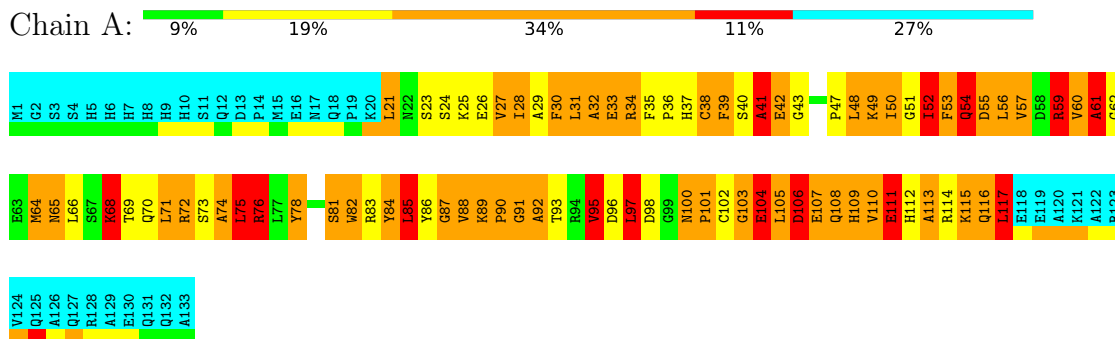
| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| A     | 1       | MET      | -      | initiating methionine | UNP B7MBN8 |
| A     | 2       | GLY      | -      | expression tag        | UNP B7MBN8 |
| A     | 3       | SER      | -      | expression tag        | UNP B7MBN8 |
| A     | 4       | SER      | -      | expression tag        | UNP B7MBN8 |
| A     | 5       | HIS      | -      | expression tag        | UNP B7MBN8 |
| A     | 6       | HIS      | -      | expression tag        | UNP B7MBN8 |
| A     | 7       | HIS      | -      | expression tag        | UNP B7MBN8 |
| A     | 8       | HIS      | -      | expression tag        | UNP B7MBN8 |
| A     | 9       | HIS      | -      | expression tag        | UNP B7MBN8 |
| A     | 10      | HIS      | -      | expression tag        | UNP B7MBN8 |
| A     | 11      | SER      | -      | expression tag        | UNP B7MBN8 |
| A     | 12      | GLN      | -      | expression tag        | UNP B7MBN8 |
| A     | 13      | ASP      | -      | expression tag        | UNP B7MBN8 |
| A     | 14      | PRO      | -      | expression tag        | UNP B7MBN8 |

## 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: RNA chaperone ProQ

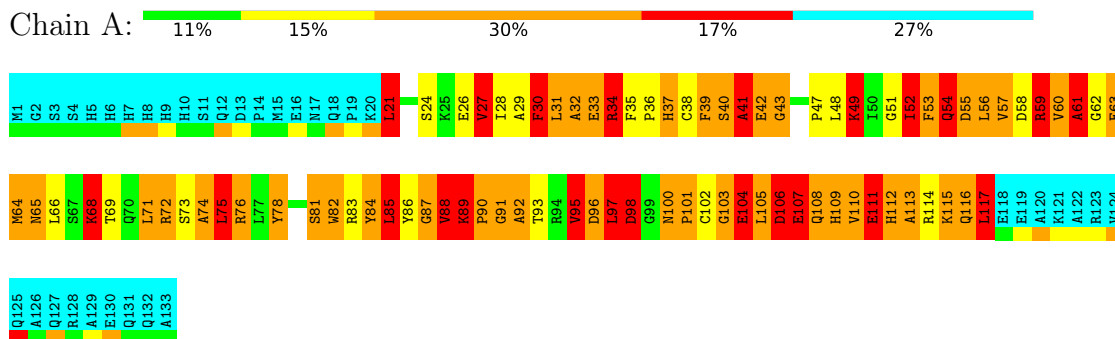


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

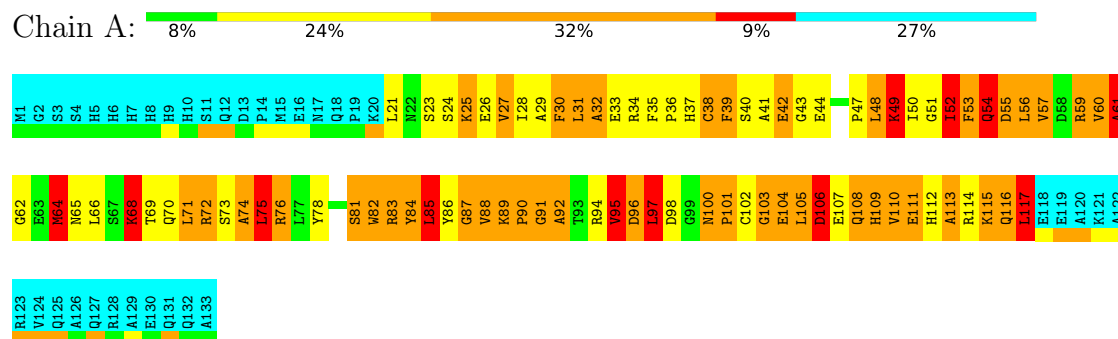
#### 4.2.1 Score per residue for model 1

- Molecule 1: RNA chaperone ProQ



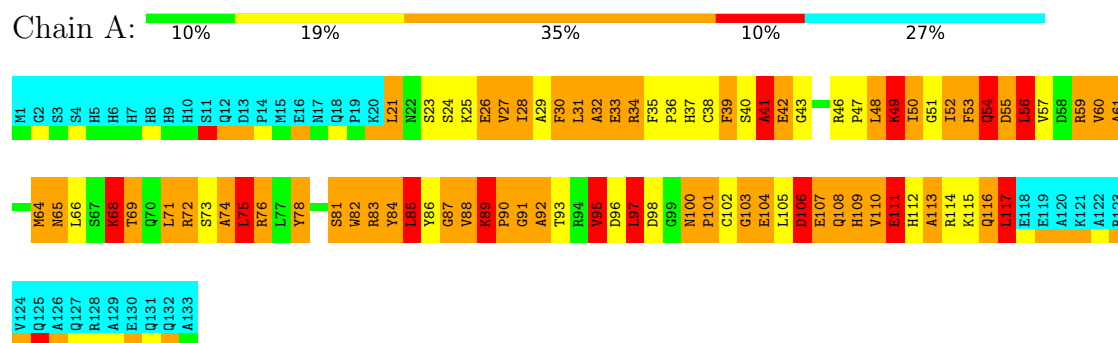
## 4.2.2 Score per residue for model 2

### • Molecule 1: RNA chaperone ProQ



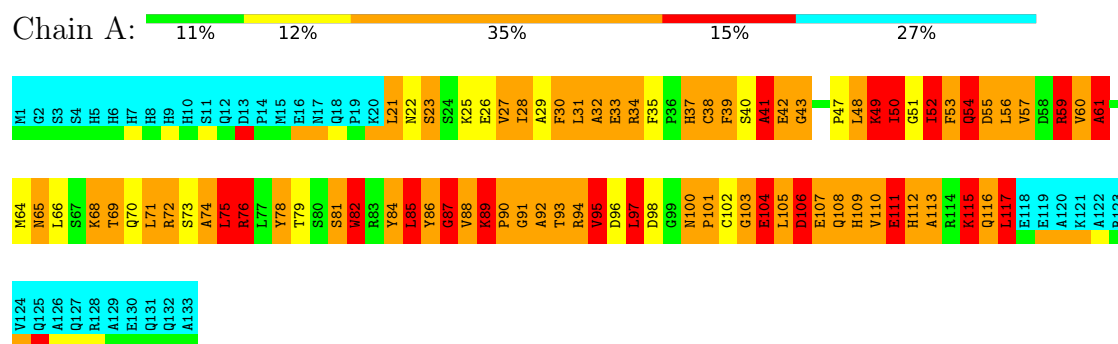
## 4.2.3 Score per residue for model 3

### • Molecule 1: RNA chaperone ProQ



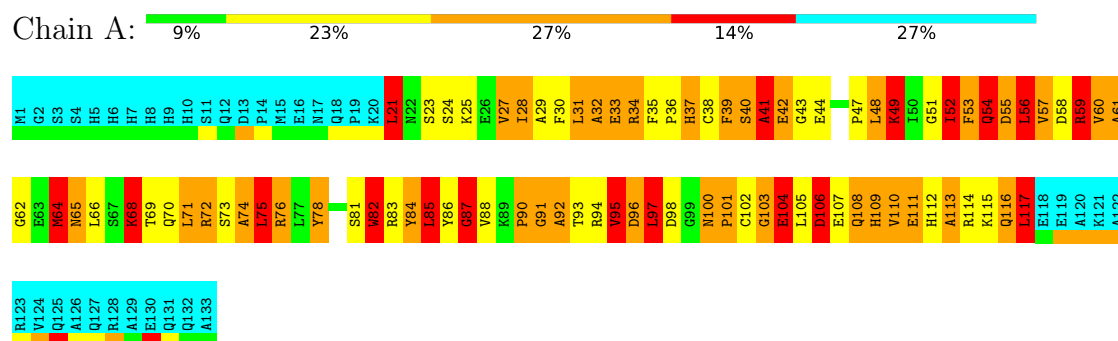
## 4.2.4 Score per residue for model 4

### • Molecule 1: RNA chaperone ProQ



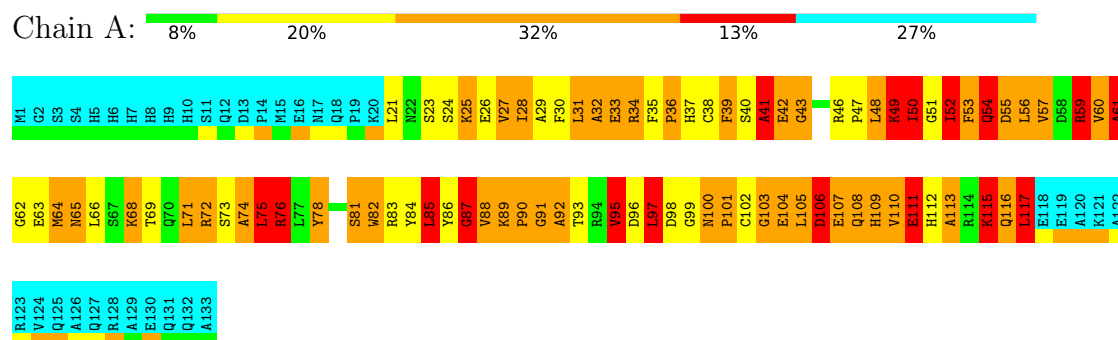
### 4.2.5 Score per residue for model 5

- Molecule 1: RNA chaperone ProQ



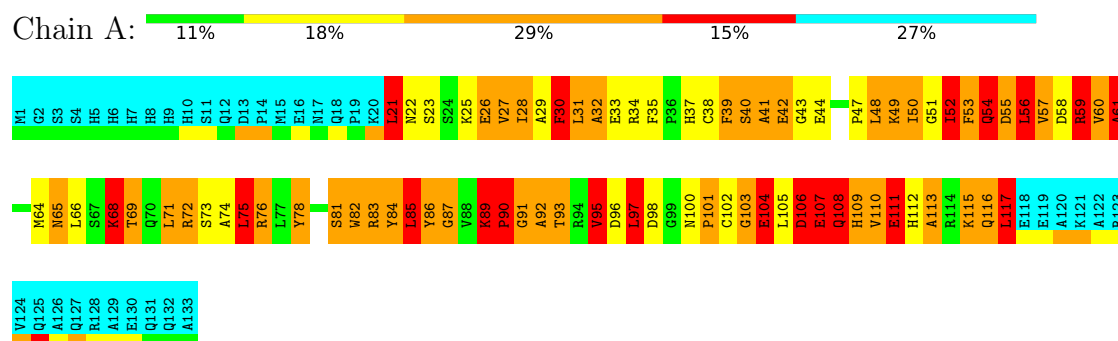
### 4.2.6 Score per residue for model 6

- Molecule 1: RNA chaperone ProQ



### 4.2.7 Score per residue for model 7

- Molecule 1: RNA chaperone ProQ

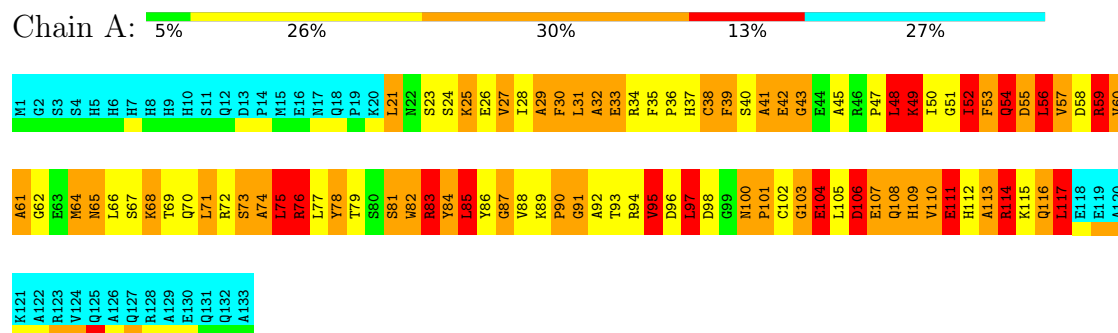






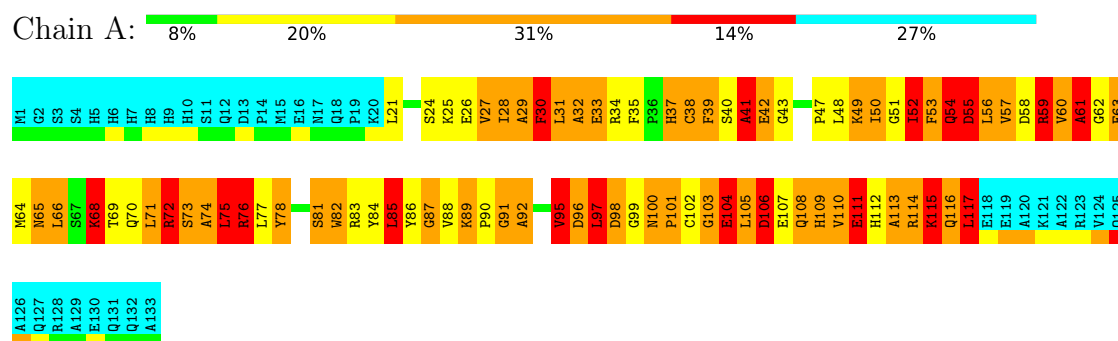
### 4.2.11 Score per residue for model 11

- Molecule 1: RNA chaperone ProQ



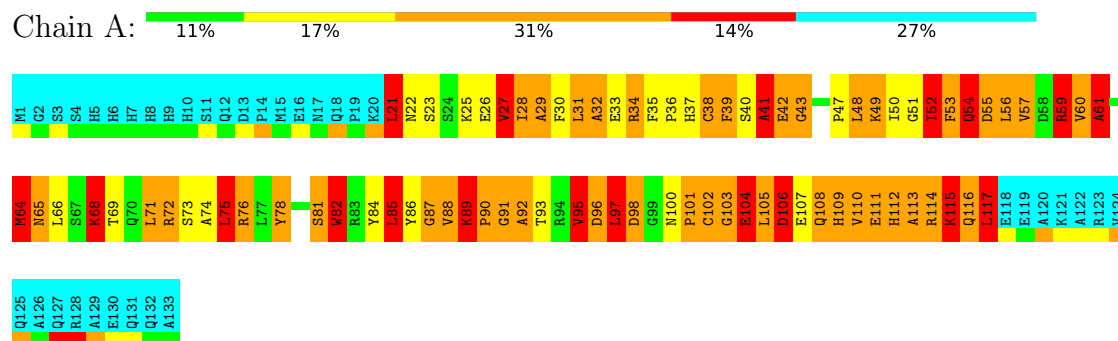
### 4.2.12 Score per residue for model 12

- Molecule 1: RNA chaperone ProQ



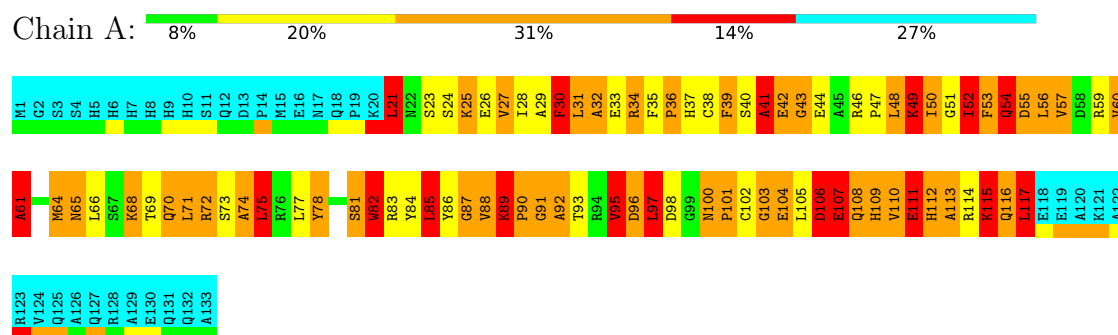
### 4.2.13 Score per residue for model 13 (medoid)

- Molecule 1: RNA chaperone ProQ



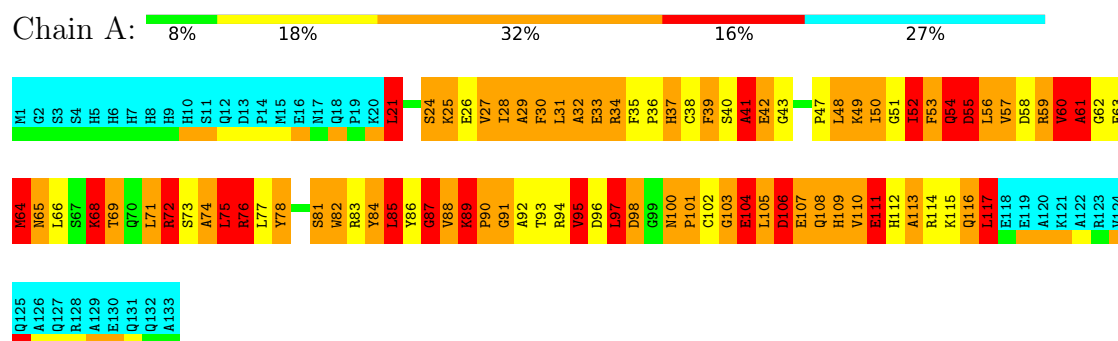
#### 4.2.14 Score per residue for model 14

- Molecule 1: RNA chaperone ProQ



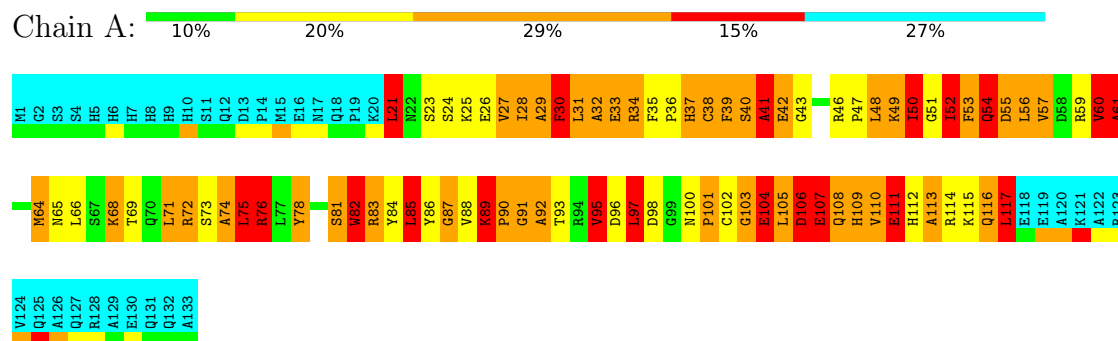
#### 4.2.15 Score per residue for model 15

- Molecule 1: RNA chaperone ProQ



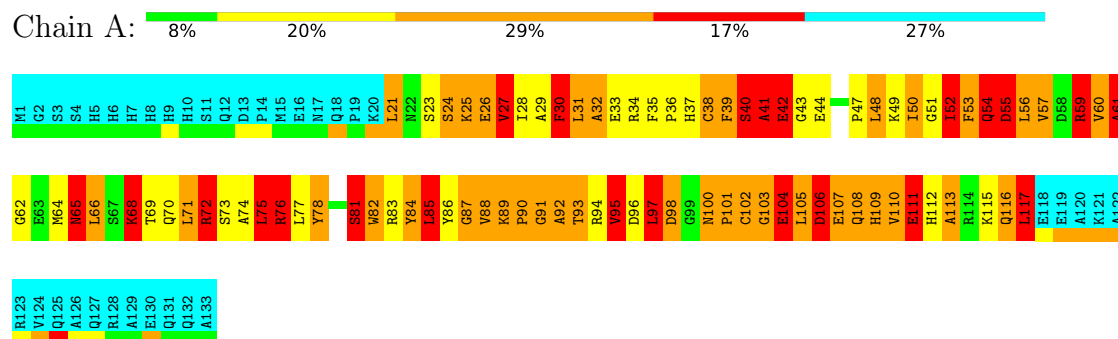
#### 4.2.16 Score per residue for model 16

- Molecule 1: RNA chaperone ProQ



## 4.2.17 Score per residue for model 17

### ● Molecule 1: RNA chaperone ProQ



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the 50 calculated structures, 17 were deposited, based on the following criterion: *structures with acceptable covalent geometry*.

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

| Software name | Classification        | Version |
|---------------|-----------------------|---------|
| ARIA          | structure calculation | 2.3     |
| CNS           | refinement            | 1.3     |

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                       | 1341           |
| Number of shifts mapped to atoms             | 1341           |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 81%            |

## 6 Model quality

### 6.1 Standard geometry

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

| Mol | Chain | Bond lengths |                        | Bond angles |                        |
|-----|-------|--------------|------------------------|-------------|------------------------|
|     |       | RMSZ         | #Z>5                   | RMSZ        | #Z>5                   |
| 1   | A     | 3.08±0.06    | 86±6/786 ( 10.9± 0.8%) | 2.01±0.03   | 29±4/1061 ( 2.7± 0.3%) |
| All | All   | 3.08         | 1461/13362 ( 10.9%)    | 2.01        | 494/18037 ( 2.7%)      |

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

| Mol | Chain | Chirality | Planarity |
|-----|-------|-----------|-----------|
| 1   | A     | 0.0±0.0   | 1.5±0.7   |
| All | All   | 0         | 26        |

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

| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) | Models |       |
|-----|-------|-----|------|-------|--------|-------------|----------|--------|-------|
|     |       |     |      |       |        |             |          | Worst  | Total |
| 1   | A     | 56  | LEU  | CA-C  | -13.45 | 1.36        | 1.52     | 1      | 17    |
| 1   | A     | 61  | ALA  | CA-CB | -12.29 | 1.32        | 1.53     | 11     | 11    |
| 1   | A     | 91  | GLY  | C-N   | -12.25 | 1.17        | 1.34     | 15     | 17    |
| 1   | A     | 61  | ALA  | C-N   | -12.17 | 1.15        | 1.33     | 9      | 17    |
| 1   | A     | 56  | LEU  | N-CA  | -12.08 | 1.32        | 1.46     | 16     | 17    |
| 1   | A     | 56  | LEU  | C-O   | -11.94 | 1.10        | 1.24     | 6      | 17    |
| 1   | A     | 55  | ASP  | CA-C  | -11.89 | 1.37        | 1.52     | 6      | 17    |
| 1   | A     | 53  | PHE  | C-O   | -11.67 | 1.10        | 1.24     | 10     | 17    |
| 1   | A     | 64  | MET  | CA-C  | -10.90 | 1.45        | 1.52     | 2      | 14    |
| 1   | A     | 49  | LYS  | C-N   | -10.75 | 1.23        | 1.33     | 7      | 13    |
| 1   | A     | 100 | ASN  | C-O   | -10.65 | 1.11        | 1.23     | 14     | 15    |
| 1   | A     | 95  | VAL  | C-N   | -10.29 | 1.19        | 1.33     | 5      | 16    |
| 1   | A     | 43  | GLY  | N-CA  | -10.04 | 1.35        | 1.45     | 16     | 14    |
| 1   | A     | 56  | LEU  | C-N   | -9.97  | 1.23        | 1.34     | 14     | 17    |
| 1   | A     | 53  | PHE  | C-N   | -9.89  | 1.20        | 1.33     | 2      | 17    |
| 1   | A     | 65  | ASN  | N-CA  | -9.80  | 1.33        | 1.46     | 3      | 10    |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) | Models |       |
|-----|-------|-----|------|--------|-------|-------------|----------|--------|-------|
|     |       |     |      |        |       |             |          | Worst  | Total |
| 1   | A     | 115 | LYS  | N-CA   | -9.49 | 1.33        | 1.45     | 9      | 17    |
| 1   | A     | 117 | LEU  | N-CA   | -9.48 | 1.33        | 1.46     | 7      | 17    |
| 1   | A     | 54  | GLN  | C-N    | -9.37 | 1.21        | 1.33     | 1      | 17    |
| 1   | A     | 75  | LEU  | N-CA   | -9.26 | 1.35        | 1.46     | 14     | 17    |
| 1   | A     | 39  | PHE  | N-CA   | -9.25 | 1.34        | 1.45     | 17     | 17    |
| 1   | A     | 40  | SER  | C-N    | -9.18 | 1.20        | 1.33     | 2      | 1     |
| 1   | A     | 61  | ALA  | N-CA   | -9.02 | 1.34        | 1.46     | 7      | 14    |
| 1   | A     | 96  | ASP  | C-N    | -8.95 | 1.21        | 1.33     | 2      | 2     |
| 1   | A     | 100 | ASN  | CG-ND2 | -8.61 | 1.15        | 1.33     | 11     | 1     |
| 1   | A     | 42  | GLU  | C-N    | -8.59 | 1.25        | 1.33     | 14     | 16    |
| 1   | A     | 82  | TRP  | CA-C   | -8.56 | 1.41        | 1.52     | 6      | 17    |
| 1   | A     | 56  | LEU  | CA-CB  | -8.54 | 1.40        | 1.53     | 2      | 17    |
| 1   | A     | 113 | ALA  | N-CA   | -8.51 | 1.35        | 1.46     | 1      | 17    |
| 1   | A     | 110 | VAL  | CA-CB  | -8.48 | 1.43        | 1.54     | 7      | 17    |
| 1   | A     | 42  | GLU  | N-CA   | -8.47 | 1.36        | 1.46     | 12     | 15    |
| 1   | A     | 113 | ALA  | CA-CB  | -8.41 | 1.40        | 1.53     | 13     | 17    |
| 1   | A     | 117 | LEU  | CA-CB  | -8.40 | 1.39        | 1.53     | 11     | 8     |
| 1   | A     | 110 | VAL  | C-N    | -8.35 | 1.22        | 1.33     | 7      | 17    |
| 1   | A     | 81  | SER  | C-N    | -8.30 | 1.22        | 1.33     | 2      | 15    |
| 1   | A     | 64  | MET  | N-CA   | -8.28 | 1.38        | 1.46     | 13     | 14    |
| 1   | A     | 29  | ALA  | N-CA   | -8.27 | 1.36        | 1.46     | 3      | 17    |
| 1   | A     | 59  | ARG  | N-CA   | -8.23 | 1.37        | 1.47     | 11     | 17    |
| 1   | A     | 97  | LEU  | N-CA   | -8.16 | 1.35        | 1.46     | 5      | 4     |
| 1   | A     | 84  | TYR  | N-CA   | -8.04 | 1.35        | 1.46     | 4      | 10    |
| 1   | A     | 85  | LEU  | C-N    | -7.96 | 1.22        | 1.33     | 4      | 17    |
| 1   | A     | 97  | LEU  | CA-CB  | -7.91 | 1.41        | 1.53     | 16     | 17    |
| 1   | A     | 34  | ARG  | N-CA   | -7.90 | 1.36        | 1.46     | 16     | 17    |
| 1   | A     | 74  | ALA  | C-N    | -7.82 | 1.24        | 1.33     | 14     | 17    |
| 1   | A     | 31  | LEU  | C-O    | -7.74 | 1.15        | 1.24     | 8      | 17    |
| 1   | A     | 73  | SER  | N-CA   | -7.71 | 1.36        | 1.46     | 9      | 17    |
| 1   | A     | 87  | GLY  | C-O    | -7.67 | 1.13        | 1.23     | 15     | 16    |
| 1   | A     | 108 | GLN  | N-CA   | -7.58 | 1.36        | 1.46     | 7      | 5     |
| 1   | A     | 57  | VAL  | CA-CB  | -7.57 | 1.42        | 1.54     | 6      | 16    |
| 1   | A     | 55  | ASP  | C-N    | -7.50 | 1.24        | 1.33     | 12     | 17    |
| 1   | A     | 60  | VAL  | C-N    | -7.48 | 1.24        | 1.33     | 5      | 15    |
| 1   | A     | 56  | LEU  | CB-CG  | -7.46 | 1.38        | 1.53     | 6      | 17    |
| 1   | A     | 43  | GLY  | CA-C   | -7.43 | 1.47        | 1.52     | 14     | 1     |
| 1   | A     | 42  | GLU  | CA-C   | -7.42 | 1.43        | 1.52     | 12     | 13    |
| 1   | A     | 101 | PRO  | CA-C   | -7.33 | 1.45        | 1.53     | 4      | 17    |
| 1   | A     | 52  | ILE  | C-O    | -7.27 | 1.15        | 1.24     | 8      | 16    |
| 1   | A     | 53  | PHE  | N-CA   | -7.26 | 1.37        | 1.46     | 10     | 14    |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) | Models |       |
|-----|-------|-----|------|--------|-------|-------------|----------|--------|-------|
|     |       |     |      |        |       |             |          | Worst  | Total |
| 1   | A     | 28  | ILE  | CA-C   | -7.19 | 1.43        | 1.52     | 5      | 17    |
| 1   | A     | 111 | GLU  | N-CA   | -7.12 | 1.37        | 1.46     | 7      | 17    |
| 1   | A     | 32  | ALA  | CA-CB  | -7.09 | 1.41        | 1.53     | 5      | 17    |
| 1   | A     | 43  | GLY  | C-N    | -7.08 | 1.23        | 1.33     | 17     | 1     |
| 1   | A     | 73  | SER  | CA-CB  | -7.01 | 1.42        | 1.53     | 2      | 17    |
| 1   | A     | 97  | LEU  | CB-CG  | -6.97 | 1.39        | 1.53     | 11     | 8     |
| 1   | A     | 62  | GLY  | C-N    | -6.97 | 1.25        | 1.33     | 1      | 8     |
| 1   | A     | 60  | VAL  | N-CA   | -6.95 | 1.38        | 1.46     | 1      | 3     |
| 1   | A     | 40  | SER  | N-CA   | -6.94 | 1.36        | 1.46     | 2      | 2     |
| 1   | A     | 73  | SER  | C-N    | -6.91 | 1.23        | 1.33     | 11     | 5     |
| 1   | A     | 31  | LEU  | C-N    | -6.91 | 1.23        | 1.33     | 1      | 17    |
| 1   | A     | 87  | GLY  | CA-C   | -6.90 | 1.42        | 1.51     | 10     | 13    |
| 1   | A     | 92  | ALA  | C-N    | -6.89 | 1.25        | 1.33     | 17     | 14    |
| 1   | A     | 68  | LYS  | C-O    | -6.87 | 1.15        | 1.24     | 11     | 17    |
| 1   | A     | 65  | ASN  | CA-CB  | -6.85 | 1.48        | 1.53     | 2      | 1     |
| 1   | A     | 49  | LYS  | C-O    | -6.78 | 1.15        | 1.23     | 12     | 5     |
| 1   | A     | 28  | ILE  | C-O    | -6.77 | 1.16        | 1.24     | 7      | 11    |
| 1   | A     | 49  | LYS  | CA-CB  | -6.74 | 1.43        | 1.53     | 4      | 2     |
| 1   | A     | 92  | ALA  | CA-C   | -6.74 | 1.44        | 1.52     | 7      | 7     |
| 1   | A     | 109 | HIS  | N-CA   | -6.72 | 1.37        | 1.45     | 1      | 17    |
| 1   | A     | 112 | HIS  | C-N    | -6.72 | 1.24        | 1.33     | 1      | 17    |
| 1   | A     | 41  | ALA  | CA-CB  | -6.70 | 1.42        | 1.53     | 10     | 15    |
| 1   | A     | 46  | ARG  | NE-CZ  | 6.70  | 1.40        | 1.33     | 16     | 1     |
| 1   | A     | 117 | LEU  | C-O    | -6.66 | 1.15        | 1.24     | 7      | 4     |
| 1   | A     | 28  | ILE  | C-N    | -6.61 | 1.25        | 1.33     | 9      | 17    |
| 1   | A     | 49  | LYS  | N-CA   | -6.57 | 1.38        | 1.45     | 7      | 6     |
| 1   | A     | 109 | HIS  | CA-CB  | -6.51 | 1.45        | 1.54     | 1      | 17    |
| 1   | A     | 25  | LYS  | N-CA   | -6.47 | 1.38        | 1.46     | 14     | 8     |
| 1   | A     | 65  | ASN  | CG-ND2 | -6.46 | 1.19        | 1.33     | 1      | 6     |
| 1   | A     | 81  | SER  | N-CA   | -6.43 | 1.37        | 1.45     | 2      | 2     |
| 1   | A     | 53  | PHE  | CG-CD2 | -6.40 | 1.25        | 1.38     | 11     | 10    |
| 1   | A     | 40  | SER  | CA-C   | -6.38 | 1.49        | 1.52     | 7      | 3     |
| 1   | A     | 89  | LYS  | CA-C   | -6.34 | 1.44        | 1.52     | 7      | 1     |
| 1   | A     | 62  | GLY  | N-CA   | -6.34 | 1.36        | 1.45     | 11     | 2     |
| 1   | A     | 103 | GLY  | C-N    | -6.30 | 1.24        | 1.33     | 6      | 17    |
| 1   | A     | 109 | HIS  | C-N    | -6.27 | 1.27        | 1.33     | 3      | 5     |
| 1   | A     | 53  | PHE  | CA-CB  | -6.23 | 1.43        | 1.53     | 10     | 12    |
| 1   | A     | 82  | TRP  | C-N    | -6.21 | 1.25        | 1.33     | 3      | 3     |
| 1   | A     | 64  | MET  | C-N    | -6.20 | 1.25        | 1.33     | 11     | 9     |
| 1   | A     | 59  | ARG  | CA-C   | -6.18 | 1.47        | 1.52     | 7      | 2     |
| 1   | A     | 37  | HIS  | C-N    | -6.17 | 1.25        | 1.33     | 17     | 3     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) | Models |       |
|-----|-------|-----|------|--------|-------|-------------|----------|--------|-------|
|     |       |     |      |        |       |             |          | Worst  | Total |
| 1   | A     | 29  | ALA  | CA-CB  | -6.16 | 1.43        | 1.53     | 11     | 17    |
| 1   | A     | 21  | LEU  | N-CA   | -6.16 | 1.38        | 1.46     | 7      | 5     |
| 1   | A     | 63  | GLU  | N-CA   | -6.16 | 1.39        | 1.46     | 15     | 4     |
| 1   | A     | 52  | ILE  | CB-CG1 | -6.15 | 1.41        | 1.53     | 10     | 3     |
| 1   | A     | 38  | CYS  | C-N    | -6.12 | 1.25        | 1.33     | 10     | 6     |
| 1   | A     | 33  | GLU  | C-N    | -6.10 | 1.25        | 1.33     | 4      | 12    |
| 1   | A     | 104 | GLU  | N-CA   | -6.09 | 1.38        | 1.46     | 13     | 13    |
| 1   | A     | 42  | GLU  | CA-CB  | -6.07 | 1.43        | 1.53     | 13     | 9     |
| 1   | A     | 117 | LEU  | CA-C   | -5.99 | 1.44        | 1.52     | 2      | 5     |
| 1   | A     | 94  | ARG  | N-CA   | -5.97 | 1.38        | 1.46     | 11     | 4     |
| 1   | A     | 38  | CYS  | N-CA   | -5.97 | 1.39        | 1.46     | 4      | 3     |
| 1   | A     | 65  | ASN  | C-N    | -5.97 | 1.25        | 1.33     | 10     | 4     |
| 1   | A     | 107 | GLU  | CA-CB  | -5.95 | 1.45        | 1.54     | 14     | 7     |
| 1   | A     | 66  | LEU  | C-N    | -5.92 | 1.26        | 1.33     | 10     | 3     |
| 1   | A     | 53  | PHE  | CG-CD1 | -5.92 | 1.26        | 1.38     | 15     | 7     |
| 1   | A     | 25  | LYS  | C-N    | -5.92 | 1.25        | 1.33     | 5      | 2     |
| 1   | A     | 75  | LEU  | CA-CB  | -5.91 | 1.45        | 1.53     | 2      | 17    |
| 1   | A     | 22  | ASN  | CG-ND2 | -5.86 | 1.21        | 1.33     | 7      | 3     |
| 1   | A     | 101 | PRO  | N-CD   | -5.85 | 1.39        | 1.47     | 8      | 13    |
| 1   | A     | 105 | LEU  | N-CA   | -5.83 | 1.38        | 1.45     | 17     | 12    |
| 1   | A     | 114 | ARG  | N-CA   | -5.79 | 1.38        | 1.46     | 11     | 6     |
| 1   | A     | 92  | ALA  | CA-CB  | -5.78 | 1.43        | 1.53     | 5      | 4     |
| 1   | A     | 100 | ASN  | CA-C   | -5.78 | 1.45        | 1.52     | 4      | 5     |
| 1   | A     | 41  | ALA  | CA-C   | -5.75 | 1.45        | 1.52     | 9      | 4     |
| 1   | A     | 97  | LEU  | CG-CD2 | -5.74 | 1.33        | 1.52     | 14     | 7     |
| 1   | A     | 50  | ILE  | C-N    | -5.71 | 1.27        | 1.33     | 10     | 9     |
| 1   | A     | 97  | LEU  | C-N    | -5.70 | 1.25        | 1.33     | 1      | 1     |
| 1   | A     | 30  | PHE  | CA-C   | -5.66 | 1.45        | 1.52     | 12     | 6     |
| 1   | A     | 69  | THR  | N-CA   | -5.64 | 1.39        | 1.46     | 3      | 1     |
| 1   | A     | 60  | VAL  | CB-CG1 | -5.60 | 1.34        | 1.52     | 12     | 12    |
| 1   | A     | 54  | GLN  | CG-CD  | -5.57 | 1.38        | 1.52     | 3      | 6     |
| 1   | A     | 40  | SER  | C-O    | -5.56 | 1.17        | 1.24     | 16     | 1     |
| 1   | A     | 21  | LEU  | CA-CB  | -5.56 | 1.44        | 1.53     | 1      | 1     |
| 1   | A     | 110 | VAL  | CA-C   | -5.54 | 1.45        | 1.52     | 5      | 2     |
| 1   | A     | 115 | LYS  | C-O    | -5.52 | 1.17        | 1.23     | 6      | 2     |
| 1   | A     | 77  | LEU  | CA-C   | -5.51 | 1.47        | 1.53     | 11     | 1     |
| 1   | A     | 56  | LEU  | CG-CD2 | -5.50 | 1.34        | 1.52     | 17     | 16    |
| 1   | A     | 21  | LEU  | C-N    | -5.46 | 1.26        | 1.33     | 15     | 1     |
| 1   | A     | 95  | VAL  | CA-C   | 5.44  | 1.59        | 1.52     | 14     | 2     |
| 1   | A     | 93  | THR  | N-CA   | -5.43 | 1.39        | 1.46     | 7      | 2     |
| 1   | A     | 108 | GLN  | CA-C   | -5.40 | 1.44        | 1.52     | 10     | 3     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) | Models |       |
|-----|-------|-----|------|--------|-------|-------------|----------|--------|-------|
|     |       |     |      |        |       |             |          | Worst  | Total |
| 1   | A     | 90  | PRO  | N-CA   | -5.39 | 1.40        | 1.47     | 7      | 1     |
| 1   | A     | 55  | ASP  | C-O    | -5.34 | 1.16        | 1.23     | 7      | 1     |
| 1   | A     | 31  | LEU  | N-CA   | -5.33 | 1.39        | 1.46     | 16     | 1     |
| 1   | A     | 113 | ALA  | CA-C   | -5.33 | 1.45        | 1.52     | 11     | 1     |
| 1   | A     | 83  | ARG  | CA-CB  | -5.32 | 1.44        | 1.53     | 7      | 1     |
| 1   | A     | 69  | THR  | C-N    | -5.31 | 1.25        | 1.33     | 15     | 3     |
| 1   | A     | 30  | PHE  | C-O    | -5.29 | 1.18        | 1.24     | 10     | 3     |
| 1   | A     | 82  | TRP  | CG-CD2 | -5.29 | 1.34        | 1.43     | 2      | 1     |
| 1   | A     | 45  | ALA  | C-N    | -5.25 | 1.26        | 1.33     | 11     | 1     |
| 1   | A     | 72  | ARG  | C-N    | -5.22 | 1.26        | 1.33     | 17     | 3     |
| 1   | A     | 106 | ASP  | C-N    | -5.20 | 1.25        | 1.33     | 7      | 3     |
| 1   | A     | 40  | SER  | CA-CB  | -5.19 | 1.47        | 1.53     | 7      | 2     |
| 1   | A     | 27  | VAL  | C-O    | -5.17 | 1.18        | 1.24     | 1      | 2     |
| 1   | A     | 60  | VAL  | CA-CB  | -5.16 | 1.48        | 1.54     | 1      | 1     |
| 1   | A     | 27  | VAL  | CA-C   | -5.16 | 1.46        | 1.52     | 17     | 1     |
| 1   | A     | 61  | ALA  | CA-C   | -5.15 | 1.45        | 1.52     | 3      | 2     |
| 1   | A     | 83  | ARG  | C-N    | -5.15 | 1.26        | 1.33     | 3      | 2     |
| 1   | A     | 62  | GLY  | CA-C   | -5.14 | 1.44        | 1.51     | 15     | 1     |
| 1   | A     | 21  | LEU  | CG-CD1 | -5.13 | 1.35        | 1.52     | 1      | 2     |
| 1   | A     | 50  | ILE  | CA-CB  | -5.12 | 1.47        | 1.54     | 2      | 2     |
| 1   | A     | 107 | GLU  | C-N    | -5.11 | 1.26        | 1.33     | 7      | 2     |
| 1   | A     | 81  | SER  | CA-C   | -5.09 | 1.46        | 1.53     | 8      | 3     |
| 1   | A     | 109 | HIS  | CA-C   | -5.07 | 1.45        | 1.52     | 5      | 1     |
| 1   | A     | 51  | GLY  | C-O    | -5.05 | 1.18        | 1.24     | 10     | 1     |
| 1   | A     | 110 | VAL  | N-CA   | -5.04 | 1.40        | 1.46     | 10     | 1     |
| 1   | A     | 48  | LEU  | C-O    | -5.02 | 1.17        | 1.24     | 11     | 1     |
| 1   | A     | 86  | TYR  | CA-CB  | -5.01 | 1.44        | 1.53     | 7      | 1     |
| 1   | A     | 100 | ASN  | CA-CB  | -5.00 | 1.47        | 1.53     | 1      | 1     |

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

| Mol | Chain | Res | Type | Atoms    | Z      | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|----------|--------|-------------|----------|--------|-------|
|     |       |     |      |          |        |             |          | Worst  | Total |
| 1   | A     | 65  | ASN  | CA-CB-CG | 10.99  | 123.59      | 112.60   | 4      | 13    |
| 1   | A     | 96  | ASP  | N-CA-C   | -10.92 | 92.81       | 109.41   | 16     | 9     |
| 1   | A     | 60  | VAL  | N-CA-C   | 9.57   | 119.61      | 110.42   | 8      | 17    |
| 1   | A     | 61  | ALA  | N-CA-C   | 9.37   | 124.11      | 112.87   | 3      | 4     |
| 1   | A     | 55  | ASP  | CA-CB-CG | 8.87   | 121.47      | 112.60   | 17     | 11    |
| 1   | A     | 41  | ALA  | CA-C-N   | 8.55   | 131.56      | 120.44   | 7      | 13    |
| 1   | A     | 41  | ALA  | C-N-CA   | 8.55   | 131.56      | 120.44   | 7      | 13    |
| 1   | A     | 75  | LEU  | N-CA-CB  | -8.08  | 98.83       | 110.79   | 14     | 17    |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|----------|-------|-------------|----------|--------|-------|
|     |       |     |      |          |       |             |          | Worst  | Total |
| 1   | A     | 106 | ASP  | CA-CB-CG | 7.83  | 120.43      | 112.60   | 17     | 16    |
| 1   | A     | 95  | VAL  | CA-C-N   | 7.76  | 135.86      | 122.82   | 16     | 6     |
| 1   | A     | 95  | VAL  | C-N-CA   | 7.76  | 135.86      | 122.82   | 16     | 6     |
| 1   | A     | 91  | GLY  | CA-C-N   | 7.69  | 130.59      | 120.28   | 7      | 16    |
| 1   | A     | 91  | GLY  | C-N-CA   | 7.69  | 130.59      | 120.28   | 7      | 16    |
| 1   | A     | 54  | GLN  | N-CA-CB  | -7.57 | 96.56       | 110.18   | 2      | 17    |
| 1   | A     | 95  | VAL  | N-CA-C   | 7.43  | 118.46      | 108.27   | 1      | 8     |
| 1   | A     | 98  | ASP  | N-CA-C   | -7.27 | 104.21      | 113.23   | 12     | 17    |
| 1   | A     | 110 | VAL  | CA-C-N   | 7.18  | 129.90      | 120.28   | 8      | 16    |
| 1   | A     | 110 | VAL  | C-N-CA   | 7.18  | 129.90      | 120.28   | 8      | 16    |
| 1   | A     | 108 | GLN  | N-CA-C   | -6.83 | 104.52      | 112.92   | 15     | 16    |
| 1   | A     | 100 | ASN  | CA-CB-CG | 6.75  | 119.35      | 112.60   | 11     | 2     |
| 1   | A     | 76  | ARG  | CA-CB-CG | 6.73  | 127.55      | 114.10   | 11     | 1     |
| 1   | A     | 42  | GLU  | CB-CA-C  | -6.71 | 100.35      | 110.88   | 12     | 5     |
| 1   | A     | 46  | ARG  | N-CA-C   | -6.68 | 102.21      | 108.22   | 6      | 1     |
| 1   | A     | 21  | LEU  | N-CA-CB  | -6.63 | 99.74       | 109.82   | 4      | 3     |
| 1   | A     | 56  | LEU  | N-CA-CB  | -6.62 | 100.25      | 109.91   | 7      | 17    |
| 1   | A     | 58  | ASP  | CB-CA-C  | -6.61 | 100.24      | 110.81   | 1      | 5     |
| 1   | A     | 100 | ASN  | N-CA-C   | -6.45 | 102.01      | 110.39   | 4      | 15    |
| 1   | A     | 88  | VAL  | CB-CA-C  | -6.38 | 101.44      | 110.12   | 13     | 12    |
| 1   | A     | 50  | ILE  | CB-CA-C  | 6.33  | 116.63      | 111.06   | 6      | 3     |
| 1   | A     | 52  | ILE  | CB-CA-C  | -6.30 | 103.78      | 112.04   | 12     | 14    |
| 1   | A     | 40  | SER  | CA-C-N   | 6.27  | 133.52      | 121.54   | 17     | 1     |
| 1   | A     | 40  | SER  | C-N-CA   | 6.27  | 133.52      | 121.54   | 17     | 1     |
| 1   | A     | 89  | LYS  | N-CA-CB  | 6.24  | 121.47      | 110.37   | 7      | 2     |
| 1   | A     | 73  | SER  | N-CA-CB  | -6.20 | 100.76      | 110.44   | 1      | 6     |
| 1   | A     | 115 | LYS  | N-CA-C   | -6.18 | 106.06      | 113.97   | 17     | 12    |
| 1   | A     | 106 | ASP  | N-CA-CB  | -6.12 | 100.15      | 110.49   | 17     | 17    |
| 1   | A     | 39  | PHE  | N-CA-CB  | -6.09 | 101.91      | 111.05   | 1      | 15    |
| 1   | A     | 76  | ARG  | N-CA-C   | -6.06 | 106.49      | 114.31   | 16     | 7     |
| 1   | A     | 74  | ALA  | N-CA-C   | -6.04 | 104.63      | 112.23   | 11     | 1     |
| 1   | A     | 56  | LEU  | N-CA-C   | -6.00 | 104.43      | 110.97   | 16     | 15    |
| 1   | A     | 96  | ASP  | N-CA-CB  | -5.90 | 104.71      | 111.79   | 10     | 2     |
| 1   | A     | 21  | LEU  | N-CA-C   | 5.84  | 123.23      | 110.80   | 1      | 2     |
| 1   | A     | 49  | LYS  | N-CA-C   | -5.78 | 101.45      | 110.42   | 10     | 2     |
| 1   | A     | 96  | ASP  | CA-C-N   | 5.78  | 132.59      | 121.54   | 4      | 5     |
| 1   | A     | 96  | ASP  | C-N-CA   | 5.78  | 132.59      | 121.54   | 4      | 5     |
| 1   | A     | 62  | GLY  | CA-C-N   | 5.78  | 127.95      | 120.44   | 1      | 1     |
| 1   | A     | 62  | GLY  | C-N-CA   | 5.78  | 127.95      | 120.44   | 1      | 1     |
| 1   | A     | 97  | LEU  | N-CA-C   | 5.75  | 123.04      | 110.80   | 1      | 5     |
| 1   | A     | 114 | ARG  | N-CA-C   | -5.68 | 106.31      | 113.18   | 16     | 5     |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|-----------|-------|-------------|----------|--------|-------|
|     |       |     |      |           |       |             |          | Worst  | Total |
| 1   | A     | 58  | ASP  | CA-CB-CG  | 5.64  | 118.24      | 112.60   | 7      | 1     |
| 1   | A     | 67  | SER  | N-CA-CB   | -5.59 | 103.82      | 111.65   | 11     | 1     |
| 1   | A     | 42  | GLU  | N-CA-CB   | -5.56 | 101.95      | 110.01   | 7      | 1     |
| 1   | A     | 37  | HIS  | CA-C-N    | 5.55  | 128.03      | 120.54   | 14     | 4     |
| 1   | A     | 37  | HIS  | C-N-CA    | 5.55  | 128.03      | 120.54   | 14     | 4     |
| 1   | A     | 60  | VAL  | CB-CA-C   | -5.53 | 104.89      | 111.97   | 10     | 11    |
| 1   | A     | 40  | SER  | N-CA-CB   | -5.48 | 101.22      | 110.49   | 17     | 1     |
| 1   | A     | 85  | LEU  | N-CA-C    | 5.41  | 119.59      | 113.15   | 3      | 4     |
| 1   | A     | 68  | LYS  | N-CA-CB   | 5.38  | 119.58      | 110.49   | 4      | 5     |
| 1   | A     | 110 | VAL  | CA-CB-CG1 | -5.38 | 101.26      | 110.40   | 5      | 2     |
| 1   | A     | 58  | ASP  | CA-C-N    | 5.35  | 129.15      | 121.71   | 11     | 1     |
| 1   | A     | 58  | ASP  | C-N-CA    | 5.35  | 129.15      | 121.71   | 11     | 1     |
| 1   | A     | 75  | LEU  | CA-C-N    | 5.35  | 131.75      | 121.54   | 10     | 7     |
| 1   | A     | 75  | LEU  | C-N-CA    | 5.35  | 131.75      | 121.54   | 10     | 7     |
| 1   | A     | 34  | ARG  | N-CA-CB   | -5.33 | 102.31      | 110.26   | 11     | 1     |
| 1   | A     | 110 | VAL  | O-C-N     | 5.29  | 126.86      | 122.09   | 6      | 4     |
| 1   | A     | 65  | ASN  | N-CA-CB   | -5.26 | 103.91      | 111.54   | 7      | 2     |
| 1   | A     | 95  | VAL  | CA-C-O    | 5.26  | 126.27      | 120.64   | 1      | 1     |
| 1   | A     | 55  | ASP  | N-CA-C    | -5.15 | 106.69      | 113.12   | 7      | 1     |
| 1   | A     | 97  | LEU  | CB-CA-C   | 5.11  | 120.43      | 110.57   | 14     | 1     |
| 1   | A     | 100 | ASN  | CA-C-O    | -5.08 | 115.92      | 120.19   | 11     | 1     |
| 1   | A     | 86  | TYR  | N-CA-C    | -5.06 | 106.94      | 113.01   | 4      | 1     |
| 1   | A     | 50  | ILE  | N-CA-C    | 5.06  | 116.95      | 111.58   | 16     | 1     |
| 1   | A     | 63  | GLU  | N-CA-CB   | -5.06 | 102.67      | 110.01   | 1      | 1     |

There are no chirality outliers.

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

| Mol | Chain | Res | Type | Group     | Models (Total) |
|-----|-------|-----|------|-----------|----------------|
| 1   | A     | 59  | ARG  | Sidechain | 12             |
| 1   | A     | 76  | ARG  | Sidechain | 7              |
| 1   | A     | 60  | VAL  | Peptide   | 3              |
| 1   | A     | 83  | ARG  | Sidechain | 2              |
| 1   | A     | 95  | VAL  | Peptide   | 1              |
| 1   | A     | 42  | GLU  | Peptide   | 1              |

## 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     | 770   | 767      | 764      | 141±7   |
| All | All   | 13090 | 13039    | 12978    | 2394    |

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 92.

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

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:52:ILE:HD11  | 1:A:97:LEU:HD21  | 1.05     | 1.28        | 2      | 17    |
| 1:A:38:CYS:SG    | 1:A:97:LEU:HA    | 0.95     | 2.01        | 15     | 14    |
| 1:A:105:LEU:HD13 | 1:A:110:VAL:HG13 | 0.94     | 1.39        | 9      | 17    |
| 1:A:21:LEU:HB3   | 1:A:27:VAL:HG12  | 0.93     | 1.39        | 12     | 16    |
| 1:A:105:LEU:HD21 | 1:A:109:HIS:HB2  | 0.93     | 1.40        | 2      | 17    |
| 1:A:21:LEU:HD13  | 1:A:27:VAL:HB    | 0.87     | 1.47        | 17     | 14    |
| 1:A:38:CYS:HA    | 1:A:95:VAL:HG11  | 0.84     | 1.47        | 4      | 12    |
| 1:A:105:LEU:HD23 | 1:A:106:ASP:N    | 0.83     | 1.89        | 4      | 17    |
| 1:A:31:LEU:HD11  | 1:A:71:LEU:HD21  | 0.82     | 1.48        | 6      | 17    |
| 1:A:73:SER:HA    | 1:A:76:ARG:HG3   | 0.82     | 1.49        | 11     | 1     |
| 1:A:53:PHE:O     | 1:A:57:VAL:HG13  | 0.81     | 1.75        | 10     | 17    |
| 1:A:54:GLN:HE22  | 1:A:55:ASP:HB2   | 0.81     | 1.34        | 1      | 12    |
| 1:A:105:LEU:HD13 | 1:A:110:VAL:CG1  | 0.77     | 2.10        | 2      | 17    |
| 1:A:48:LEU:HD11  | 1:A:52:ILE:HG21  | 0.76     | 1.56        | 6      | 14    |
| 1:A:56:LEU:C     | 1:A:60:VAL:HG22  | 0.76     | 2.05        | 16     | 17    |
| 1:A:86:TYR:CD1   | 1:A:117:LEU:HD12 | 0.76     | 2.15        | 2      | 5     |
| 1:A:56:LEU:HD21  | 1:A:75:LEU:HD11  | 0.74     | 1.59        | 16     | 17    |
| 1:A:53:PHE:HA    | 1:A:56:LEU:HD23  | 0.74     | 1.60        | 2      | 17    |
| 1:A:76:ARG:HD2   | 1:A:76:ARG:C     | 0.74     | 2.08        | 11     | 1     |
| 1:A:49:LYS:HG3   | 1:A:52:ILE:HB    | 0.73     | 1.59        | 10     | 8     |
| 1:A:61:ALA:HB1   | 1:A:68:LYS:HD3   | 0.73     | 1.59        | 5      | 3     |
| 1:A:38:CYS:SG    | 1:A:95:VAL:HG21  | 0.73     | 2.23        | 8      | 3     |
| 1:A:60:VAL:HG21  | 1:A:71:LEU:HD11  | 0.73     | 1.59        | 12     | 17    |
| 1:A:21:LEU:HD22  | 1:A:65:ASN:HB2   | 0.73     | 1.60        | 4      | 3     |
| 1:A:49:LYS:CG    | 1:A:52:ILE:HB    | 0.72     | 2.14        | 10     | 7     |
| 1:A:31:LEU:HD11  | 1:A:71:LEU:CD2   | 0.72     | 2.13        | 16     | 17    |
| 1:A:61:ALA:O     | 1:A:66:LEU:HB2   | 0.72     | 1.84        | 17     | 14    |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:30:PHE:O     | 1:A:33:GLU:HG2   | 0.72     | 1.85        | 1      | 17    |
| 1:A:47:PRO:HB3   | 1:A:87:GLY:O     | 0.72     | 1.85        | 7      | 16    |
| 1:A:105:LEU:HD22 | 1:A:110:VAL:HG13 | 0.71     | 1.60        | 11     | 17    |
| 1:A:31:LEU:HB3   | 1:A:39:PHE:CD1   | 0.71     | 2.20        | 16     | 8     |
| 1:A:54:GLN:C     | 1:A:57:VAL:HG22  | 0.70     | 2.11        | 8      | 17    |
| 1:A:21:LEU:HB3   | 1:A:27:VAL:CG1   | 0.70     | 2.17        | 12     | 10    |
| 1:A:92:ALA:N     | 1:A:110:VAL:HG11 | 0.70     | 2.02        | 10     | 17    |
| 1:A:21:LEU:HD21  | 1:A:30:PHE:HB2   | 0.69     | 1.65        | 13     | 10    |
| 1:A:52:ILE:HD11  | 1:A:97:LEU:CD2   | 0.69     | 2.14        | 10     | 9     |
| 1:A:53:PHE:CZ    | 1:A:72:ARG:HB3   | 0.69     | 2.23        | 3      | 17    |
| 1:A:61:ALA:HB1   | 1:A:68:LYS:CD    | 0.68     | 2.18        | 5      | 3     |
| 1:A:60:VAL:HG23  | 1:A:61:ALA:N     | 0.68     | 2.04        | 8      | 17    |
| 1:A:66:LEU:HD13  | 1:A:71:LEU:HG    | 0.68     | 1.67        | 7      | 17    |
| 1:A:56:LEU:CD2   | 1:A:75:LEU:HD11  | 0.67     | 2.19        | 12     | 17    |
| 1:A:71:LEU:HD22  | 1:A:75:LEU:HD12  | 0.67     | 1.66        | 9      | 17    |
| 1:A:60:VAL:HG21  | 1:A:71:LEU:CD1   | 0.67     | 2.19        | 1      | 17    |
| 1:A:54:GLN:HE21  | 1:A:55:ASP:N     | 0.67     | 1.87        | 10     | 11    |
| 1:A:48:LEU:HD12  | 1:A:52:ILE:HG21  | 0.67     | 1.66        | 17     | 3     |
| 1:A:53:PHE:HA    | 1:A:56:LEU:CD2   | 0.67     | 2.19        | 2      | 17    |
| 1:A:86:TYR:CD2   | 1:A:117:LEU:HD12 | 0.67     | 2.24        | 12     | 3     |
| 1:A:31:LEU:HB3   | 1:A:39:PHE:CD2   | 0.66     | 2.26        | 6      | 9     |
| 1:A:35:PHE:CD2   | 1:A:97:LEU:HB3   | 0.66     | 2.26        | 6      | 7     |
| 1:A:83:ARG:HA    | 1:A:86:TYR:CD1   | 0.66     | 2.26        | 2      | 8     |
| 1:A:105:LEU:CD1  | 1:A:110:VAL:HG13 | 0.65     | 2.21        | 14     | 17    |
| 1:A:115:LYS:O    | 1:A:115:LYS:HE3  | 0.65     | 1.91        | 8      | 2     |
| 1:A:54:GLN:NE2   | 1:A:55:ASP:HB2   | 0.65     | 2.05        | 1      | 12    |
| 1:A:105:LEU:HD21 | 1:A:109:HIS:CB   | 0.64     | 2.22        | 6      | 17    |
| 1:A:53:PHE:CE2   | 1:A:71:LEU:HD13  | 0.64     | 2.28        | 11     | 10    |
| 1:A:56:LEU:HG    | 1:A:60:VAL:HG11  | 0.64     | 1.68        | 12     | 16    |
| 1:A:61:ALA:C     | 1:A:66:LEU:HB2   | 0.64     | 2.18        | 4      | 14    |
| 1:A:91:GLY:O     | 1:A:101:PRO:HB3  | 0.64     | 1.93        | 5      | 17    |
| 1:A:105:LEU:HD22 | 1:A:110:VAL:HG22 | 0.63     | 1.70        | 5      | 17    |
| 1:A:105:LEU:CD2  | 1:A:109:HIS:HB2  | 0.63     | 2.22        | 6      | 17    |
| 1:A:21:LEU:HB2   | 1:A:65:ASN:OD1   | 0.63     | 1.93        | 14     | 2     |
| 1:A:95:VAL:HG23  | 1:A:97:LEU:H     | 0.63     | 1.53        | 6      | 4     |
| 1:A:21:LEU:HD13  | 1:A:27:VAL:CB    | 0.63     | 2.21        | 17     | 13    |
| 1:A:21:LEU:HD23  | 1:A:21:LEU:N     | 0.63     | 2.09        | 14     | 9     |
| 1:A:91:GLY:C     | 1:A:110:VAL:HG11 | 0.63     | 2.18        | 5      | 17    |
| 1:A:30:PHE:O     | 1:A:34:ARG:HB2   | 0.62     | 1.94        | 1      | 9     |
| 1:A:49:LYS:HG3   | 1:A:102:CYS:CB   | 0.62     | 2.24        | 4      | 4     |
| 1:A:21:LEU:HG    | 1:A:65:ASN:OD1   | 0.62     | 1.94        | 12     | 7     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:107:GLU:HA   | 1:A:110:VAL:CG2  | 0.62     | 2.24        | 4      | 17    |
| 1:A:89:LYS:HB3   | 1:A:90:PRO:HD3   | 0.62     | 1.71        | 16     | 12    |
| 1:A:31:LEU:HD13  | 1:A:39:PHE:CZ    | 0.62     | 2.29        | 6      | 17    |
| 1:A:87:GLY:O     | 1:A:113:ALA:HB1  | 0.62     | 1.95        | 1      | 1     |
| 1:A:57:VAL:HA    | 1:A:60:VAL:HG22  | 0.62     | 1.70        | 1      | 17    |
| 1:A:48:LEU:HG    | 1:A:49:LYS:O     | 0.62     | 1.95        | 6      | 13    |
| 1:A:37:HIS:HD2   | 1:A:38:CYS:SG    | 0.62     | 2.17        | 5      | 7     |
| 1:A:53:PHE:CE1   | 1:A:71:LEU:HD13  | 0.61     | 2.30        | 5      | 7     |
| 1:A:54:GLN:NE2   | 1:A:55:ASP:N     | 0.61     | 2.48        | 17     | 17    |
| 1:A:48:LEU:HD22  | 1:A:78:TYR:CE1   | 0.61     | 2.30        | 14     | 8     |
| 1:A:61:ALA:HA    | 1:A:66:LEU:HD12  | 0.61     | 1.71        | 4      | 14    |
| 1:A:82:TRP:CD1   | 1:A:85:LEU:HD21  | 0.61     | 2.31        | 15     | 17    |
| 1:A:73:SER:CA    | 1:A:76:ARG:HG3   | 0.61     | 2.23        | 11     | 1     |
| 1:A:86:TYR:CE1   | 1:A:117:LEU:HD12 | 0.61     | 2.30        | 2      | 3     |
| 1:A:52:ILE:CD1   | 1:A:97:LEU:HD21  | 0.61     | 2.18        | 2      | 11    |
| 1:A:52:ILE:O     | 1:A:52:ILE:HG12  | 0.61     | 1.95        | 10     | 14    |
| 1:A:55:ASP:O     | 1:A:59:ARG:HD2   | 0.60     | 1.96        | 12     | 11    |
| 1:A:95:VAL:HA    | 1:A:100:ASN:O    | 0.60     | 1.96        | 1      | 4     |
| 1:A:48:LEU:HD22  | 1:A:78:TYR:CE2   | 0.60     | 2.31        | 5      | 6     |
| 1:A:81:SER:O     | 1:A:84:TYR:HB3   | 0.60     | 1.96        | 2      | 17    |
| 1:A:48:LEU:O     | 1:A:88:VAL:HG13  | 0.60     | 1.96        | 4      | 5     |
| 1:A:21:LEU:HG    | 1:A:27:VAL:HA    | 0.60     | 1.73        | 9      | 3     |
| 1:A:35:PHE:HB3   | 1:A:38:CYS:SG    | 0.60     | 2.37        | 1      | 3     |
| 1:A:78:TYR:O     | 1:A:81:SER:HB3   | 0.59     | 1.98        | 15     | 11    |
| 1:A:66:LEU:CD1   | 1:A:71:LEU:HG    | 0.59     | 2.27        | 5      | 17    |
| 1:A:50:ILE:HG23  | 1:A:76:ARG:NH2   | 0.59     | 2.13        | 4      | 7     |
| 1:A:21:LEU:H     | 1:A:21:LEU:CD1   | 0.59     | 2.11        | 7      | 2     |
| 1:A:96:ASP:OD1   | 1:A:102:CYS:HA   | 0.59     | 1.98        | 13     | 1     |
| 1:A:90:PRO:C     | 1:A:92:ALA:H     | 0.58     | 2.06        | 2      | 10    |
| 1:A:101:PRO:C    | 1:A:103:GLY:H    | 0.58     | 2.07        | 1      | 17    |
| 1:A:105:LEU:HD11 | 1:A:109:HIS:HB2  | 0.58     | 1.75        | 15     | 17    |
| 1:A:30:PHE:CD1   | 1:A:64:MET:HE1   | 0.58     | 2.34        | 3      | 5     |
| 1:A:85:LEU:HD23  | 1:A:117:LEU:CD2  | 0.58     | 2.29        | 15     | 8     |
| 1:A:87:GLY:O     | 1:A:92:ALA:HB1   | 0.58     | 1.98        | 13     | 15    |
| 1:A:40:SER:O     | 1:A:42:GLU:HG3   | 0.58     | 1.99        | 6      | 2     |
| 1:A:48:LEU:HG    | 1:A:49:LYS:N     | 0.58     | 2.14        | 1      | 14    |
| 1:A:86:TYR:HA    | 1:A:117:LEU:CB   | 0.58     | 2.29        | 9      | 10    |
| 1:A:83:ARG:HA    | 1:A:86:TYR:CD2   | 0.58     | 2.34        | 3      | 6     |
| 1:A:32:ALA:HA    | 1:A:39:PHE:HB2   | 0.58     | 1.75        | 9      | 15    |
| 1:A:90:PRO:HA    | 1:A:104:GLU:OE2  | 0.57     | 1.98        | 7      | 1     |
| 1:A:32:ALA:HB1   | 1:A:40:SER:O     | 0.57     | 1.99        | 7      | 12    |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:40:SER:C     | 1:A:42:GLU:H     | 0.57     | 2.07        | 7      | 14    |
| 1:A:38:CYS:SG    | 1:A:97:LEU:HD23  | 0.56     | 2.41        | 5      | 13    |
| 1:A:31:LEU:HD22  | 1:A:56:LEU:HD11  | 0.56     | 1.77        | 13     | 17    |
| 1:A:73:SER:HA    | 1:A:76:ARG:CG    | 0.56     | 2.26        | 11     | 1     |
| 1:A:76:ARG:NE    | 1:A:76:ARG:HA    | 0.56     | 2.15        | 1      | 2     |
| 1:A:57:VAL:HB    | 1:A:68:LYS:HD2   | 0.56     | 1.76        | 9      | 5     |
| 1:A:51:GLY:O     | 1:A:54:GLN:HB3   | 0.56     | 2.00        | 11     | 17    |
| 1:A:56:LEU:CG    | 1:A:60:VAL:HG11  | 0.56     | 2.30        | 12     | 15    |
| 1:A:69:THR:HA    | 1:A:72:ARG:HG3   | 0.56     | 1.76        | 14     | 16    |
| 1:A:30:PHE:CD2   | 1:A:64:MET:HE1   | 0.56     | 2.36        | 13     | 2     |
| 1:A:69:THR:O     | 1:A:72:ARG:HG3   | 0.56     | 2.01        | 4      | 16    |
| 1:A:101:PRO:C    | 1:A:103:GLY:N    | 0.55     | 2.65        | 5      | 17    |
| 1:A:87:GLY:C     | 1:A:92:ALA:HB1   | 0.55     | 2.26        | 7      | 16    |
| 1:A:52:ILE:O     | 1:A:55:ASP:HB2   | 0.55     | 2.01        | 8      | 5     |
| 1:A:86:TYR:CD1   | 1:A:117:LEU:HD13 | 0.55     | 2.35        | 14     | 6     |
| 1:A:72:ARG:O     | 1:A:76:ARG:HD2   | 0.55     | 2.02        | 13     | 12    |
| 1:A:53:PHE:HD2   | 1:A:75:LEU:HD13  | 0.55     | 1.61        | 17     | 10    |
| 1:A:113:ALA:O    | 1:A:116:GLN:HG3  | 0.55     | 2.00        | 1      | 16    |
| 1:A:60:VAL:CG2   | 1:A:61:ALA:N     | 0.55     | 2.69        | 12     | 17    |
| 1:A:105:LEU:HD11 | 1:A:109:HIS:CB   | 0.55     | 2.32        | 15     | 17    |
| 1:A:105:LEU:HD23 | 1:A:106:ASP:C    | 0.55     | 2.26        | 11     | 17    |
| 1:A:44:GLU:OE2   | 1:A:83:ARG:HB2   | 0.55     | 2.02        | 7      | 1     |
| 1:A:57:VAL:HA    | 1:A:60:VAL:CG2   | 0.55     | 2.32        | 1      | 17    |
| 1:A:112:HIS:HA   | 1:A:115:LYS:HG2  | 0.55     | 1.79        | 13     | 3     |
| 1:A:49:LYS:HG3   | 1:A:52:ILE:CB    | 0.54     | 2.32        | 10     | 4     |
| 1:A:52:ILE:HG12  | 1:A:52:ILE:O     | 0.54     | 1.94        | 7      | 2     |
| 1:A:68:LYS:N     | 1:A:68:LYS:HD3   | 0.54     | 2.15        | 17     | 4     |
| 1:A:106:ASP:CG   | 1:A:107:GLU:H    | 0.54     | 2.10        | 5      | 17    |
| 1:A:53:PHE:HD1   | 1:A:75:LEU:HD13  | 0.54     | 1.62        | 2      | 7     |
| 1:A:56:LEU:O     | 1:A:60:VAL:HG22  | 0.54     | 2.02        | 6      | 17    |
| 1:A:108:GLN:HA   | 1:A:111:GLU:HB2  | 0.54     | 1.79        | 7      | 17    |
| 1:A:91:GLY:N     | 1:A:104:GLU:HG2  | 0.54     | 2.18        | 7      | 1     |
| 1:A:101:PRO:HG2  | 1:A:105:LEU:O    | 0.53     | 2.02        | 11     | 17    |
| 1:A:86:TYR:CD2   | 1:A:117:LEU:HD13 | 0.53     | 2.38        | 16     | 3     |
| 1:A:105:LEU:CD2  | 1:A:110:VAL:HG13 | 0.53     | 2.33        | 11     | 17    |
| 1:A:54:GLN:C     | 1:A:54:GLN:NE2   | 0.53     | 2.67        | 10     | 16    |
| 1:A:107:GLU:HA   | 1:A:110:VAL:HG22 | 0.53     | 1.78        | 13     | 17    |
| 1:A:114:ARG:O    | 1:A:114:ARG:HD3  | 0.53     | 2.03        | 11     | 1     |
| 1:A:82:TRP:CE2   | 1:A:117:LEU:HD11 | 0.53     | 2.39        | 2      | 8     |
| 1:A:31:LEU:HB3   | 1:A:39:PHE:CE1   | 0.53     | 2.39        | 8      | 8     |
| 1:A:35:PHE:CD1   | 1:A:97:LEU:HB3   | 0.52     | 2.39        | 5      | 8     |

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| Atom-1           | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|------------------|-----------------|----------|-------------|--------|-------|
|                  |                 |          |             | Worst  | Total |
| 1:A:37:HIS:CD2   | 1:A:38:CYS:SG   | 0.52     | 3.02        | 1      | 5     |
| 1:A:38:CYS:CB    | 1:A:95:VAL:HG21 | 0.52     | 2.34        | 1      | 5     |
| 1:A:30:PHE:CG    | 1:A:64:MET:HE1  | 0.52     | 2.39        | 16     | 2     |
| 1:A:49:LYS:HE2   | 1:A:96:ASP:HA   | 0.52     | 1.81        | 15     | 1     |
| 1:A:96:ASP:CG    | 1:A:100:ASN:HB2 | 0.52     | 2.29        | 6      | 5     |
| 1:A:89:LYS:HB2   | 1:A:90:PRO:HD3  | 0.52     | 1.81        | 10     | 2     |
| 1:A:111:GLU:O    | 1:A:114:ARG:HB3 | 0.52     | 2.03        | 13     | 3     |
| 1:A:52:ILE:HG23  | 1:A:53:PHE:N    | 0.52     | 2.19        | 12     | 10    |
| 1:A:117:LEU:O    | 1:A:117:LEU:HG  | 0.52     | 2.04        | 6      | 9     |
| 1:A:55:ASP:HB3   | 1:A:97:LEU:HD12 | 0.52     | 1.82        | 15     | 10    |
| 1:A:40:SER:HB3   | 1:A:43:GLY:H    | 0.51     | 1.65        | 15     | 9     |
| 1:A:31:LEU:HB3   | 1:A:39:PHE:CE2  | 0.51     | 2.40        | 6      | 9     |
| 1:A:44:GLU:HB3   | 1:A:83:ARG:HD3  | 0.51     | 1.81        | 10     | 2     |
| 1:A:48:LEU:HD23  | 1:A:84:TYR:HE1  | 0.51     | 1.65        | 5      | 5     |
| 1:A:31:LEU:O     | 1:A:35:PHE:HB2  | 0.51     | 2.05        | 3      | 17    |
| 1:A:25:LYS:HG2   | 1:A:26:GLU:CD   | 0.51     | 2.31        | 11     | 6     |
| 1:A:48:LEU:HD22  | 1:A:78:TYR:HE1  | 0.51     | 1.66        | 7      | 7     |
| 1:A:27:VAL:O     | 1:A:31:LEU:HG   | 0.50     | 2.06        | 1      | 16    |
| 1:A:37:HIS:CD2   | 1:A:95:VAL:HG12 | 0.50     | 2.42        | 12     | 3     |
| 1:A:28:ILE:HG13  | 1:A:78:TYR:HB3  | 0.50     | 1.82        | 10     | 10    |
| 1:A:35:PHE:CE2   | 1:A:97:LEU:HB3  | 0.50     | 2.42        | 6      | 2     |
| 1:A:88:VAL:O     | 1:A:89:LYS:HG2  | 0.50     | 2.07        | 10     | 2     |
| 1:A:21:LEU:HD23  | 1:A:27:VAL:HB   | 0.50     | 1.83        | 4      | 3     |
| 1:A:92:ALA:HA    | 1:A:110:VAL:HB  | 0.50     | 1.84        | 2      | 11    |
| 1:A:32:ALA:HB3   | 1:A:41:ALA:HB2  | 0.50     | 1.82        | 9      | 14    |
| 1:A:72:ARG:HD3   | 1:A:72:ARG:C    | 0.50     | 2.32        | 11     | 17    |
| 1:A:25:LYS:HG3   | 1:A:26:GLU:OE2  | 0.49     | 2.07        | 14     | 1     |
| 1:A:25:LYS:HB3   | 1:A:26:GLU:OE2  | 0.49     | 2.07        | 7      | 3     |
| 1:A:115:LYS:O    | 1:A:115:LYS:HE2 | 0.49     | 2.08        | 9      | 2     |
| 1:A:48:LEU:HD21  | 1:A:75:LEU:HD23 | 0.49     | 1.84        | 8      | 1     |
| 1:A:69:THR:HA    | 1:A:72:ARG:CG   | 0.49     | 2.37        | 3      | 17    |
| 1:A:48:LEU:CD1   | 1:A:52:ILE:HG21 | 0.49     | 2.37        | 2      | 4     |
| 1:A:88:VAL:HA    | 1:A:92:ALA:HB3  | 0.49     | 1.85        | 14     | 5     |
| 1:A:105:LEU:HD23 | 1:A:106:ASP:H   | 0.49     | 1.67        | 9      | 9     |
| 1:A:66:LEU:HA    | 1:A:70:GLN:CD   | 0.49     | 2.33        | 14     | 2     |
| 1:A:30:PHE:CE1   | 1:A:60:VAL:HB   | 0.48     | 2.43        | 13     | 6     |
| 1:A:85:LEU:HA    | 1:A:88:VAL:HG23 | 0.48     | 1.84        | 2      | 9     |
| 1:A:54:GLN:C     | 1:A:54:GLN:HE21 | 0.48     | 2.15        | 10     | 9     |
| 1:A:21:LEU:CD1   | 1:A:27:VAL:HB   | 0.48     | 2.32        | 17     | 3     |
| 1:A:87:GLY:HA2   | 1:A:113:ALA:O   | 0.48     | 2.08        | 1      | 5     |
| 1:A:85:LEU:HD13  | 1:A:85:LEU:H    | 0.48     | 1.68        | 17     | 16    |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:A:113:ALA:HA  | 1:A:116:GLN:CG   | 0.48     | 2.39        | 9      | 14    |
| 1:A:116:GLN:NE2 | 1:A:117:LEU:HD23 | 0.48     | 2.24        | 2      | 2     |
| 1:A:95:VAL:HA   | 1:A:99:GLY:HA2   | 0.48     | 1.86        | 12     | 3     |
| 1:A:35:PHE:CD1  | 1:A:97:LEU:HD22  | 0.48     | 2.43        | 16     | 3     |
| 1:A:91:GLY:CA   | 1:A:104:GLU:HG2  | 0.48     | 2.38        | 8      | 15    |
| 1:A:21:LEU:HD11 | 1:A:30:PHE:HB2   | 0.48     | 1.85        | 4      | 3     |
| 1:A:30:PHE:CE1  | 1:A:66:LEU:HD11  | 0.48     | 2.44        | 1      | 5     |
| 1:A:113:ALA:HA  | 1:A:116:GLN:HG3  | 0.48     | 1.84        | 14     | 6     |
| 1:A:48:LEU:HD22 | 1:A:78:TYR:HE2   | 0.48     | 1.69        | 13     | 5     |
| 1:A:53:PHE:CE1  | 1:A:72:ARG:HB3   | 0.48     | 2.44        | 1      | 2     |
| 1:A:85:LEU:HA   | 1:A:88:VAL:CG2   | 0.48     | 2.39        | 2      | 5     |
| 1:A:23:SER:HA   | 1:A:70:GLN:NE2   | 0.48     | 2.24        | 5      | 1     |
| 1:A:71:LEU:O    | 1:A:75:LEU:HB2   | 0.48     | 2.09        | 11     | 2     |
| 1:A:32:ALA:CB   | 1:A:41:ALA:HB2   | 0.47     | 2.39        | 15     | 6     |
| 1:A:86:TYR:CG   | 1:A:117:LEU:HD22 | 0.47     | 2.44        | 6      | 3     |
| 1:A:86:TYR:CE2  | 1:A:117:LEU:HD12 | 0.47     | 2.45        | 12     | 2     |
| 1:A:24:SER:HB2  | 1:A:77:LEU:HD13  | 0.47     | 1.85        | 8      | 2     |
| 1:A:27:VAL:HG22 | 1:A:74:ALA:CB    | 0.47     | 2.40        | 14     | 9     |
| 1:A:30:PHE:CE2  | 1:A:60:VAL:HB    | 0.47     | 2.45        | 3      | 9     |
| 1:A:47:PRO:HA   | 1:A:88:VAL:CG2   | 0.47     | 2.40        | 15     | 7     |
| 1:A:25:LYS:HG3  | 1:A:26:GLU:CD    | 0.47     | 2.35        | 2      | 1     |
| 1:A:83:ARG:HA   | 1:A:86:TYR:CE1   | 0.47     | 2.45        | 7      | 3     |
| 1:A:90:PRO:HB2  | 1:A:110:VAL:CG1  | 0.47     | 2.39        | 7      | 1     |
| 1:A:79:THR:HA   | 1:A:84:TYR:CG    | 0.47     | 2.45        | 11     | 2     |
| 1:A:48:LEU:HB3  | 1:A:84:TYR:CE1   | 0.47     | 2.45        | 8      | 3     |
| 1:A:21:LEU:HD23 | 1:A:21:LEU:H     | 0.47     | 1.69        | 15     | 2     |
| 1:A:68:LYS:O    | 1:A:71:LEU:HB3   | 0.47     | 2.10        | 8      | 17    |
| 1:A:112:HIS:O   | 1:A:115:LYS:HG3  | 0.47     | 2.10        | 1      | 1     |
| 1:A:57:VAL:CA   | 1:A:60:VAL:HG22  | 0.46     | 2.39        | 1      | 15    |
| 1:A:39:PHE:CE1  | 1:A:48:LEU:HD11  | 0.46     | 2.46        | 4      | 2     |
| 1:A:49:LYS:HG3  | 1:A:102:CYS:SG   | 0.46     | 2.51        | 1      | 3     |
| 1:A:106:ASP:CG  | 1:A:107:GLU:N    | 0.46     | 2.74        | 5      | 16    |
| 1:A:96:ASP:OD2  | 1:A:100:ASN:HB2  | 0.46     | 2.11        | 15     | 1     |
| 1:A:89:LYS:CB   | 1:A:90:PRO:HD3   | 0.46     | 2.40        | 10     | 3     |
| 1:A:82:TRP:O    | 1:A:86:TYR:HD1   | 0.46     | 1.93        | 15     | 1     |
| 1:A:53:PHE:CD1  | 1:A:75:LEU:HD13  | 0.46     | 2.45        | 2      | 5     |
| 1:A:110:VAL:O   | 1:A:113:ALA:HB3  | 0.46     | 2.10        | 13     | 3     |
| 1:A:38:CYS:HG   | 1:A:97:LEU:HA    | 0.46     | 1.71        | 3      | 2     |
| 1:A:25:LYS:HB3  | 1:A:26:GLU:OE1   | 0.46     | 2.11        | 8      | 3     |
| 1:A:61:ALA:HA   | 1:A:66:LEU:CD1   | 0.46     | 2.40        | 7      | 4     |
| 1:A:48:LEU:C    | 1:A:93:THR:HB    | 0.46     | 2.36        | 17     | 1     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:A:35:PHE:HB2  | 1:A:39:PHE:HD2   | 0.46     | 1.71        | 11     | 6     |
| 1:A:91:GLY:HA2  | 1:A:101:PRO:O    | 0.46     | 2.11        | 7      | 1     |
| 1:A:44:GLU:CD   | 1:A:83:ARG:HD2   | 0.45     | 2.35        | 2      | 1     |
| 1:A:30:PHE:CE2  | 1:A:66:LEU:HD11  | 0.45     | 2.47        | 6      | 7     |
| 1:A:90:PRO:HD2  | 1:A:92:ALA:HB2   | 0.45     | 1.87        | 17     | 1     |
| 1:A:53:PHE:CD2  | 1:A:75:LEU:HD13  | 0.45     | 2.46        | 17     | 8     |
| 1:A:48:LEU:HD23 | 1:A:84:TYR:HE2   | 0.45     | 1.71        | 7      | 3     |
| 1:A:21:LEU:N    | 1:A:21:LEU:CD2   | 0.45     | 2.76        | 16     | 4     |
| 1:A:48:LEU:HD11 | 1:A:52:ILE:CD1   | 0.45     | 2.41        | 1      | 1     |
| 1:A:81:SER:OG   | 1:A:83:ARG:HG2   | 0.45     | 2.11        | 14     | 2     |
| 1:A:85:LEU:HD23 | 1:A:117:LEU:HD21 | 0.45     | 1.88        | 15     | 3     |
| 1:A:84:TYR:O    | 1:A:88:VAL:HG23  | 0.45     | 2.12        | 1      | 1     |
| 1:A:35:PHE:HB2  | 1:A:39:PHE:HD1   | 0.45     | 1.72        | 5      | 2     |
| 1:A:23:SER:CB   | 1:A:70:GLN:HB2   | 0.45     | 2.41        | 8      | 2     |
| 1:A:54:GLN:CA   | 1:A:57:VAL:HG22  | 0.45     | 2.41        | 14     | 15    |
| 1:A:86:TYR:HA   | 1:A:117:LEU:HB2  | 0.45     | 1.88        | 1      | 1     |
| 1:A:94:ARG:CA   | 1:A:101:PRO:HA   | 0.45     | 2.42        | 4      | 3     |
| 1:A:54:GLN:C    | 1:A:54:GLN:CD    | 0.44     | 2.85        | 9      | 6     |
| 1:A:49:LYS:HG3  | 1:A:102:CYS:HB2  | 0.44     | 1.88        | 4      | 1     |
| 1:A:84:TYR:CZ   | 1:A:88:VAL:HG11  | 0.44     | 2.47        | 5      | 1     |
| 1:A:30:PHE:HA   | 1:A:33:GLU:OE1   | 0.44     | 2.12        | 7      | 2     |
| 1:A:38:CYS:HB2  | 1:A:39:PHE:CD1   | 0.44     | 2.46        | 10     | 4     |
| 1:A:32:ALA:HB1  | 1:A:40:SER:C     | 0.44     | 2.38        | 11     | 1     |
| 1:A:21:LEU:CB   | 1:A:27:VAL:HG12  | 0.44     | 2.30        | 14     | 2     |
| 1:A:88:VAL:HA   | 1:A:92:ALA:CB    | 0.44     | 2.42        | 6      | 3     |
| 1:A:50:ILE:N    | 1:A:52:ILE:HG22  | 0.44     | 2.27        | 8      | 1     |
| 1:A:115:LYS:HE3 | 1:A:115:LYS:C    | 0.44     | 2.37        | 8      | 1     |
| 1:A:54:GLN:HA   | 1:A:57:VAL:HG22  | 0.44     | 1.88        | 11     | 12    |
| 1:A:23:SER:HB2  | 1:A:70:GLN:HB2   | 0.44     | 1.89        | 9      | 2     |
| 1:A:85:LEU:C    | 1:A:87:GLY:N     | 0.44     | 2.76        | 15     | 11    |
| 1:A:49:LYS:HZ2  | 1:A:104:GLU:CD   | 0.44     | 2.21        | 4      | 2     |
| 1:A:49:LYS:O    | 1:A:52:ILE:HG22  | 0.44     | 2.12        | 12     | 1     |
| 1:A:56:LEU:HD13 | 1:A:97:LEU:HD11  | 0.44     | 1.89        | 3      | 4     |
| 1:A:52:ILE:HG13 | 1:A:97:LEU:HG    | 0.44     | 1.90        | 11     | 1     |
| 1:A:29:ALA:HA   | 1:A:41:ALA:HB2   | 0.44     | 1.88        | 16     | 2     |
| 1:A:35:PHE:CE1  | 1:A:97:LEU:HB3   | 0.44     | 2.47        | 15     | 1     |
| 1:A:90:PRO:HA   | 1:A:104:GLU:CD   | 0.43     | 2.38        | 7      | 1     |
| 1:A:37:HIS:ND1  | 1:A:99:GLY:HA3   | 0.43     | 2.27        | 6      | 1     |
| 1:A:66:LEU:HD23 | 1:A:70:GLN:NE2   | 0.43     | 2.29        | 17     | 3     |
| 1:A:21:LEU:HD22 | 1:A:27:VAL:HA    | 0.43     | 1.90        | 16     | 2     |
| 1:A:35:PHE:CD2  | 1:A:97:LEU:HD22  | 0.43     | 2.48        | 14     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:56:LEU:HG    | 1:A:71:LEU:HD11  | 0.43     | 1.91        | 11     | 5     |
| 1:A:89:LYS:HB2   | 1:A:89:LYS:NZ    | 0.43     | 2.29        | 15     | 3     |
| 1:A:40:SER:C     | 1:A:42:GLU:HG3   | 0.43     | 2.39        | 12     | 2     |
| 1:A:54:GLN:HA    | 1:A:57:VAL:CG2   | 0.43     | 2.44        | 14     | 4     |
| 1:A:30:PHE:HA    | 1:A:33:GLU:HG2   | 0.43     | 1.90        | 17     | 3     |
| 1:A:21:LEU:O     | 1:A:26:GLU:HG2   | 0.43     | 2.13        | 3      | 1     |
| 1:A:46:ARG:HD2   | 1:A:47:PRO:HD2   | 0.43     | 1.91        | 14     | 1     |
| 1:A:52:ILE:CG1   | 1:A:97:LEU:HD11  | 0.43     | 2.44        | 12     | 4     |
| 1:A:56:LEU:O     | 1:A:59:ARG:HB2   | 0.43     | 2.13        | 6      | 3     |
| 1:A:49:LYS:HD3   | 1:A:102:CYS:SG   | 0.43     | 2.53        | 15     | 1     |
| 1:A:49:LYS:HE3   | 1:A:52:ILE:HA    | 0.43     | 1.89        | 15     | 1     |
| 1:A:46:ARG:HG2   | 1:A:47:PRO:HD2   | 0.43     | 1.91        | 3      | 1     |
| 1:A:68:LYS:HD3   | 1:A:68:LYS:N     | 0.43     | 2.29        | 11     | 1     |
| 1:A:83:ARG:HA    | 1:A:86:TYR:CE2   | 0.43     | 2.48        | 17     | 2     |
| 1:A:52:ILE:O     | 1:A:53:PHE:C     | 0.43     | 2.61        | 12     | 6     |
| 1:A:96:ASP:HB3   | 1:A:100:ASN:HB2  | 0.43     | 1.90        | 12     | 2     |
| 1:A:95:VAL:CA    | 1:A:100:ASN:O    | 0.43     | 2.66        | 11     | 6     |
| 1:A:46:ARG:HG2   | 1:A:47:PRO:CD    | 0.43     | 2.44        | 3      | 1     |
| 1:A:26:GLU:O     | 1:A:29:ALA:HB3   | 0.43     | 2.13        | 12     | 6     |
| 1:A:105:LEU:HD23 | 1:A:106:ASP:CA   | 0.42     | 2.44        | 5      | 4     |
| 1:A:34:ARG:O     | 1:A:36:PRO:HD2   | 0.42     | 2.13        | 6      | 2     |
| 1:A:90:PRO:HB2   | 1:A:110:VAL:HG12 | 0.42     | 1.90        | 7      | 1     |
| 1:A:29:ALA:HA    | 1:A:41:ALA:CB    | 0.42     | 2.45        | 9      | 1     |
| 1:A:92:ALA:CA    | 1:A:110:VAL:HB   | 0.42     | 2.44        | 7      | 1     |
| 1:A:21:LEU:CD2   | 1:A:30:PHE:HB2   | 0.42     | 2.42        | 13     | 1     |
| 1:A:44:GLU:CD    | 1:A:83:ARG:HD3   | 0.42     | 2.39        | 14     | 1     |
| 1:A:28:ILE:HD11  | 1:A:74:ALA:O     | 0.42     | 2.14        | 16     | 4     |
| 1:A:96:ASP:C     | 1:A:98:ASP:H     | 0.42     | 2.21        | 15     | 1     |
| 1:A:91:GLY:HA3   | 1:A:105:LEU:HB3  | 0.42     | 1.92        | 7      | 5     |
| 1:A:48:LEU:CD2   | 1:A:78:TYR:HE1   | 0.42     | 2.28        | 11     | 1     |
| 1:A:58:ASP:HB3   | 1:A:59:ARG:HD2   | 0.42     | 1.91        | 5      | 1     |
| 1:A:21:LEU:CG    | 1:A:65:ASN:OD1   | 0.42     | 2.67        | 12     | 1     |
| 1:A:100:ASN:O    | 1:A:102:CYS:N    | 0.42     | 2.53        | 17     | 6     |
| 1:A:38:CYS:HB2   | 1:A:39:PHE:CD2   | 0.42     | 2.49        | 17     | 2     |
| 1:A:53:PHE:CZ    | 1:A:68:LYS:HB3   | 0.42     | 2.50        | 17     | 1     |
| 1:A:21:LEU:HD11  | 1:A:64:MET:HE1   | 0.42     | 1.91        | 11     | 1     |
| 1:A:73:SER:CB    | 1:A:76:ARG:HG3   | 0.42     | 2.44        | 11     | 1     |
| 1:A:105:LEU:CD1  | 1:A:109:HIS:HB2  | 0.42     | 2.43        | 15     | 6     |
| 1:A:107:GLU:O    | 1:A:111:GLU:HB2  | 0.42     | 2.15        | 2      | 1     |
| 1:A:49:LYS:HG2   | 1:A:93:THR:CG2   | 0.42     | 2.44        | 4      | 1     |
| 1:A:85:LEU:CD2   | 1:A:117:LEU:HD21 | 0.42     | 2.45        | 15     | 1     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:A:21:LEU:CD1  | 1:A:21:LEU:N     | 0.41     | 2.84        | 4      | 1     |
| 1:A:40:SER:CA   | 1:A:42:GLU:HG3   | 0.41     | 2.45        | 17     | 1     |
| 1:A:50:ILE:HD13 | 1:A:76:ARG:HH21  | 0.41     | 1.75        | 3      | 1     |
| 1:A:64:MET:HE3  | 1:A:64:MET:HB2   | 0.41     | 1.72        | 11     | 1     |
| 1:A:60:VAL:O    | 1:A:63:GLU:HG3   | 0.41     | 2.16        | 12     | 2     |
| 1:A:82:TRP:O    | 1:A:86:TYR:CD1   | 0.41     | 2.74        | 4      | 1     |
| 1:A:33:GLU:HG3  | 1:A:34:ARG:N     | 0.41     | 2.29        | 5      | 1     |
| 1:A:53:PHE:O    | 1:A:56:LEU:HB2   | 0.41     | 2.15        | 5      | 1     |
| 1:A:91:GLY:N    | 1:A:110:VAL:HG11 | 0.41     | 2.30        | 6      | 2     |
| 1:A:85:LEU:H    | 1:A:85:LEU:HD13  | 0.41     | 1.76        | 9      | 1     |
| 1:A:55:ASP:CG   | 1:A:97:LEU:HD12  | 0.41     | 2.40        | 16     | 1     |
| 1:A:24:SER:HB3  | 1:A:77:LEU:HD13  | 0.41     | 1.91        | 17     | 1     |
| 1:A:56:LEU:O    | 1:A:60:VAL:HG13  | 0.41     | 2.15        | 1      | 2     |
| 1:A:95:VAL:C    | 1:A:100:ASN:O    | 0.41     | 2.64        | 8      | 2     |
| 1:A:21:LEU:HD22 | 1:A:26:GLU:O     | 0.41     | 2.15        | 10     | 1     |
| 1:A:30:PHE:CE2  | 1:A:31:LEU:HD23  | 0.41     | 2.51        | 11     | 1     |
| 1:A:65:ASN:O    | 1:A:66:LEU:HD23  | 0.41     | 2.15        | 14     | 1     |
| 1:A:89:LYS:HG3  | 1:A:90:PRO:HD3   | 0.41     | 1.92        | 4      | 1     |
| 1:A:56:LEU:HD13 | 1:A:97:LEU:HD21  | 0.41     | 1.92        | 11     | 2     |
| 1:A:109:HIS:C   | 1:A:111:GLU:H    | 0.41     | 2.19        | 4      | 1     |
| 1:A:95:VAL:HG23 | 1:A:97:LEU:N     | 0.41     | 2.29        | 11     | 1     |
| 1:A:21:LEU:HD11 | 1:A:64:MET:CE    | 0.41     | 2.46        | 5      | 1     |
| 1:A:30:PHE:CE1  | 1:A:34:ARG:HG2   | 0.41     | 2.51        | 6      | 1     |
| 1:A:25:LYS:HD3  | 1:A:77:LEU:HD21  | 0.41     | 1.92        | 14     | 1     |
| 1:A:52:ILE:O    | 1:A:55:ASP:HB3   | 0.41     | 2.16        | 16     | 1     |
| 1:A:105:LEU:CG  | 1:A:109:HIS:HB2  | 0.41     | 2.46        | 17     | 1     |
| 1:A:30:PHE:CZ   | 1:A:60:VAL:HB    | 0.40     | 2.51        | 16     | 2     |
| 1:A:96:ASP:O    | 1:A:98:ASP:N     | 0.40     | 2.49        | 1      | 1     |
| 1:A:53:PHE:CE2  | 1:A:72:ARG:HB3   | 0.40     | 2.52        | 2      | 1     |
| 1:A:44:GLU:HB3  | 1:A:83:ARG:CD    | 0.40     | 2.46        | 10     | 1     |
| 1:A:30:PHE:HZ   | 1:A:60:VAL:CA    | 0.40     | 2.29        | 1      | 1     |
| 1:A:54:GLN:O    | 1:A:57:VAL:HG22  | 0.40     | 2.15        | 1      | 1     |
| 1:A:28:ILE:CD1  | 1:A:74:ALA:HB1   | 0.40     | 2.46        | 10     | 1     |
| 1:A:38:CYS:SG   | 1:A:97:LEU:CA    | 0.40     | 3.08        | 1      | 1     |
| 1:A:38:CYS:HB3  | 1:A:95:VAL:HG21  | 0.40     | 1.94        | 1      | 1     |
| 1:A:71:LEU:O    | 1:A:74:ALA:HB3   | 0.40     | 2.16        | 2      | 1     |
| 1:A:88:VAL:C    | 1:A:92:ALA:HB3   | 0.40     | 2.41        | 5      | 1     |
| 1:A:38:CYS:SG   | 1:A:48:LEU:HD13  | 0.40     | 2.56        | 6      | 1     |
| 1:A:89:LYS:HB2  | 1:A:116:GLN:OE1  | 0.40     | 2.15        | 11     | 1     |
| 1:A:21:LEU:HD11 | 1:A:30:PHE:CB    | 0.40     | 2.47        | 7      | 1     |
| 1:A:47:PRO:HB2  | 1:A:92:ALA:O     | 0.40     | 2.16        | 1      | 1     |

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| Atom-1           | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|------------------|-----------------|----------|-------------|--------|-------|
|                  |                 |          |             | Worst  | Total |
| 1:A:48:LEU:HD23  | 1:A:84:TYR:CE1  | 0.40     | 2.48        | 5      | 1     |
| 1:A:105:LEU:HD22 | 1:A:110:VAL:CG1 | 0.40     | 2.40        | 11     | 1     |
| 1:A:73:SER:O     | 1:A:77:LEU:HB2  | 0.40     | 2.16        | 12     | 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     | 97/133 (73%)    | 70±2 (73±2%) | 18±2 (18±2%) | 9±1 (9±1%) | <b>1</b>    | <b>11</b> |
| All | All   | 1649/2261 (73%) | 1197 (73%)   | 302 (18%)    | 150 (9%)   | <b>1</b>    | <b>11</b> |

All 17 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 90  | PRO  | 17             |
| 1   | A     | 106 | ASP  | 17             |
| 1   | A     | 41  | ALA  | 15             |
| 1   | A     | 89  | LYS  | 15             |
| 1   | A     | 61  | ALA  | 14             |
| 1   | A     | 24  | SER  | 13             |
| 1   | A     | 36  | PRO  | 13             |
| 1   | A     | 23  | SER  | 11             |
| 1   | A     | 68  | LYS  | 9              |
| 1   | A     | 97  | LEU  | 9              |
| 1   | A     | 87  | GLY  | 6              |
| 1   | A     | 21  | LEU  | 5              |
| 1   | A     | 44  | GLU  | 2              |
| 1   | A     | 88  | VAL  | 1              |
| 1   | A     | 40  | SER  | 1              |
| 1   | A     | 42  | GLU  | 1              |
| 1   | A     | 65  | ASN  | 1              |

### 6.3.2 Protein sidechains ⓘ

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

| Mol | Chain | Analysed        | Rotameric    | Outliers     | Percentiles |    |
|-----|-------|-----------------|--------------|--------------|-------------|----|
| 1   | A     | 82/112 (73%)    | 56±2 (69±2%) | 26±2 (31±2%) | 1           | 15 |
| All | All   | 1394/1904 (73%) | 960 (69%)    | 434 (31%)    | 1           | 15 |

All 43 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     | 27  | VAL  | 17             |
| 1   | A     | 52  | ILE  | 17             |
| 1   | A     | 54  | GLN  | 17             |
| 1   | A     | 71  | LEU  | 17             |
| 1   | A     | 75  | LEU  | 17             |
| 1   | A     | 78  | TYR  | 17             |
| 1   | A     | 85  | LEU  | 17             |
| 1   | A     | 95  | VAL  | 17             |
| 1   | A     | 104 | GLU  | 17             |
| 1   | A     | 116 | GLN  | 17             |
| 1   | A     | 117 | LEU  | 17             |
| 1   | A     | 72  | ARG  | 16             |
| 1   | A     | 76  | ARG  | 16             |
| 1   | A     | 97  | LEU  | 16             |
| 1   | A     | 48  | LEU  | 15             |
| 1   | A     | 106 | ASP  | 15             |
| 1   | A     | 30  | PHE  | 14             |
| 1   | A     | 111 | GLU  | 14             |
| 1   | A     | 93  | THR  | 13             |
| 1   | A     | 50  | ILE  | 12             |
| 1   | A     | 107 | GLU  | 11             |
| 1   | A     | 89  | LYS  | 10             |
| 1   | A     | 49  | LYS  | 9              |
| 1   | A     | 68  | LYS  | 8              |
| 1   | A     | 21  | LEU  | 8              |
| 1   | A     | 115 | LYS  | 8              |
| 1   | A     | 26  | GLU  | 7              |
| 1   | A     | 64  | MET  | 7              |
| 1   | A     | 82  | TRP  | 7              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 102 | CYS  | 7              |
| 1   | A     | 37  | HIS  | 6              |
| 1   | A     | 98  | ASP  | 6              |
| 1   | A     | 56  | LEU  | 5              |
| 1   | A     | 55  | ASP  | 5              |
| 1   | A     | 34  | ARG  | 2              |
| 1   | A     | 81  | SER  | 2              |
| 1   | A     | 114 | ARG  | 2              |
| 1   | A     | 59  | ARG  | 1              |
| 1   | A     | 108 | GLN  | 1              |
| 1   | A     | 83  | ARG  | 1              |
| 1   | A     | 96  | ASP  | 1              |
| 1   | A     | 70  | GLN  | 1              |
| 1   | A     | 42  | GLU  | 1              |

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

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

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 1   | 10-A  | 3                |
| 1   | 14-A  | 3                |
| 1   | 15-A  | 3                |
| 1   | 5-A   | 3                |
| 1   | 1-A   | 2                |
| 1   | 2-A   | 2                |
| 1   | 4-A   | 2                |
| 1   | 6-A   | 2                |
| 1   | 11-A  | 2                |
| 1   | 17-A  | 2                |
| 1   | 3-A   | 2                |
| 1   | 8-A   | 2                |
| 1   | 9-A   | 2                |
| 1   | 12-A  | 2                |
| 1   | 13-A  | 2                |
| 1   | 16-A  | 2                |
| 1   | 7-A   | 1                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 10    | A     | 17:ASN    | C      | 18:GLN    | N      | 1.20         |
| 14    | A     | 95:VAL    | C      | 96:ASP    | N      | 1.20         |
| 15    | A     | 121:LYS   | C      | 122:ALA   | N      | 1.20         |
| 1     | A     | 91:GLY    | C      | 92:ALA    | N      | 1.19         |
| 2     | A     | 91:GLY    | C      | 92:ALA    | N      | 1.19         |
| 4     | A     | 91:GLY    | C      | 92:ALA    | N      | 1.19         |
| 5     | A     | 61:ALA    | C      | 62:GLY    | N      | 1.19         |
| 5     | A     | 91:GLY    | C      | 92:ALA    | N      | 1.19         |
| 5     | A     | 95:VAL    | C      | 96:ASP    | N      | 1.19         |
| 6     | A     | 91:GLY    | C      | 92:ALA    | N      | 1.19         |
| 11    | A     | 91:GLY    | C      | 92:ALA    | N      | 1.19         |
| 14    | A     | 91:GLY    | C      | 92:ALA    | N      | 1.19         |
| 17    | A     | 91:GLY    | C      | 92:ALA    | N      | 1.19         |
| 1     | A     | 61:ALA    | C      | 62:GLY    | N      | 1.18         |
| 3     | A     | 61:ALA    | C      | 62:GLY    | N      | 1.18         |
| 3     | A     | 91:GLY    | C      | 92:ALA    | N      | 1.18         |
| 8     | A     | 91:GLY    | C      | 92:ALA    | N      | 1.18         |
| 9     | A     | 91:GLY    | C      | 92:ALA    | N      | 1.18         |
| 10    | A     | 91:GLY    | C      | 92:ALA    | N      | 1.18         |
| 11    | A     | 61:ALA    | C      | 62:GLY    | N      | 1.18         |
| 12    | A     | 91:GLY    | C      | 92:ALA    | N      | 1.18         |
| 13    | A     | 91:GLY    | C      | 92:ALA    | N      | 1.18         |
| 16    | A     | 91:GLY    | C      | 92:ALA    | N      | 1.18         |

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| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 8     | A     | 61:ALA    | C      | 62:GLY    | N      | 1.17         |
| 12    | A     | 61:ALA    | C      | 62:GLY    | N      | 1.17         |
| 15    | A     | 91:GLY    | C      | 92:ALA    | N      | 1.17         |
| 2     | A     | 61:ALA    | C      | 62:GLY    | N      | 1.16         |
| 4     | A     | 61:ALA    | C      | 62:GLY    | N      | 1.16         |
| 6     | A     | 61:ALA    | C      | 62:GLY    | N      | 1.16         |
| 10    | A     | 61:ALA    | C      | 62:GLY    | N      | 1.16         |
| 13    | A     | 61:ALA    | C      | 62:GLY    | N      | 1.16         |
| 14    | A     | 61:ALA    | C      | 62:GLY    | N      | 1.16         |
| 15    | A     | 61:ALA    | C      | 62:GLY    | N      | 1.16         |
| 16    | A     | 61:ALA    | C      | 62:GLY    | N      | 1.16         |
| 17    | A     | 61:ALA    | C      | 62:GLY    | N      | 1.16         |
| 7     | A     | 61:ALA    | C      | 62:GLY    | N      | 1.15         |
| 9     | A     | 61:ALA    | C      | 62:GLY    | N      | 1.15         |

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 81% for the well-defined parts and 73% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

Chemical shift list name: *NT\_170227\_b.txt*

#### 7.1.1 Bookkeeping

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

|                                         |      |
|-----------------------------------------|------|
| Total number of shifts                  | 1341 |
| Number of shifts mapped to atoms        | 1341 |
| Number of unparsed shifts               | 0    |
| Number of shifts with mapping errors    | 0    |
| Number of shifts with mapping warnings  | 0    |
| Number of shift outliers (ShiftChecker) | 0    |

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 124      | $0.22 \pm 0.10$                 | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}_\beta$  | 116      | $0.37 \pm 0.10$                 | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}'$       | 117      | $-0.10 \pm 0.10$                | None needed ( $< 0.5$ ppm) |
| $^{15}\text{N}$        | 117      | $0.23 \pm 0.27$                 | None needed ( $< 0.5$ ppm) |

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 81%, i.e. 1082 atoms were assigned a chemical shift out of a possible 1344. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total         | $^1\text{H}$  | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|---------------|---------------|-----------------|-----------------|
| Backbone  | 477/484 (99%) | 194/197 (98%) | 190/194 (98%)   | 93/93 (100%)    |
| Sidechain | 532/757 (70%) | 354/490 (72%) | 170/231 (74%)   | 8/36 (22%)      |

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|          | Total           | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|----------|-----------------|----------------|-----------------|-----------------|
| Aromatic | 73/103 (71%)    | 38/50 (76%)    | 34/46 (74%)     | 1/7 (14%)       |
| Overall  | 1082/1344 (81%) | 586/737 (80%)  | 394/471 (84%)   | 102/136 (75%)   |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 73%, i.e. 1340 atoms were assigned a chemical shift out of a possible 1825. 0 out of 19 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total           | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|-----------|-----------------|----------------|-----------------|-----------------|
| Backbone  | 603/661 (91%)   | 245/268 (91%)  | 241/266 (91%)   | 117/127 (92%)   |
| Sidechain | 664/1013 (66%)  | 438/652 (67%)  | 218/310 (70%)   | 8/51 (16%)      |
| Aromatic  | 73/151 (48%)    | 38/74 (51%)    | 34/58 (59%)     | 1/19 (5%)       |
| Overall   | 1340/1825 (73%) | 721/994 (73%)  | 493/634 (78%)   | 126/197 (64%)   |

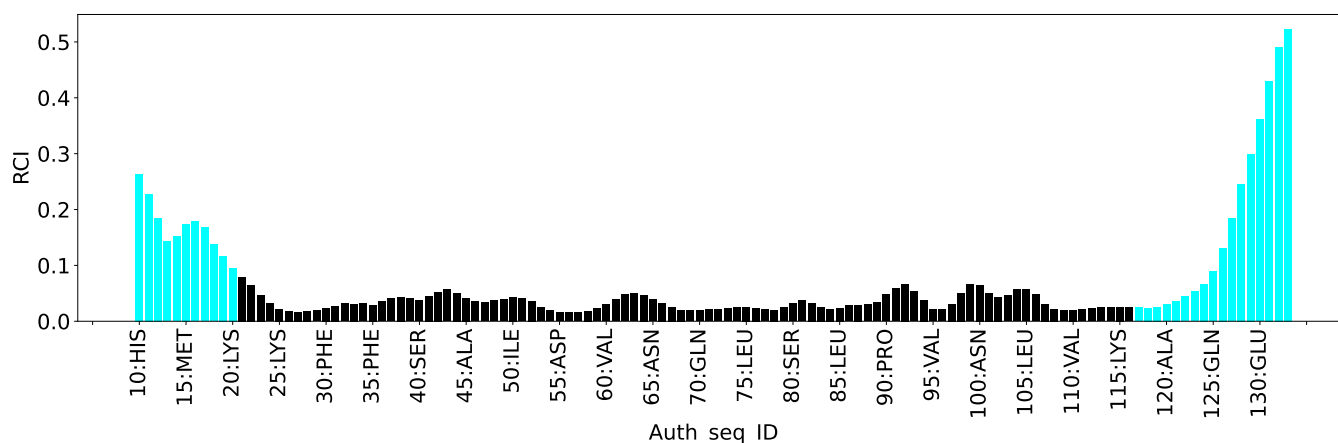
#### 7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain A:



## 8 NMR restraints analysis

### 8.1 Conformationally restricting restraints

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

| Description                                              | Value |
|----------------------------------------------------------|-------|
| Total distance restraints                                | 4503  |
| Intra-residue ( $ i-j =0$ )                              | 1798  |
| Sequential ( $ i-j =1$ )                                 | 1115  |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 812   |
| Long range ( $ i-j \geq 5$ )                             | 778   |
| 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                         | 33.9  |
| Number of long range restraints per residue <sup>1</sup> | 5.8   |

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

### 8.2 Residual restraint violations

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

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

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

| Bins (Å)         | Average number of violations per model | Max (Å) |
|------------------|----------------------------------------|---------|
| 0.1-0.2 (Small)  | 299.8                                  | 0.2     |
| 0.2-0.5 (Medium) | 448.9                                  | 0.5     |
| >0.5 (Large)     | 203.5                                  | 2.33    |

### 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 ⓘ

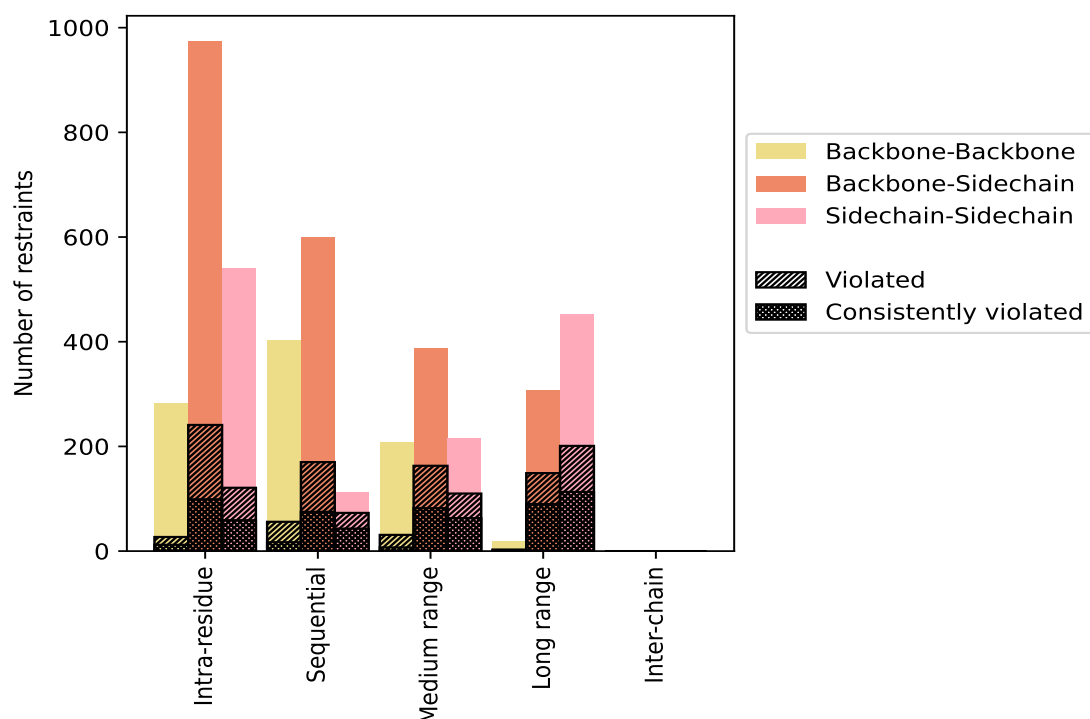
### 9.1 Summary of distance violations ⓘ

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.

| Restraints type                                            | Count                | % <sup>1</sup>        | Violated <sup>3</sup> |                      |                      | Consistently Violated <sup>4</sup> |                      |                      |
|------------------------------------------------------------|----------------------|-----------------------|-----------------------|----------------------|----------------------|------------------------------------|----------------------|----------------------|
|                                                            |                      |                       | Count                 | % <sup>2</sup>       | % <sup>1</sup>       | Count                              | % <sup>2</sup>       | % <sup>1</sup>       |
| <a href="#">Intra-residue ( i-j =0)</a>                    | <a href="#">1798</a> | <a href="#">39.9</a>  | <a href="#">389</a>   | <a href="#">21.6</a> | <a href="#">8.6</a>  | <a href="#">170</a>                | <a href="#">9.5</a>  | <a href="#">3.8</a>  |
| Backbone-Backbone                                          | 283                  | 6.3                   | 27                    | 9.5                  | 0.6                  | 12                                 | 4.2                  | 0.3                  |
| Backbone-Sidechain                                         | 974                  | 21.6                  | 241                   | 24.7                 | 5.4                  | 99                                 | 10.2                 | 2.2                  |
| Sidechain-Sidechain                                        | 541                  | 12.0                  | 121                   | 22.4                 | 2.7                  | 59                                 | 10.9                 | 1.3                  |
| <a href="#">Sequential ( i-j =1)</a>                       | <a href="#">1115</a> | <a href="#">24.8</a>  | <a href="#">299</a>   | <a href="#">26.8</a> | <a href="#">6.6</a>  | <a href="#">135</a>                | <a href="#">12.1</a> | <a href="#">3.0</a>  |
| Backbone-Backbone                                          | 402                  | 8.9                   | 56                    | 13.9                 | 1.2                  | 17                                 | 4.2                  | 0.4                  |
| Backbone-Sidechain                                         | 600                  | 13.3                  | 170                   | 28.3                 | 3.8                  | 75                                 | 12.5                 | 1.7                  |
| Sidechain-Sidechain                                        | 113                  | 2.5                   | 73                    | 64.6                 | 1.6                  | 43                                 | 38.1                 | 1.0                  |
| <a href="#">Medium range ( i-j &gt;1 &amp;  i-j &lt;5)</a> | <a href="#">812</a>  | <a href="#">18.0</a>  | <a href="#">304</a>   | <a href="#">37.4</a> | <a href="#">6.8</a>  | <a href="#">152</a>                | <a href="#">18.7</a> | <a href="#">3.4</a>  |
| Backbone-Backbone                                          | 208                  | 4.6                   | 31                    | 14.9                 | 0.7                  | 7                                  | 3.4                  | 0.2                  |
| Backbone-Sidechain                                         | 388                  | 8.6                   | 163                   | 42.0                 | 3.6                  | 82                                 | 21.1                 | 1.8                  |
| Sidechain-Sidechain                                        | 216                  | 4.8                   | 110                   | 50.9                 | 2.4                  | 63                                 | 29.2                 | 1.4                  |
| <a href="#">Long range ( i-j ≥5)</a>                       | <a href="#">778</a>  | <a href="#">17.3</a>  | <a href="#">353</a>   | <a href="#">45.4</a> | <a href="#">7.8</a>  | <a href="#">204</a>                | <a href="#">26.2</a> | <a href="#">4.5</a>  |
| Backbone-Backbone                                          | 18                   | 0.4                   | 3                     | 16.7                 | 0.1                  | 1                                  | 5.6                  | 0.0                  |
| Backbone-Sidechain                                         | 307                  | 6.8                   | 149                   | 48.5                 | 3.3                  | 90                                 | 29.3                 | 2.0                  |
| Sidechain-Sidechain                                        | 453                  | 10.1                  | 201                   | 44.4                 | 4.5                  | 113                                | 24.9                 | 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="#">4503</a> | <a href="#">100.0</a> | <a href="#">1345</a>  | <a href="#">29.9</a> | <a href="#">29.9</a> | <a href="#">661</a>                | <a href="#">14.7</a> | <a href="#">14.7</a> |
| Backbone-Backbone                                          | 911                  | 20.2                  | 117                   | 12.8                 | 2.6                  | 37                                 | 4.1                  | 0.8                  |
| Backbone-Sidechain                                         | 2269                 | 50.4                  | 723                   | 31.9                 | 16.1                 | 346                                | 15.2                 | 7.7                  |
| Sidechain-Sidechain                                        | 1323                 | 29.4                  | 505                   | 38.2                 | 11.2                 | 278                                | 21.0                 | 6.2                  |

<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        | 274                  | 197             | 223             | 279             | 0               | 973   | 0.36     | 2.21    | 0.25                | 0.28       |
| 2        | 269                  | 195             | 214             | 278             | 0               | 956   | 0.36     | 2.23    | 0.25                | 0.29       |
| 3        | 270                  | 203             | 202             | 280             | 0               | 955   | 0.36     | 2.15    | 0.25                | 0.28       |
| 4        | 275                  | 201             | 216             | 289             | 0               | 981   | 0.35     | 2.33    | 0.24                | 0.27       |
| 5        | 285                  | 207             | 219             | 274             | 0               | 985   | 0.35     | 2.14    | 0.24                | 0.27       |
| 6        | 273                  | 212             | 222             | 279             | 0               | 986   | 0.35     | 2.12    | 0.24                | 0.28       |
| 7        | 267                  | 197             | 214             | 277             | 0               | 955   | 0.36     | 2.2     | 0.25                | 0.28       |
| 8        | 277                  | 207             | 220             | 273             | 0               | 977   | 0.35     | 2.07    | 0.25                | 0.28       |
| 9        | 268                  | 204             | 217             | 281             | 0               | 970   | 0.36     | 2.25    | 0.25                | 0.28       |
| 10       | 281                  | 194             | 215             | 273             | 0               | 963   | 0.36     | 2.07    | 0.25                | 0.28       |

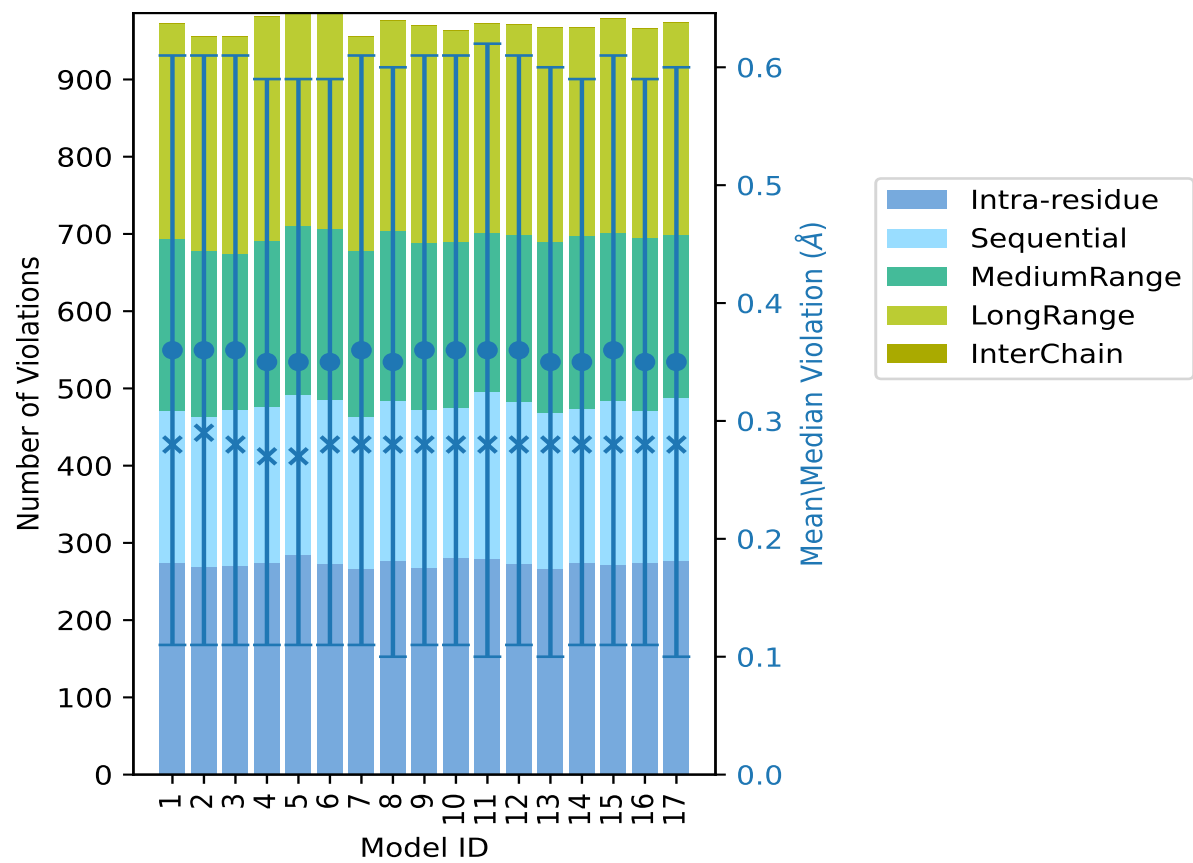
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| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 11       | 279                  | 216             | 207             | 270             | 0               | 972   | 0.36     | 2.18    | 0.26                | 0.28       |
| 12       | 273                  | 210             | 216             | 272             | 0               | 971   | 0.36     | 2.2     | 0.25                | 0.28       |
| 13       | 267                  | 202             | 221             | 277             | 0               | 967   | 0.35     | 2.14    | 0.25                | 0.28       |
| 14       | 274                  | 200             | 224             | 269             | 0               | 967   | 0.35     | 2.13    | 0.24                | 0.28       |
| 15       | 272                  | 212             | 217             | 278             | 0               | 979   | 0.36     | 2.21    | 0.25                | 0.28       |
| 16       | 274                  | 197             | 224             | 271             | 0               | 966   | 0.35     | 2.06    | 0.24                | 0.28       |
| 17       | 277                  | 211             | 211             | 275             | 0               | 974   | 0.35     | 2.16    | 0.25                | 0.28       |

<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

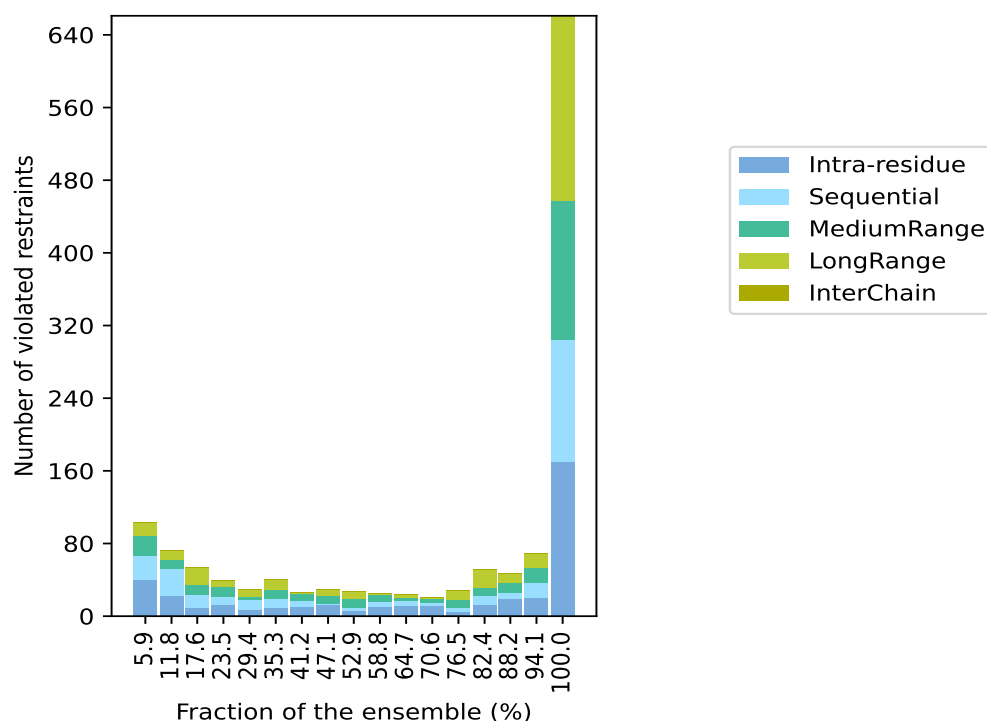
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 3158(IR:1409, SQ:816, MR:508, LR:425, IC:0) restraints are 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>       | %     |
| 40                            | 26              | 22              | 15              | 0               | 103   | 1                        | 5.9   |
| 23                            | 29              | 10              | 10              | 0               | 72    | 2                        | 11.8  |
| 9                             | 14              | 12              | 19              | 0               | 54    | 3                        | 17.6  |
| 13                            | 8               | 11              | 7               | 0               | 39    | 4                        | 23.5  |
| 7                             | 11              | 4               | 7               | 0               | 29    | 5                        | 29.4  |
| 10                            | 9               | 10              | 11              | 0               | 40    | 6                        | 35.3  |
| 10                            | 7               | 7               | 2               | 0               | 26    | 7                        | 41.2  |
| 12                            | 2               | 9               | 6               | 0               | 29    | 8                        | 47.1  |
| 6                             | 4               | 9               | 8               | 0               | 27    | 9                        | 52.9  |
| 10                            | 6               | 7               | 2               | 0               | 25    | 10                       | 58.8  |
| 12                            | 5               | 3               | 4               | 0               | 24    | 11                       | 64.7  |
| 11                            | 4               | 4               | 2               | 0               | 21    | 12                       | 70.6  |
| 5                             | 4               | 9               | 10              | 0               | 28    | 13                       | 76.5  |
| 12                            | 11              | 8               | 20              | 0               | 51    | 14                       | 82.4  |
| 19                            | 7               | 11              | 10              | 0               | 47    | 15                       | 88.2  |
| 20                            | 17              | 16              | 16              | 0               | 69    | 16                       | 94.1  |
| 170                           | 135             | 152             | 204             | 0               | 661   | 17                       | 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

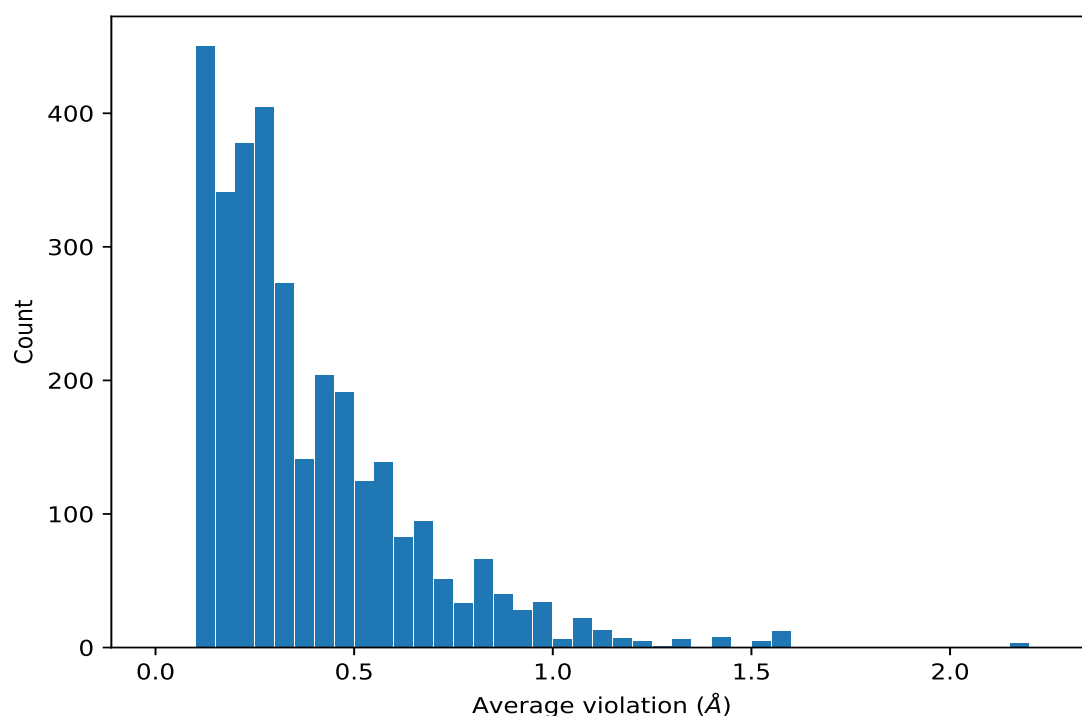
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



## 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) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,4095) | 1:116:A:GLN:HE22 | 1:85:A:LEU:HD13 | 17                  | 2.17     | 0.07                | 2.16       |
| (1,4095) | 1:116:A:GLN:HE22 | 1:85:A:LEU:HD11 | 17                  | 2.17     | 0.07                | 2.16       |
| (1,4095) | 1:116:A:GLN:HE22 | 1:85:A:LEU:HD12 | 17                  | 2.17     | 0.07                | 2.16       |
| (1,1386) | 1:56:A:LEU:HB3   | 1:53:A:PHE:HD1  | 17                  | 1.57     | 0.02                | 1.57       |
| (1,1386) | 1:56:A:LEU:HB3   | 1:53:A:PHE:HD2  | 17                  | 1.57     | 0.02                | 1.57       |
| (3,128)  | 1:97:A:LEU:HD22  | 1:75:A:LEU:HD12 | 17                  | 1.55     | 0.05                | 1.57       |
| (3,128)  | 1:57:A:VAL:HG11  | 1:75:A:LEU:HD13 | 17                  | 1.55     | 0.05                | 1.57       |
| (3,128)  | 1:97:A:LEU:HD23  | 1:75:A:LEU:HD12 | 17                  | 1.55     | 0.05                | 1.57       |
| (3,128)  | 1:97:A:LEU:HD21  | 1:75:A:LEU:HD13 | 17                  | 1.55     | 0.05                | 1.57       |
| (3,128)  | 1:97:A:LEU:HD23  | 1:75:A:LEU:HD11 | 17                  | 1.55     | 0.05                | 1.57       |
| (3,128)  | 1:97:A:LEU:HD21  | 1:75:A:LEU:HD12 | 17                  | 1.55     | 0.05                | 1.57       |
| (3,128)  | 1:97:A:LEU:HD21  | 1:75:A:LEU:HD11 | 17                  | 1.55     | 0.05                | 1.57       |
| (3,128)  | 1:97:A:LEU:HD23  | 1:75:A:LEU:HD13 | 17                  | 1.55     | 0.05                | 1.57       |
| (3,128)  | 1:97:A:LEU:HD22  | 1:75:A:LEU:HD13 | 17                  | 1.55     | 0.05                | 1.57       |
| (3,128)  | 1:57:A:VAL:HG11  | 1:75:A:LEU:HD11 | 17                  | 1.55     | 0.05                | 1.57       |
| (3,17)   | 1:60:A:VAL:HG12  | 1:62:A:GLY:H    | 17                  | 1.54     | 0.22                | 1.61       |

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| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (3,17)   | 1:60:A:VAL:HG13  | 1:62:A:GLY:H    | 17                  | 1.54     | 0.22                | 1.61       |
| (3,17)   | 1:60:A:VAL:HG11  | 1:62:A:GLY:H    | 17                  | 1.54     | 0.22                | 1.61       |
| (1,2917) | 1:56:A:LEU:HB3   | 1:53:A:PHE:HD1  | 17                  | 1.53     | 0.02                | 1.52       |
| (1,2917) | 1:56:A:LEU:HB3   | 1:53:A:PHE:HD2  | 17                  | 1.53     | 0.02                | 1.52       |
| (3,39)   | 1:31:A:LEU:HD21  | 1:32:A:ALA:HB3  | 17                  | 1.43     | 0.04                | 1.42       |
| (3,39)   | 1:31:A:LEU:HD23  | 1:32:A:ALA:HB1  | 17                  | 1.43     | 0.04                | 1.42       |
| (3,39)   | 1:31:A:LEU:HD22  | 1:32:A:ALA:HB2  | 17                  | 1.43     | 0.04                | 1.42       |
| (3,39)   | 1:31:A:LEU:HD22  | 1:32:A:ALA:HB1  | 17                  | 1.43     | 0.04                | 1.42       |
| (3,39)   | 1:31:A:LEU:HD21  | 1:32:A:ALA:HB1  | 17                  | 1.43     | 0.04                | 1.42       |
| (3,39)   | 1:31:A:LEU:HD23  | 1:32:A:ALA:HB2  | 17                  | 1.43     | 0.04                | 1.42       |
| (3,39)   | 1:31:A:LEU:HD22  | 1:32:A:ALA:HB3  | 17                  | 1.43     | 0.04                | 1.42       |
| (3,39)   | 1:31:A:LEU:HD23  | 1:32:A:ALA:HB3  | 17                  | 1.43     | 0.04                | 1.42       |
| (3,120)  | 1:49:A:LYS:HB2   | 1:52:A:ILE:HD11 | 17                  | 1.33     | 0.28                | 1.4        |
| (3,120)  | 1:49:A:LYS:HB2   | 1:52:A:ILE:HD13 | 17                  | 1.33     | 0.28                | 1.4        |
| (3,120)  | 1:48:A:LEU:HD21  | 1:49:A:LYS:HB2  | 17                  | 1.33     | 0.28                | 1.4        |
| (3,120)  | 1:49:A:LYS:HB2   | 1:52:A:ILE:HD12 | 17                  | 1.33     | 0.28                | 1.4        |
| (3,120)  | 1:50:A:ILE:HG21  | 1:49:A:LYS:HB2  | 17                  | 1.33     | 0.28                | 1.4        |
| (3,120)  | 1:50:A:ILE:HG23  | 1:49:A:LYS:HB2  | 17                  | 1.33     | 0.28                | 1.4        |
| (1,4121) | 1:116:A:GLN:HE21 | 1:116:A:GLN:HA  | 17                  | 1.28     | 0.06                | 1.28       |
| (1,558)  | 1:116:A:GLN:HE21 | 1:116:A:GLN:HA  | 17                  | 1.23     | 0.06                | 1.23       |
| (3,104)  | 1:66:A:LEU:HD11  | 1:70:A:GLN:H    | 17                  | 1.23     | 0.06                | 1.24       |
| (3,104)  | 1:66:A:LEU:HD12  | 1:70:A:GLN:H    | 17                  | 1.23     | 0.06                | 1.24       |
| (3,104)  | 1:66:A:LEU:HD12  | 1:57:A:VAL:H    | 17                  | 1.23     | 0.06                | 1.24       |
| (3,104)  | 1:66:A:LEU:HD13  | 1:70:A:GLN:H    | 17                  | 1.23     | 0.06                | 1.24       |
| (1,3486) | 1:97:A:LEU:HD12  | 1:31:A:LEU:HD13 | 17                  | 1.16     | 0.05                | 1.15       |
| (1,3486) | 1:97:A:LEU:HD12  | 1:31:A:LEU:HD12 | 17                  | 1.16     | 0.05                | 1.15       |
| (1,3486) | 1:97:A:LEU:HD13  | 1:31:A:LEU:HD12 | 17                  | 1.16     | 0.05                | 1.15       |
| (1,3486) | 1:97:A:LEU:HD11  | 1:31:A:LEU:HD11 | 17                  | 1.16     | 0.05                | 1.15       |
| (1,3486) | 1:97:A:LEU:HD11  | 1:31:A:LEU:HD13 | 17                  | 1.16     | 0.05                | 1.15       |
| (1,3486) | 1:97:A:LEU:HD13  | 1:31:A:LEU:HD13 | 17                  | 1.16     | 0.05                | 1.15       |
| (1,3486) | 1:97:A:LEU:HD12  | 1:31:A:LEU:HD11 | 17                  | 1.16     | 0.05                | 1.15       |
| (3,127)  | 1:31:A:LEU:HD21  | 1:97:A:LEU:HD21 | 17                  | 1.15     | 0.03                | 1.16       |
| (3,127)  | 1:31:A:LEU:HD23  | 1:97:A:LEU:HD22 | 17                  | 1.15     | 0.03                | 1.16       |
| (3,127)  | 1:31:A:LEU:HD23  | 1:97:A:LEU:HD23 | 17                  | 1.15     | 0.03                | 1.16       |
| (3,127)  | 1:31:A:LEU:HD22  | 1:97:A:LEU:HD23 | 17                  | 1.15     | 0.03                | 1.16       |
| (3,127)  | 1:31:A:LEU:HD22  | 1:97:A:LEU:HD22 | 17                  | 1.15     | 0.03                | 1.16       |
| (3,127)  | 1:31:A:LEU:HD21  | 1:97:A:LEU:HD22 | 17                  | 1.15     | 0.03                | 1.16       |
| (3,127)  | 1:31:A:LEU:HD23  | 1:97:A:LEU:HD21 | 17                  | 1.15     | 0.03                | 1.16       |
| (3,127)  | 1:31:A:LEU:HD22  | 1:97:A:LEU:HD21 | 17                  | 1.15     | 0.03                | 1.16       |
| (1,2191) | 1:32:A:ALA:HB3   | 1:39:A:PHE:HE2  | 17                  | 1.13     | 0.05                | 1.13       |
| (1,2191) | 1:32:A:ALA:HB1   | 1:39:A:PHE:HE1  | 17                  | 1.13     | 0.05                | 1.13       |
| (1,2191) | 1:32:A:ALA:HB2   | 1:39:A:PHE:HE1  | 17                  | 1.13     | 0.05                | 1.13       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,2191) | 1:32:A:ALA:HB2  | 1:39:A:PHE:HE2  | 17                  | 1.13     | 0.05                | 1.13       |
| (1,2191) | 1:32:A:ALA:HB3  | 1:39:A:PHE:HE1  | 17                  | 1.13     | 0.05                | 1.13       |
| (3,95)   | 1:75:A:LEU:HD11 | 1:78:A:TYR:H    | 17                  | 1.09     | 0.4                 | 1.22       |
| (3,95)   | 1:75:A:LEU:HD13 | 1:50:A:ILE:H    | 17                  | 1.09     | 0.4                 | 1.22       |
| (3,95)   | 1:75:A:LEU:HD11 | 1:50:A:ILE:H    | 17                  | 1.09     | 0.4                 | 1.22       |
| (3,95)   | 1:75:A:LEU:HD13 | 1:78:A:TYR:H    | 17                  | 1.09     | 0.4                 | 1.22       |
| (3,95)   | 1:75:A:LEU:HD12 | 1:78:A:TYR:H    | 17                  | 1.09     | 0.4                 | 1.22       |
| (3,82)   | 1:57:A:VAL:HG12 | 1:71:A:LEU:HD21 | 17                  | 1.06     | 0.04                | 1.06       |
| (3,82)   | 1:57:A:VAL:HG12 | 1:71:A:LEU:HD23 | 17                  | 1.06     | 0.04                | 1.06       |
| (3,82)   | 1:57:A:VAL:HG12 | 1:71:A:LEU:HD22 | 17                  | 1.06     | 0.04                | 1.06       |
| (3,82)   | 1:57:A:VAL:HG13 | 1:71:A:LEU:HD22 | 17                  | 1.06     | 0.04                | 1.06       |
| (3,82)   | 1:57:A:VAL:HG11 | 1:71:A:LEU:HD22 | 17                  | 1.06     | 0.04                | 1.06       |
| (3,82)   | 1:57:A:VAL:HG13 | 1:71:A:LEU:HD21 | 17                  | 1.06     | 0.04                | 1.06       |
| (3,82)   | 1:57:A:VAL:HG13 | 1:71:A:LEU:HD23 | 17                  | 1.06     | 0.04                | 1.06       |
| (3,82)   | 1:57:A:VAL:HG11 | 1:71:A:LEU:HD23 | 17                  | 1.06     | 0.04                | 1.06       |
| (1,836)  | 1:64:A:MET:HE1  | 1:60:A:VAL:HG13 | 17                  | 1.05     | 0.14                | 0.99       |
| (1,836)  | 1:64:A:MET:HE3  | 1:60:A:VAL:HG11 | 17                  | 1.05     | 0.14                | 0.99       |
| (1,836)  | 1:64:A:MET:HE2  | 1:60:A:VAL:HG13 | 17                  | 1.05     | 0.14                | 0.99       |
| (1,836)  | 1:64:A:MET:HE3  | 1:60:A:VAL:HG12 | 17                  | 1.05     | 0.14                | 0.99       |
| (1,836)  | 1:64:A:MET:HE2  | 1:60:A:VAL:HG11 | 17                  | 1.05     | 0.14                | 0.99       |
| (1,836)  | 1:64:A:MET:HE1  | 1:60:A:VAL:HG12 | 17                  | 1.05     | 0.14                | 0.99       |
| (1,836)  | 1:64:A:MET:HE2  | 1:60:A:VAL:HG12 | 17                  | 1.05     | 0.14                | 0.99       |
| (1,836)  | 1:64:A:MET:HE3  | 1:60:A:VAL:HG13 | 17                  | 1.05     | 0.14                | 0.99       |
| (1,836)  | 1:64:A:MET:HE1  | 1:60:A:VAL:HG11 | 17                  | 1.05     | 0.14                | 0.99       |
| (3,5)    | 1:28:A:ILE:HD12 | 1:25:A:LYS:HA   | 17                  | 1.04     | 0.1                 | 1.04       |
| (3,5)    | 1:28:A:ILE:HD13 | 1:25:A:LYS:HA   | 17                  | 1.04     | 0.1                 | 1.04       |
| (3,5)    | 1:28:A:ILE:HD11 | 1:25:A:LYS:HA   | 17                  | 1.04     | 0.1                 | 1.04       |
| (1,4026) | 1:32:A:ALA:H    | 1:29:A:ALA:HB1  | 17                  | 1.0      | 0.02                | 1.0        |
| (1,4026) | 1:32:A:ALA:H    | 1:29:A:ALA:HB2  | 17                  | 1.0      | 0.02                | 1.0        |
| (1,4026) | 1:32:A:ALA:H    | 1:29:A:ALA:HB3  | 17                  | 1.0      | 0.02                | 1.0        |
| (1,1758) | 1:79:A:THR:HG22 | 1:48:A:LEU:HD11 | 17                  | 0.99     | 0.18                | 1.05       |
| (1,1758) | 1:79:A:THR:HG21 | 1:48:A:LEU:HD13 | 17                  | 0.99     | 0.18                | 1.05       |
| (1,1758) | 1:79:A:THR:HG21 | 1:48:A:LEU:HD11 | 17                  | 0.99     | 0.18                | 1.05       |
| (1,1758) | 1:79:A:THR:HG23 | 1:48:A:LEU:HD12 | 17                  | 0.99     | 0.18                | 1.05       |
| (1,1758) | 1:79:A:THR:HG22 | 1:48:A:LEU:HD12 | 17                  | 0.99     | 0.18                | 1.05       |
| (1,1758) | 1:79:A:THR:HG23 | 1:48:A:LEU:HD13 | 17                  | 0.99     | 0.18                | 1.05       |
| (1,1758) | 1:79:A:THR:HG21 | 1:48:A:LEU:HD12 | 17                  | 0.99     | 0.18                | 1.05       |
| (1,2421) | 1:64:A:MET:HE1  | 1:60:A:VAL:HG13 | 17                  | 0.99     | 0.14                | 0.92       |
| (1,2421) | 1:64:A:MET:HE3  | 1:60:A:VAL:HG11 | 17                  | 0.99     | 0.14                | 0.92       |
| (1,2421) | 1:64:A:MET:HE2  | 1:60:A:VAL:HG13 | 17                  | 0.99     | 0.14                | 0.92       |
| (1,2421) | 1:64:A:MET:HE3  | 1:60:A:VAL:HG12 | 17                  | 0.99     | 0.14                | 0.92       |
| (1,2421) | 1:64:A:MET:HE2  | 1:60:A:VAL:HG11 | 17                  | 0.99     | 0.14                | 0.92       |

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| Key      | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,2421) | 1:64:A:MET:HE1  | 1:60:A:VAL:HG12  | 17                  | 0.99     | 0.14                | 0.92       |
| (1,2421) | 1:64:A:MET:HE2  | 1:60:A:VAL:HG12  | 17                  | 0.99     | 0.14                | 0.92       |
| (1,2421) | 1:64:A:MET:HE3  | 1:60:A:VAL:HG13  | 17                  | 0.99     | 0.14                | 0.92       |
| (1,2421) | 1:64:A:MET:HE1  | 1:60:A:VAL:HG11  | 17                  | 0.99     | 0.14                | 0.92       |
| (3,20)   | 1:88:A:VAL:HG13 | 1:93:A:THR:HG22  | 17                  | 0.97     | 0.1                 | 0.99       |
| (3,20)   | 1:93:A:THR:HG23 | 1:110:A:VAL:HG11 | 17                  | 0.97     | 0.1                 | 0.99       |
| (3,20)   | 1:88:A:VAL:HG12 | 1:93:A:THR:HG21  | 17                  | 0.97     | 0.1                 | 0.99       |
| (3,20)   | 1:93:A:THR:HG22 | 1:110:A:VAL:HG12 | 17                  | 0.97     | 0.1                 | 0.99       |
| (3,20)   | 1:93:A:THR:HG22 | 1:110:A:VAL:HG13 | 17                  | 0.97     | 0.1                 | 0.99       |
| (3,20)   | 1:93:A:THR:HG23 | 1:110:A:VAL:HG13 | 17                  | 0.97     | 0.1                 | 0.99       |
| (3,20)   | 1:88:A:VAL:HG13 | 1:93:A:THR:HG23  | 17                  | 0.97     | 0.1                 | 0.99       |
| (3,20)   | 1:93:A:THR:HG21 | 1:110:A:VAL:HG13 | 17                  | 0.97     | 0.1                 | 0.99       |
| (3,20)   | 1:88:A:VAL:HG13 | 1:93:A:THR:HG21  | 17                  | 0.97     | 0.1                 | 0.99       |
| (3,20)   | 1:93:A:THR:HG23 | 1:110:A:VAL:HG12 | 17                  | 0.97     | 0.1                 | 0.99       |
| (3,20)   | 1:88:A:VAL:HG12 | 1:93:A:THR:HG22  | 17                  | 0.97     | 0.1                 | 0.99       |
| (3,20)   | 1:93:A:THR:HG22 | 1:110:A:VAL:HG11 | 17                  | 0.97     | 0.1                 | 0.99       |
| (3,20)   | 1:93:A:THR:HG21 | 1:110:A:VAL:HG12 | 17                  | 0.97     | 0.1                 | 0.99       |
| (3,134)  | 1:75:A:LEU:HD21 | 1:97:A:LEU:HD22  | 17                  | 0.94     | 0.05                | 0.94       |
| (3,134)  | 1:75:A:LEU:HD23 | 1:97:A:LEU:HD23  | 17                  | 0.94     | 0.05                | 0.94       |
| (3,134)  | 1:75:A:LEU:HD21 | 1:97:A:LEU:HD23  | 17                  | 0.94     | 0.05                | 0.94       |
| (3,134)  | 1:75:A:LEU:HD23 | 1:97:A:LEU:HD21  | 17                  | 0.94     | 0.05                | 0.94       |
| (3,134)  | 1:75:A:LEU:HD22 | 1:97:A:LEU:HD21  | 17                  | 0.94     | 0.05                | 0.94       |
| (3,134)  | 1:75:A:LEU:HD21 | 1:97:A:LEU:HD21  | 17                  | 0.94     | 0.05                | 0.94       |
| (3,134)  | 1:75:A:LEU:HD22 | 1:97:A:LEU:HD23  | 17                  | 0.94     | 0.05                | 0.94       |
| (3,134)  | 1:75:A:LEU:HD22 | 1:97:A:LEU:HD22  | 17                  | 0.94     | 0.05                | 0.94       |
| (1,3352) | 1:79:A:THR:HG22 | 1:48:A:LEU:HD11  | 17                  | 0.93     | 0.18                | 1.0        |
| (1,3352) | 1:79:A:THR:HG21 | 1:48:A:LEU:HD13  | 17                  | 0.93     | 0.18                | 1.0        |
| (1,3352) | 1:79:A:THR:HG21 | 1:48:A:LEU:HD11  | 17                  | 0.93     | 0.18                | 1.0        |
| (1,3352) | 1:79:A:THR:HG23 | 1:48:A:LEU:HD12  | 17                  | 0.93     | 0.18                | 1.0        |
| (1,3352) | 1:79:A:THR:HG22 | 1:48:A:LEU:HD12  | 17                  | 0.93     | 0.18                | 1.0        |
| (1,3352) | 1:79:A:THR:HG23 | 1:48:A:LEU:HD13  | 17                  | 0.93     | 0.18                | 1.0        |
| (1,3352) | 1:79:A:THR:HG21 | 1:48:A:LEU:HD12  | 17                  | 0.93     | 0.18                | 1.0        |
| (1,2883) | 1:32:A:ALA:HB1  | 1:39:A:PHE:H     | 17                  | 0.92     | 0.04                | 0.91       |
| (1,2883) | 1:32:A:ALA:HB2  | 1:39:A:PHE:H     | 17                  | 0.92     | 0.04                | 0.91       |
| (1,2883) | 1:32:A:ALA:HB3  | 1:39:A:PHE:H     | 17                  | 0.92     | 0.04                | 0.91       |
| (1,1415) | 1:48:A:LEU:HD13 | 1:75:A:LEU:HD12  | 17                  | 0.91     | 0.07                | 0.89       |
| (1,1415) | 1:48:A:LEU:HD11 | 1:75:A:LEU:HD13  | 17                  | 0.91     | 0.07                | 0.89       |
| (1,1415) | 1:48:A:LEU:HD13 | 1:75:A:LEU:HD11  | 17                  | 0.91     | 0.07                | 0.89       |
| (1,1415) | 1:48:A:LEU:HD12 | 1:75:A:LEU:HD12  | 17                  | 0.91     | 0.07                | 0.89       |
| (1,1415) | 1:48:A:LEU:HD12 | 1:75:A:LEU:HD11  | 17                  | 0.91     | 0.07                | 0.89       |
| (1,1415) | 1:48:A:LEU:HD12 | 1:75:A:LEU:HD13  | 17                  | 0.91     | 0.07                | 0.89       |
| (1,1415) | 1:48:A:LEU:HD13 | 1:75:A:LEU:HD13  | 17                  | 0.91     | 0.07                | 0.89       |

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| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (3,107)  | 1:95:A:VAL:HG21  | 1:102:A:CYS:HB3 | 17                  | 0.91     | 0.19                | 0.92       |
| (3,107)  | 1:95:A:VAL:HG23  | 1:102:A:CYS:HB3 | 17                  | 0.91     | 0.19                | 0.92       |
| (3,107)  | 1:95:A:VAL:HG22  | 1:102:A:CYS:HB3 | 17                  | 0.91     | 0.19                | 0.92       |
| (3,70)   | 1:58:A:ASP:HA    | 1:57:A:VAL:HG12 | 17                  | 0.89     | 0.05                | 0.9        |
| (3,70)   | 1:58:A:ASP:HA    | 1:57:A:VAL:HG13 | 17                  | 0.89     | 0.05                | 0.9        |
| (3,70)   | 1:58:A:ASP:HA    | 1:57:A:VAL:HG11 | 17                  | 0.89     | 0.05                | 0.9        |
| (3,52)   | 1:95:A:VAL:HG22  | 1:37:A:HIS:HB2  | 17                  | 0.88     | 0.3                 | 0.95       |
| (3,52)   | 1:99:A:GLY:HA3   | 1:95:A:VAL:HG22 | 17                  | 0.88     | 0.3                 | 0.95       |
| (3,52)   | 1:95:A:VAL:HG21  | 1:37:A:HIS:HB2  | 17                  | 0.88     | 0.3                 | 0.95       |
| (3,52)   | 1:99:A:GLY:HA3   | 1:95:A:VAL:HG23 | 17                  | 0.88     | 0.3                 | 0.95       |
| (3,52)   | 1:95:A:VAL:HG23  | 1:37:A:HIS:HB2  | 17                  | 0.88     | 0.3                 | 0.95       |
| (3,52)   | 1:99:A:GLY:HA3   | 1:95:A:VAL:HG21 | 17                  | 0.88     | 0.3                 | 0.95       |
| (1,4118) | 1:71:A:LEU:H     | 1:70:A:GLN:HE21 | 17                  | 0.88     | 0.13                | 0.9        |
| (1,4341) | 1:113:A:ALA:HB1  | 1:116:A:GLN:H   | 17                  | 0.88     | 0.03                | 0.88       |
| (1,4341) | 1:113:A:ALA:HB3  | 1:116:A:GLN:H   | 17                  | 0.88     | 0.03                | 0.88       |
| (1,4341) | 1:113:A:ALA:HB2  | 1:116:A:GLN:H   | 17                  | 0.88     | 0.03                | 0.88       |
| (1,1534) | 1:56:A:LEU:HB2   | 1:35:A:PHE:HE2  | 17                  | 0.88     | 0.07                | 0.86       |
| (1,1534) | 1:56:A:LEU:HB2   | 1:35:A:PHE:HE1  | 17                  | 0.88     | 0.07                | 0.86       |
| (1,1862) | 1:32:A:ALA:HB3   | 1:31:A:LEU:HD11 | 17                  | 0.87     | 0.03                | 0.86       |
| (1,1862) | 1:32:A:ALA:HB1   | 1:31:A:LEU:HD11 | 17                  | 0.87     | 0.03                | 0.86       |
| (1,1862) | 1:32:A:ALA:HB1   | 1:31:A:LEU:HD13 | 17                  | 0.87     | 0.03                | 0.86       |
| (1,1862) | 1:32:A:ALA:HB2   | 1:31:A:LEU:HD13 | 17                  | 0.87     | 0.03                | 0.86       |
| (1,1862) | 1:32:A:ALA:HB2   | 1:31:A:LEU:HD12 | 17                  | 0.87     | 0.03                | 0.86       |
| (1,1862) | 1:32:A:ALA:HB2   | 1:31:A:LEU:HD11 | 17                  | 0.87     | 0.03                | 0.86       |
| (1,1862) | 1:32:A:ALA:HB3   | 1:31:A:LEU:HD13 | 17                  | 0.87     | 0.03                | 0.86       |
| (1,3098) | 1:56:A:LEU:HD13  | 1:57:A:VAL:H    | 17                  | 0.87     | 0.01                | 0.87       |
| (1,3098) | 1:56:A:LEU:HD11  | 1:57:A:VAL:H    | 17                  | 0.87     | 0.01                | 0.87       |
| (1,3098) | 1:56:A:LEU:HD12  | 1:57:A:VAL:H    | 17                  | 0.87     | 0.01                | 0.87       |
| (1,4080) | 1:54:A:GLN:HE22  | 1:57:A:VAL:HG22 | 17                  | 0.86     | 0.21                | 0.73       |
| (1,4080) | 1:54:A:GLN:HE22  | 1:57:A:VAL:HG21 | 17                  | 0.86     | 0.21                | 0.73       |
| (1,4080) | 1:54:A:GLN:HE22  | 1:57:A:VAL:HG23 | 17                  | 0.86     | 0.21                | 0.73       |
| (1,4120) | 1:116:A:GLN:HE21 | 1:119:A:GLU:HB2 | 17                  | 0.86     | 0.15                | 0.88       |
| (1,4116) | 1:70:A:GLN:HA    | 1:70:A:GLN:HE21 | 17                  | 0.86     | 0.08                | 0.87       |
| (1,2956) | 1:48:A:LEU:HD13  | 1:75:A:LEU:HD12 | 17                  | 0.86     | 0.07                | 0.84       |
| (1,2956) | 1:48:A:LEU:HD11  | 1:75:A:LEU:HD13 | 17                  | 0.86     | 0.07                | 0.84       |
| (1,2956) | 1:48:A:LEU:HD13  | 1:75:A:LEU:HD11 | 17                  | 0.86     | 0.07                | 0.84       |
| (1,2956) | 1:48:A:LEU:HD12  | 1:75:A:LEU:HD12 | 17                  | 0.86     | 0.07                | 0.84       |
| (1,2956) | 1:48:A:LEU:HD12  | 1:75:A:LEU:HD11 | 17                  | 0.86     | 0.07                | 0.84       |
| (1,2956) | 1:48:A:LEU:HD12  | 1:75:A:LEU:HD13 | 17                  | 0.86     | 0.07                | 0.84       |
| (1,2956) | 1:48:A:LEU:HD13  | 1:75:A:LEU:HD13 | 17                  | 0.86     | 0.07                | 0.84       |
| (1,1503) | 1:52:A:ILE:HG12  | 1:54:A:GLN:HE21 | 17                  | 0.86     | 0.13                | 0.84       |
| (3,142)  | 1:59:A:ARG:H     | 1:57:A:VAL:HG12 | 17                  | 0.84     | 0.04                | 0.84       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (3,142)  | 1:59:A:ARG:H    | 1:57:A:VAL:HG13 | 17                  | 0.84     | 0.04                | 0.84       |
| (3,142)  | 1:59:A:ARG:H    | 1:57:A:VAL:HG11 | 17                  | 0.84     | 0.04                | 0.84       |
| (1,3060) | 1:52:A:ILE:HG22 | 1:97:A:LEU:HD22 | 17                  | 0.84     | 0.14                | 0.9        |
| (1,3060) | 1:52:A:ILE:HG23 | 1:97:A:LEU:HD23 | 17                  | 0.84     | 0.14                | 0.9        |
| (1,3060) | 1:52:A:ILE:HG22 | 1:97:A:LEU:HD21 | 17                  | 0.84     | 0.14                | 0.9        |
| (1,3060) | 1:52:A:ILE:HG21 | 1:97:A:LEU:HD23 | 17                  | 0.84     | 0.14                | 0.9        |
| (1,3060) | 1:52:A:ILE:HG22 | 1:97:A:LEU:HD23 | 17                  | 0.84     | 0.14                | 0.9        |
| (1,3060) | 1:52:A:ILE:HG23 | 1:97:A:LEU:HD21 | 17                  | 0.84     | 0.14                | 0.9        |
| (1,3060) | 1:52:A:ILE:HG21 | 1:97:A:LEU:HD21 | 17                  | 0.84     | 0.14                | 0.9        |
| (1,3060) | 1:52:A:ILE:HG21 | 1:97:A:LEU:HD22 | 17                  | 0.84     | 0.14                | 0.9        |
| (1,2326) | 1:31:A:LEU:HD12 | 1:27:A:VAL:HG13 | 17                  | 0.83     | 0.08                | 0.84       |
| (1,2326) | 1:31:A:LEU:HD12 | 1:27:A:VAL:HG11 | 17                  | 0.83     | 0.08                | 0.84       |
| (1,2326) | 1:31:A:LEU:HD11 | 1:27:A:VAL:HG11 | 17                  | 0.83     | 0.08                | 0.84       |
| (1,2326) | 1:31:A:LEU:HD11 | 1:27:A:VAL:HG13 | 17                  | 0.83     | 0.08                | 0.84       |
| (1,2326) | 1:31:A:LEU:HD13 | 1:27:A:VAL:HG13 | 17                  | 0.83     | 0.08                | 0.84       |
| (1,2326) | 1:31:A:LEU:HD12 | 1:27:A:VAL:HG12 | 17                  | 0.83     | 0.08                | 0.84       |
| (1,2326) | 1:31:A:LEU:HD13 | 1:27:A:VAL:HG12 | 17                  | 0.83     | 0.08                | 0.84       |
| (1,3893) | 1:79:A:THR:HG21 | 1:81:A:SER:H    | 17                  | 0.83     | 0.04                | 0.83       |
| (1,3893) | 1:79:A:THR:HG22 | 1:81:A:SER:H    | 17                  | 0.83     | 0.04                | 0.83       |
| (1,3893) | 1:79:A:THR:HG23 | 1:81:A:SER:H    | 17                  | 0.83     | 0.04                | 0.83       |
| (1,556)  | 1:71:A:LEU:H    | 1:70:A:GLN:HE21 | 17                  | 0.82     | 0.13                | 0.85       |
| (3,30)   | 1:64:A:MET:HE1  | 1:34:A:ARG:HB3  | 17                  | 0.82     | 0.09                | 0.79       |
| (3,30)   | 1:64:A:MET:HE3  | 1:34:A:ARG:HB3  | 17                  | 0.82     | 0.09                | 0.79       |
| (3,30)   | 1:64:A:MET:HE2  | 1:34:A:ARG:HB3  | 17                  | 0.82     | 0.09                | 0.79       |
| (1,522)  | 1:54:A:GLN:HE22 | 1:57:A:VAL:HG22 | 17                  | 0.82     | 0.21                | 0.69       |
| (1,522)  | 1:54:A:GLN:HE22 | 1:57:A:VAL:HG21 | 17                  | 0.82     | 0.21                | 0.69       |
| (1,522)  | 1:54:A:GLN:HE22 | 1:57:A:VAL:HG23 | 17                  | 0.82     | 0.21                | 0.69       |
| (1,3088) | 1:56:A:LEU:HB2  | 1:35:A:PHE:HE2  | 17                  | 0.82     | 0.07                | 0.81       |
| (1,3088) | 1:56:A:LEU:HB2  | 1:35:A:PHE:HE1  | 17                  | 0.82     | 0.07                | 0.81       |
| (3,146)  | 1:52:A:ILE:H    | 1:52:A:ILE:HD13 | 17                  | 0.82     | 0.1                 | 0.85       |
| (3,146)  | 1:52:A:ILE:H    | 1:52:A:ILE:HD11 | 17                  | 0.82     | 0.1                 | 0.85       |
| (3,146)  | 1:52:A:ILE:H    | 1:52:A:ILE:HD12 | 17                  | 0.82     | 0.1                 | 0.85       |
| (1,2903) | 1:50:A:ILE:HD11 | 1:51:A:GLY:H    | 17                  | 0.81     | 0.07                | 0.82       |
| (1,2903) | 1:50:A:ILE:HD12 | 1:51:A:GLY:H    | 17                  | 0.81     | 0.07                | 0.82       |
| (1,2903) | 1:50:A:ILE:HD13 | 1:51:A:GLY:H    | 17                  | 0.81     | 0.07                | 0.82       |
| (1,3474) | 1:32:A:ALA:HB3  | 1:31:A:LEU:HD11 | 17                  | 0.81     | 0.03                | 0.8        |
| (1,3474) | 1:32:A:ALA:HB1  | 1:31:A:LEU:HD11 | 17                  | 0.81     | 0.03                | 0.8        |
| (1,3474) | 1:32:A:ALA:HB1  | 1:31:A:LEU:HD13 | 17                  | 0.81     | 0.03                | 0.8        |
| (1,3474) | 1:32:A:ALA:HB2  | 1:31:A:LEU:HD13 | 17                  | 0.81     | 0.03                | 0.8        |
| (1,3474) | 1:32:A:ALA:HB2  | 1:31:A:LEU:HD12 | 17                  | 0.81     | 0.03                | 0.8        |
| (1,3474) | 1:32:A:ALA:HB2  | 1:31:A:LEU:HD11 | 17                  | 0.81     | 0.03                | 0.8        |
| (1,3474) | 1:32:A:ALA:HB3  | 1:31:A:LEU:HD13 | 17                  | 0.81     | 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) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,3951) | 1:56:A:LEU:HB2   | 1:60:A:VAL:H     | 17                  | 0.81     | 0.01                | 0.81       |
| (1,2157) | 1:99:A:GLY:HA3   | 1:95:A:VAL:HG22  | 17                  | 0.81     | 0.11                | 0.82       |
| (1,2157) | 1:99:A:GLY:HA3   | 1:95:A:VAL:HG21  | 17                  | 0.81     | 0.11                | 0.82       |
| (1,2157) | 1:99:A:GLY:HA3   | 1:95:A:VAL:HG23  | 17                  | 0.81     | 0.11                | 0.82       |
| (1,554)  | 1:70:A:GLN:HA    | 1:70:A:GLN:HE21  | 17                  | 0.8      | 0.08                | 0.82       |
| (1,3046) | 1:52:A:ILE:HG12  | 1:54:A:GLN:HE21  | 17                  | 0.8      | 0.13                | 0.78       |
| (1,1675) | 1:88:A:VAL:HG21  | 1:92:A:ALA:HB2   | 17                  | 0.8      | 0.11                | 0.82       |
| (1,1675) | 1:88:A:VAL:HG23  | 1:92:A:ALA:HB1   | 17                  | 0.8      | 0.11                | 0.82       |
| (1,1675) | 1:88:A:VAL:HG22  | 1:92:A:ALA:HB1   | 17                  | 0.8      | 0.11                | 0.82       |
| (1,1675) | 1:88:A:VAL:HG21  | 1:92:A:ALA:HB1   | 17                  | 0.8      | 0.11                | 0.82       |
| (1,1675) | 1:88:A:VAL:HG23  | 1:92:A:ALA:HB3   | 17                  | 0.8      | 0.11                | 0.82       |
| (1,1675) | 1:88:A:VAL:HG23  | 1:92:A:ALA:HB2   | 17                  | 0.8      | 0.11                | 0.82       |
| (1,1675) | 1:88:A:VAL:HG21  | 1:92:A:ALA:HB3   | 17                  | 0.8      | 0.11                | 0.82       |
| (1,1675) | 1:88:A:VAL:HG22  | 1:92:A:ALA:HB2   | 17                  | 0.8      | 0.11                | 0.82       |
| (1,2308) | 1:82:A:TRP:HB2   | 1:117:A:LEU:HD12 | 17                  | 0.8      | 0.15                | 0.89       |
| (1,2308) | 1:82:A:TRP:HB2   | 1:117:A:LEU:HD11 | 17                  | 0.8      | 0.15                | 0.89       |
| (1,2308) | 1:82:A:TRP:HB2   | 1:117:A:LEU:HD13 | 17                  | 0.8      | 0.15                | 0.89       |
| (1,4124) | 1:116:A:GLN:HE21 | 1:120:A:ALA:H    | 17                  | 0.77     | 0.14                | 0.71       |
| (1,1676) | 1:94:A:ARG:HD2   | 1:92:A:ALA:HB2   | 17                  | 0.77     | 0.05                | 0.76       |
| (1,1676) | 1:94:A:ARG:HD2   | 1:92:A:ALA:HB1   | 17                  | 0.77     | 0.05                | 0.76       |
| (1,1676) | 1:94:A:ARG:HD2   | 1:92:A:ALA:HB3   | 17                  | 0.77     | 0.05                | 0.76       |
| (1,2820) | 1:97:A:LEU:HD12  | 1:52:A:ILE:H     | 17                  | 0.77     | 0.03                | 0.77       |
| (1,2820) | 1:97:A:LEU:HD11  | 1:52:A:ILE:H     | 17                  | 0.77     | 0.03                | 0.77       |
| (1,2820) | 1:97:A:LEU:HD13  | 1:52:A:ILE:H     | 17                  | 0.77     | 0.03                | 0.77       |
| (1,376)  | 1:56:A:LEU:HB2   | 1:60:A:VAL:H     | 17                  | 0.77     | 0.01                | 0.76       |
| (1,4122) | 1:116:A:GLN:HE21 | 1:113:A:ALA:HA   | 17                  | 0.76     | 0.09                | 0.79       |
| (1,3248) | 1:88:A:VAL:HG21  | 1:92:A:ALA:HB2   | 17                  | 0.76     | 0.11                | 0.78       |
| (1,3248) | 1:88:A:VAL:HG23  | 1:92:A:ALA:HB1   | 17                  | 0.76     | 0.11                | 0.78       |
| (1,3248) | 1:88:A:VAL:HG22  | 1:92:A:ALA:HB1   | 17                  | 0.76     | 0.11                | 0.78       |
| (1,3248) | 1:88:A:VAL:HG21  | 1:92:A:ALA:HB1   | 17                  | 0.76     | 0.11                | 0.78       |
| (1,3248) | 1:88:A:VAL:HG23  | 1:92:A:ALA:HB3   | 17                  | 0.76     | 0.11                | 0.78       |
| (1,3248) | 1:88:A:VAL:HG23  | 1:92:A:ALA:HB2   | 17                  | 0.76     | 0.11                | 0.78       |
| (1,3248) | 1:88:A:VAL:HG21  | 1:92:A:ALA:HB3   | 17                  | 0.76     | 0.11                | 0.78       |
| (1,3248) | 1:88:A:VAL:HG22  | 1:92:A:ALA:HB2   | 17                  | 0.76     | 0.11                | 0.78       |
| (1,805)  | 1:57:A:VAL:HG11  | 1:53:A:PHE:HD2   | 17                  | 0.75     | 0.04                | 0.75       |
| (1,805)  | 1:57:A:VAL:HG11  | 1:53:A:PHE:HD1   | 17                  | 0.75     | 0.04                | 0.75       |
| (1,805)  | 1:57:A:VAL:HG12  | 1:53:A:PHE:HD2   | 17                  | 0.75     | 0.04                | 0.75       |
| (1,805)  | 1:57:A:VAL:HG13  | 1:53:A:PHE:HD1   | 17                  | 0.75     | 0.04                | 0.75       |
| (1,805)  | 1:57:A:VAL:HG12  | 1:53:A:PHE:HD1   | 17                  | 0.75     | 0.04                | 0.75       |
| (1,805)  | 1:57:A:VAL:HG13  | 1:53:A:PHE:HD2   | 17                  | 0.75     | 0.04                | 0.75       |
| (1,1050) | 1:56:A:LEU:HB2   | 1:60:A:VAL:HG11  | 17                  | 0.75     | 0.03                | 0.75       |
| (1,1050) | 1:56:A:LEU:HB2   | 1:60:A:VAL:HG12  | 17                  | 0.75     | 0.03                | 0.75       |

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| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1050) | 1:56:A:LEU:HB2   | 1:60:A:VAL:HG13 | 17                  | 0.75     | 0.03                | 0.75       |
| (1,2192) | 1:55:A:ASP:HB2   | 1:52:A:ILE:HD12 | 17                  | 0.74     | 0.08                | 0.76       |
| (1,2192) | 1:55:A:ASP:HB2   | 1:52:A:ILE:HD13 | 17                  | 0.74     | 0.08                | 0.76       |
| (1,2192) | 1:55:A:ASP:HB2   | 1:52:A:ILE:HD11 | 17                  | 0.74     | 0.08                | 0.76       |
| (3,27)   | 1:71:A:LEU:HD11  | 1:71:A:LEU:H    | 17                  | 0.74     | 0.03                | 0.74       |
| (3,27)   | 1:71:A:LEU:HD13  | 1:71:A:LEU:H    | 17                  | 0.74     | 0.03                | 0.74       |
| (3,27)   | 1:71:A:LEU:HD12  | 1:71:A:LEU:H    | 17                  | 0.74     | 0.03                | 0.74       |
| (1,1800) | 1:75:A:LEU:HA    | 1:31:A:LEU:HD11 | 17                  | 0.74     | 0.05                | 0.74       |
| (1,1800) | 1:75:A:LEU:HA    | 1:31:A:LEU:HD13 | 17                  | 0.74     | 0.05                | 0.74       |
| (1,1800) | 1:75:A:LEU:HA    | 1:31:A:LEU:HD12 | 17                  | 0.74     | 0.05                | 0.74       |
| (1,2188) | 1:124:A:VAL:HG12 | 1:124:A:VAL:H   | 17                  | 0.74     | 0.01                | 0.74       |
| (1,2188) | 1:124:A:VAL:HG11 | 1:124:A:VAL:H   | 17                  | 0.74     | 0.01                | 0.74       |
| (1,2188) | 1:124:A:VAL:HG13 | 1:124:A:VAL:H   | 17                  | 0.74     | 0.01                | 0.74       |
| (1,2337) | 1:66:A:LEU:HD13  | 1:31:A:LEU:HD12 | 17                  | 0.74     | 0.05                | 0.75       |
| (1,2337) | 1:66:A:LEU:HD11  | 1:31:A:LEU:HD12 | 17                  | 0.74     | 0.05                | 0.75       |
| (1,2337) | 1:66:A:LEU:HD11  | 1:31:A:LEU:HD11 | 17                  | 0.74     | 0.05                | 0.75       |
| (1,2337) | 1:66:A:LEU:HD13  | 1:31:A:LEU:HD11 | 17                  | 0.74     | 0.05                | 0.75       |
| (1,2337) | 1:66:A:LEU:HD13  | 1:31:A:LEU:HD13 | 17                  | 0.74     | 0.05                | 0.75       |
| (1,2337) | 1:66:A:LEU:HD12  | 1:31:A:LEU:HD12 | 17                  | 0.74     | 0.05                | 0.75       |
| (1,2337) | 1:66:A:LEU:HD12  | 1:31:A:LEU:HD11 | 17                  | 0.74     | 0.05                | 0.75       |
| (1,2337) | 1:66:A:LEU:HD12  | 1:31:A:LEU:HD13 | 17                  | 0.74     | 0.05                | 0.75       |
| (3,76)   | 1:116:A:GLN:HE21 | 1:85:A:LEU:HD13 | 17                  | 0.74     | 0.08                | 0.73       |
| (3,76)   | 1:116:A:GLN:HE21 | 1:85:A:LEU:HD11 | 17                  | 0.74     | 0.08                | 0.73       |
| (3,76)   | 1:116:A:GLN:HE21 | 1:85:A:LEU:HD12 | 17                  | 0.74     | 0.08                | 0.73       |
| (1,3249) | 1:94:A:ARG:HD2   | 1:92:A:ALA:HB2  | 17                  | 0.72     | 0.05                | 0.71       |
| (1,3249) | 1:94:A:ARG:HD2   | 1:92:A:ALA:HB1  | 17                  | 0.72     | 0.05                | 0.71       |
| (1,3249) | 1:94:A:ARG:HD2   | 1:92:A:ALA:HB3  | 17                  | 0.72     | 0.05                | 0.71       |
| (1,561)  | 1:116:A:GLN:HE21 | 1:120:A:ALA:H   | 17                  | 0.72     | 0.14                | 0.66       |
| (1,2338) | 1:61:A:ALA:HB2   | 1:66:A:LEU:HD11 | 17                  | 0.72     | 0.08                | 0.69       |
| (1,2338) | 1:61:A:ALA:HB3   | 1:66:A:LEU:HD12 | 17                  | 0.72     | 0.08                | 0.69       |
| (1,2338) | 1:61:A:ALA:HB1   | 1:66:A:LEU:HD11 | 17                  | 0.72     | 0.08                | 0.69       |
| (1,2338) | 1:61:A:ALA:HB3   | 1:66:A:LEU:HD11 | 17                  | 0.72     | 0.08                | 0.69       |
| (1,2338) | 1:61:A:ALA:HB2   | 1:66:A:LEU:HD12 | 17                  | 0.72     | 0.08                | 0.69       |
| (1,2338) | 1:61:A:ALA:HB1   | 1:66:A:LEU:HD13 | 17                  | 0.72     | 0.08                | 0.69       |
| (1,2338) | 1:61:A:ALA:HB3   | 1:66:A:LEU:HD13 | 17                  | 0.72     | 0.08                | 0.69       |
| (1,2338) | 1:61:A:ALA:HB2   | 1:66:A:LEU:HD13 | 17                  | 0.72     | 0.08                | 0.69       |
| (1,2580) | 1:56:A:LEU:HB2   | 1:60:A:VAL:HG11 | 17                  | 0.72     | 0.03                | 0.72       |
| (1,2580) | 1:56:A:LEU:HB2   | 1:60:A:VAL:HG12 | 17                  | 0.72     | 0.03                | 0.72       |
| (1,2580) | 1:56:A:LEU:HB2   | 1:60:A:VAL:HG13 | 17                  | 0.72     | 0.03                | 0.72       |
| (1,4283) | 1:120:A:ALA:H    | 1:85:A:LEU:HD21 | 17                  | 0.72     | 0.23                | 0.64       |
| (1,4283) | 1:120:A:ALA:H    | 1:85:A:LEU:HD22 | 17                  | 0.72     | 0.23                | 0.64       |
| (1,4283) | 1:120:A:ALA:H    | 1:85:A:LEU:HD23 | 17                  | 0.72     | 0.23                | 0.64       |

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| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,4229) | 1:122:A:ALA:HB2  | 1:124:A:VAL:H   | 17                  | 0.71     | 0.02                | 0.72       |
| (1,4229) | 1:122:A:ALA:HB3  | 1:124:A:VAL:H   | 17                  | 0.71     | 0.02                | 0.72       |
| (1,4229) | 1:122:A:ALA:HB1  | 1:124:A:VAL:H   | 17                  | 0.71     | 0.02                | 0.72       |
| (1,559)  | 1:116:A:GLN:HE21 | 1:113:A:ALA:HA  | 17                  | 0.71     | 0.09                | 0.75       |
| (1,2384) | 1:57:A:VAL:HG11  | 1:53:A:PHE:HD2  | 17                  | 0.71     | 0.04                | 0.72       |
| (1,2384) | 1:57:A:VAL:HG11  | 1:53:A:PHE:HD1  | 17                  | 0.71     | 0.04                | 0.72       |
| (1,2384) | 1:57:A:VAL:HG12  | 1:53:A:PHE:HD2  | 17                  | 0.71     | 0.04                | 0.72       |
| (1,2384) | 1:57:A:VAL:HG13  | 1:53:A:PHE:HD1  | 17                  | 0.71     | 0.04                | 0.72       |
| (1,2384) | 1:57:A:VAL:HG12  | 1:53:A:PHE:HD1  | 17                  | 0.71     | 0.04                | 0.72       |
| (1,2384) | 1:57:A:VAL:HG13  | 1:53:A:PHE:HD2  | 17                  | 0.71     | 0.04                | 0.72       |
| (3,51)   | 1:95:A:VAL:HG22  | 1:35:A:PHE:HB2  | 17                  | 0.7      | 0.2                 | 0.7        |
| (3,51)   | 1:95:A:VAL:HG23  | 1:49:A:LYS:HA   | 17                  | 0.7      | 0.2                 | 0.7        |
| (3,51)   | 1:95:A:VAL:HG21  | 1:35:A:PHE:HB2  | 17                  | 0.7      | 0.2                 | 0.7        |
| (3,51)   | 1:95:A:VAL:HG21  | 1:49:A:LYS:HA   | 17                  | 0.7      | 0.2                 | 0.7        |
| (3,51)   | 1:95:A:VAL:HG22  | 1:49:A:LYS:HA   | 17                  | 0.7      | 0.2                 | 0.7        |
| (3,51)   | 1:95:A:VAL:HG23  | 1:35:A:PHE:HB2  | 17                  | 0.7      | 0.2                 | 0.7        |
| (3,86)   | 1:84:A:TYR:HE2   | 1:47:A:PRO:HB3  | 17                  | 0.7      | 0.19                | 0.76       |
| (3,86)   | 1:84:A:TYR:HE1   | 1:47:A:PRO:HB3  | 17                  | 0.7      | 0.19                | 0.76       |
| (1,1137) | 1:97:A:LEU:HD13  | 1:35:A:PHE:HD2  | 17                  | 0.69     | 0.11                | 0.7        |
| (1,1137) | 1:97:A:LEU:HD12  | 1:35:A:PHE:HD1  | 17                  | 0.69     | 0.11                | 0.7        |
| (1,1137) | 1:97:A:LEU:HD11  | 1:35:A:PHE:HD1  | 17                  | 0.69     | 0.11                | 0.7        |
| (1,1137) | 1:97:A:LEU:HD12  | 1:35:A:PHE:HD2  | 17                  | 0.69     | 0.11                | 0.7        |
| (1,1137) | 1:97:A:LEU:HD11  | 1:35:A:PHE:HD2  | 17                  | 0.69     | 0.11                | 0.7        |
| (1,1137) | 1:97:A:LEU:HD13  | 1:35:A:PHE:HD1  | 17                  | 0.69     | 0.11                | 0.7        |
| (1,2026) | 1:57:A:VAL:HG11  | 1:53:A:PHE:HD2  | 17                  | 0.68     | 0.04                | 0.69       |
| (1,2026) | 1:57:A:VAL:HG11  | 1:53:A:PHE:HD1  | 17                  | 0.68     | 0.04                | 0.69       |
| (1,2026) | 1:57:A:VAL:HG12  | 1:53:A:PHE:HD2  | 17                  | 0.68     | 0.04                | 0.69       |
| (1,2026) | 1:57:A:VAL:HG13  | 1:53:A:PHE:HD1  | 17                  | 0.68     | 0.04                | 0.69       |
| (1,2026) | 1:57:A:VAL:HG12  | 1:53:A:PHE:HD1  | 17                  | 0.68     | 0.04                | 0.69       |
| (1,2026) | 1:57:A:VAL:HG13  | 1:53:A:PHE:HD2  | 17                  | 0.68     | 0.04                | 0.69       |
| (1,3397) | 1:75:A:LEU:HA    | 1:31:A:LEU:HD11 | 17                  | 0.68     | 0.05                | 0.68       |
| (1,3397) | 1:75:A:LEU:HA    | 1:31:A:LEU:HD13 | 17                  | 0.68     | 0.05                | 0.68       |
| (1,3397) | 1:75:A:LEU:HA    | 1:31:A:LEU:HD12 | 17                  | 0.68     | 0.05                | 0.68       |
| (1,4168) | 1:48:A:LEU:H     | 1:48:A:LEU:HD11 | 17                  | 0.68     | 0.07                | 0.69       |
| (1,4168) | 1:48:A:LEU:H     | 1:48:A:LEU:HD12 | 17                  | 0.68     | 0.07                | 0.69       |
| (1,4168) | 1:48:A:LEU:H     | 1:48:A:LEU:HD13 | 17                  | 0.68     | 0.07                | 0.69       |
| (3,55)   | 1:97:A:LEU:HD22  | 1:75:A:LEU:HD12 | 17                  | 0.68     | 0.05                | 0.69       |
| (3,55)   | 1:57:A:VAL:HG11  | 1:75:A:LEU:HD13 | 17                  | 0.68     | 0.05                | 0.69       |
| (3,55)   | 1:97:A:LEU:HD23  | 1:75:A:LEU:HD12 | 17                  | 0.68     | 0.05                | 0.69       |
| (3,55)   | 1:97:A:LEU:HD21  | 1:75:A:LEU:HD13 | 17                  | 0.68     | 0.05                | 0.69       |
| (3,55)   | 1:97:A:LEU:HD23  | 1:75:A:LEU:HD11 | 17                  | 0.68     | 0.05                | 0.69       |
| (3,55)   | 1:97:A:LEU:HD21  | 1:75:A:LEU:HD12 | 17                  | 0.68     | 0.05                | 0.69       |

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| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (3,55)   | 1:97:A:LEU:HD21  | 1:75:A:LEU:HD11 | 17                  | 0.68     | 0.05                | 0.69       |
| (3,55)   | 1:97:A:LEU:HD23  | 1:75:A:LEU:HD13 | 17                  | 0.68     | 0.05                | 0.69       |
| (3,55)   | 1:97:A:LEU:HD22  | 1:75:A:LEU:HD13 | 17                  | 0.68     | 0.05                | 0.69       |
| (3,55)   | 1:57:A:VAL:HG11  | 1:75:A:LEU:HD11 | 17                  | 0.68     | 0.05                | 0.69       |
| (1,2206) | 1:57:A:VAL:HG21  | 1:57:A:VAL:HA   | 17                  | 0.68     | 0.02                | 0.67       |
| (1,2206) | 1:57:A:VAL:HG23  | 1:57:A:VAL:HA   | 17                  | 0.68     | 0.02                | 0.67       |
| (1,2206) | 1:57:A:VAL:HG22  | 1:57:A:VAL:HA   | 17                  | 0.68     | 0.02                | 0.67       |
| (1,2902) | 1:50:A:ILE:HD12  | 1:76:A:ARG:H    | 17                  | 0.68     | 0.11                | 0.71       |
| (1,2902) | 1:50:A:ILE:HD13  | 1:76:A:ARG:H    | 17                  | 0.68     | 0.11                | 0.71       |
| (1,2902) | 1:50:A:ILE:HD11  | 1:76:A:ARG:H    | 17                  | 0.68     | 0.11                | 0.71       |
| (3,113)  | 1:61:A:ALA:HB1   | 1:60:A:VAL:HB   | 17                  | 0.67     | 0.04                | 0.68       |
| (3,113)  | 1:61:A:ALA:HB2   | 1:60:A:VAL:HB   | 17                  | 0.67     | 0.04                | 0.68       |
| (3,113)  | 1:61:A:ALA:HB3   | 1:60:A:VAL:HB   | 17                  | 0.67     | 0.04                | 0.68       |
| (3,21)   | 1:31:A:LEU:H     | 1:21:A:LEU:HD12 | 17                  | 0.67     | 0.08                | 0.69       |
| (3,21)   | 1:31:A:LEU:H     | 1:21:A:LEU:HD13 | 17                  | 0.67     | 0.08                | 0.69       |
| (3,21)   | 1:22:A:ASN:H     | 1:21:A:LEU:HD13 | 17                  | 0.67     | 0.08                | 0.69       |
| (3,21)   | 1:22:A:ASN:H     | 1:21:A:LEU:HD12 | 17                  | 0.67     | 0.08                | 0.69       |
| (3,21)   | 1:22:A:ASN:H     | 1:21:A:LEU:HD11 | 17                  | 0.67     | 0.08                | 0.69       |
| (3,21)   | 1:31:A:LEU:H     | 1:21:A:LEU:HD11 | 17                  | 0.67     | 0.08                | 0.69       |
| (1,3826) | 1:102:A:CYS:H    | 1:95:A:VAL:HG12 | 17                  | 0.66     | 0.08                | 0.66       |
| (1,3826) | 1:102:A:CYS:H    | 1:95:A:VAL:HG11 | 17                  | 0.66     | 0.08                | 0.66       |
| (1,3826) | 1:102:A:CYS:H    | 1:95:A:VAL:HG13 | 17                  | 0.66     | 0.08                | 0.66       |
| (3,150)  | 1:77:A:LEU:H     | 1:79:A:THR:HG21 | 17                  | 0.66     | 0.13                | 0.66       |
| (3,150)  | 1:77:A:LEU:H     | 1:79:A:THR:HG22 | 17                  | 0.66     | 0.13                | 0.66       |
| (3,150)  | 1:77:A:LEU:HD23  | 1:77:A:LEU:H    | 17                  | 0.66     | 0.13                | 0.66       |
| (3,150)  | 1:77:A:LEU:H     | 1:79:A:THR:HG23 | 17                  | 0.66     | 0.13                | 0.66       |
| (3,150)  | 1:77:A:LEU:HD21  | 1:77:A:LEU:H    | 17                  | 0.66     | 0.13                | 0.66       |
| (3,150)  | 1:77:A:LEU:HD22  | 1:77:A:LEU:H    | 17                  | 0.66     | 0.13                | 0.66       |
| (1,2398) | 1:50:A:ILE:HD11  | 1:50:A:ILE:H    | 17                  | 0.66     | 0.12                | 0.6        |
| (1,2398) | 1:50:A:ILE:HD12  | 1:50:A:ILE:H    | 17                  | 0.66     | 0.12                | 0.6        |
| (1,2398) | 1:50:A:ILE:HD13  | 1:50:A:ILE:H    | 17                  | 0.66     | 0.12                | 0.6        |
| (1,2334) | 1:60:A:VAL:HG12  | 1:63:A:GLU:HG3  | 17                  | 0.66     | 0.2                 | 0.72       |
| (1,2334) | 1:60:A:VAL:HG13  | 1:63:A:GLU:HG3  | 17                  | 0.66     | 0.2                 | 0.72       |
| (1,2334) | 1:60:A:VAL:HG11  | 1:63:A:GLU:HG3  | 17                  | 0.66     | 0.2                 | 0.72       |
| (1,2610) | 1:105:A:LEU:HD12 | 1:105:A:LEU:HA  | 17                  | 0.66     | 0.02                | 0.66       |
| (1,2610) | 1:105:A:LEU:HD13 | 1:105:A:LEU:HA  | 17                  | 0.66     | 0.02                | 0.66       |
| (1,2610) | 1:105:A:LEU:HD11 | 1:105:A:LEU:HA  | 17                  | 0.66     | 0.02                | 0.66       |
| (1,2363) | 1:48:A:LEU:HD11  | 1:84:A:TYR:HE2  | 17                  | 0.66     | 0.16                | 0.72       |
| (1,2363) | 1:48:A:LEU:HD13  | 1:84:A:TYR:HE2  | 17                  | 0.66     | 0.16                | 0.72       |
| (1,2363) | 1:48:A:LEU:HD11  | 1:84:A:TYR:HE1  | 17                  | 0.66     | 0.16                | 0.72       |
| (1,2363) | 1:48:A:LEU:HD13  | 1:84:A:TYR:HE1  | 17                  | 0.66     | 0.16                | 0.72       |
| (3,11)   | 1:93:A:THR:HB    | 1:104:A:GLU:HG2 | 17                  | 0.65     | 0.04                | 0.65       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2894) | 1:52:A:ILE:HD13  | 1:53:A:PHE:HB2   | 17                  | 0.65     | 0.11                | 0.67       |
| (1,2894) | 1:52:A:ILE:HD11  | 1:53:A:PHE:HB2   | 17                  | 0.65     | 0.11                | 0.67       |
| (1,2894) | 1:52:A:ILE:HD12  | 1:53:A:PHE:HB2   | 17                  | 0.65     | 0.11                | 0.67       |
| (1,2673) | 1:97:A:LEU:HD13  | 1:35:A:PHE:HD2   | 17                  | 0.65     | 0.11                | 0.65       |
| (1,2673) | 1:97:A:LEU:HD12  | 1:35:A:PHE:HD1   | 17                  | 0.65     | 0.11                | 0.65       |
| (1,2673) | 1:97:A:LEU:HD11  | 1:35:A:PHE:HD1   | 17                  | 0.65     | 0.11                | 0.65       |
| (1,2673) | 1:97:A:LEU:HD12  | 1:35:A:PHE:HD2   | 17                  | 0.65     | 0.11                | 0.65       |
| (1,2673) | 1:97:A:LEU:HD11  | 1:35:A:PHE:HD2   | 17                  | 0.65     | 0.11                | 0.65       |
| (1,2673) | 1:97:A:LEU:HD13  | 1:35:A:PHE:HD1   | 17                  | 0.65     | 0.11                | 0.65       |
| (1,1125) | 1:97:A:LEU:HD13  | 1:60:A:VAL:HG12  | 17                  | 0.64     | 0.11                | 0.65       |
| (1,1125) | 1:97:A:LEU:HD12  | 1:60:A:VAL:HG13  | 17                  | 0.64     | 0.11                | 0.65       |
| (1,1125) | 1:97:A:LEU:HD13  | 1:60:A:VAL:HG11  | 17                  | 0.64     | 0.11                | 0.65       |
| (1,1125) | 1:97:A:LEU:HD13  | 1:60:A:VAL:HG13  | 17                  | 0.64     | 0.11                | 0.65       |
| (1,1125) | 1:97:A:LEU:HD11  | 1:60:A:VAL:HG13  | 17                  | 0.64     | 0.11                | 0.65       |
| (1,1125) | 1:97:A:LEU:HD12  | 1:60:A:VAL:HG11  | 17                  | 0.64     | 0.11                | 0.65       |
| (1,1125) | 1:97:A:LEU:HD11  | 1:60:A:VAL:HG12  | 17                  | 0.64     | 0.11                | 0.65       |
| (1,1125) | 1:97:A:LEU:HD11  | 1:60:A:VAL:HG11  | 17                  | 0.64     | 0.11                | 0.65       |
| (1,3377) | 1:40:A:SER:HB2   | 1:41:A:ALA:HB2   | 17                  | 0.64     | 0.11                | 0.68       |
| (1,3377) | 1:40:A:SER:HB2   | 1:41:A:ALA:HB3   | 17                  | 0.64     | 0.11                | 0.68       |
| (1,3377) | 1:40:A:SER:HB2   | 1:41:A:ALA:HB1   | 17                  | 0.64     | 0.11                | 0.68       |
| (1,2324) | 1:97:A:LEU:HD23  | 1:39:A:PHE:H     | 17                  | 0.64     | 0.04                | 0.65       |
| (1,2324) | 1:97:A:LEU:HD21  | 1:39:A:PHE:H     | 17                  | 0.64     | 0.04                | 0.65       |
| (1,2324) | 1:97:A:LEU:HD22  | 1:39:A:PHE:H     | 17                  | 0.64     | 0.04                | 0.65       |
| (3,117)  | 1:48:A:LEU:HD22  | 1:39:A:PHE:HD1   | 17                  | 0.64     | 0.34                | 0.64       |
| (3,117)  | 1:48:A:LEU:HD21  | 1:39:A:PHE:HD1   | 17                  | 0.64     | 0.34                | 0.64       |
| (3,117)  | 1:48:A:LEU:HD23  | 1:39:A:PHE:HD1   | 17                  | 0.64     | 0.34                | 0.64       |
| (3,117)  | 1:48:A:LEU:HD21  | 1:39:A:PHE:HD2   | 17                  | 0.64     | 0.34                | 0.64       |
| (3,117)  | 1:48:A:LEU:HD23  | 1:39:A:PHE:HD2   | 17                  | 0.64     | 0.34                | 0.64       |
| (3,117)  | 1:48:A:LEU:HD22  | 1:39:A:PHE:HD2   | 17                  | 0.64     | 0.34                | 0.64       |
| (3,8)    | 1:57:A:VAL:HB    | 1:54:A:GLN:HA    | 17                  | 0.63     | 0.02                | 0.62       |
| (3,153)  | 1:110:A:VAL:HG23 | 1:114:A:ARG:H    | 17                  | 0.63     | 0.04                | 0.64       |
| (3,153)  | 1:110:A:VAL:HG21 | 1:114:A:ARG:H    | 17                  | 0.63     | 0.04                | 0.64       |
| (3,153)  | 1:110:A:VAL:HG22 | 1:114:A:ARG:H    | 17                  | 0.63     | 0.04                | 0.64       |
| (1,3376) | 1:41:A:ALA:HB1   | 1:40:A:SER:HB3   | 17                  | 0.63     | 0.08                | 0.62       |
| (1,3376) | 1:41:A:ALA:HB2   | 1:40:A:SER:HB3   | 17                  | 0.63     | 0.08                | 0.62       |
| (1,3376) | 1:41:A:ALA:HB3   | 1:40:A:SER:HB3   | 17                  | 0.63     | 0.08                | 0.62       |
| (1,2600) | 1:105:A:LEU:HA   | 1:105:A:LEU:HD21 | 17                  | 0.63     | 0.03                | 0.63       |
| (1,2600) | 1:105:A:LEU:HA   | 1:105:A:LEU:HD23 | 17                  | 0.63     | 0.03                | 0.63       |
| (1,2600) | 1:105:A:LEU:HA   | 1:105:A:LEU:HD22 | 17                  | 0.63     | 0.03                | 0.63       |
| (3,65)   | 1:49:A:LYS:HB2   | 1:52:A:ILE:HG21  | 17                  | 0.62     | 0.11                | 0.6        |
| (3,65)   | 1:52:A:ILE:HG13  | 1:52:A:ILE:HG23  | 17                  | 0.62     | 0.11                | 0.6        |
| (3,65)   | 1:49:A:LYS:HB2   | 1:52:A:ILE:HG22  | 17                  | 0.62     | 0.11                | 0.6        |

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| Key      | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (3,65)   | 1:52:A:ILE:HG13 | 1:52:A:ILE:HG22  | 17                  | 0.62     | 0.11                | 0.6        |
| (3,65)   | 1:49:A:LYS:HB2  | 1:52:A:ILE:HG23  | 17                  | 0.62     | 0.11                | 0.6        |
| (3,65)   | 1:52:A:ILE:HG13 | 1:52:A:ILE:HG21  | 17                  | 0.62     | 0.11                | 0.6        |
| (1,3281) | 1:93:A:THR:HG22 | 1:104:A:GLU:HG2  | 17                  | 0.62     | 0.04                | 0.62       |
| (1,3281) | 1:93:A:THR:HG23 | 1:104:A:GLU:HG2  | 17                  | 0.62     | 0.04                | 0.62       |
| (1,3281) | 1:93:A:THR:HG21 | 1:104:A:GLU:HG2  | 17                  | 0.62     | 0.04                | 0.62       |
| (1,2400) | 1:28:A:ILE:HB   | 1:28:A:ILE:HD12  | 17                  | 0.62     | 0.02                | 0.62       |
| (1,2400) | 1:28:A:ILE:HB   | 1:28:A:ILE:HD13  | 17                  | 0.62     | 0.02                | 0.62       |
| (1,2400) | 1:28:A:ILE:HB   | 1:28:A:ILE:HD11  | 17                  | 0.62     | 0.02                | 0.62       |
| (1,1990) | 1:92:A:ALA:HB3  | 1:91:A:GLY:H     | 17                  | 0.62     | 0.08                | 0.64       |
| (1,1990) | 1:92:A:ALA:HB2  | 1:91:A:GLY:H     | 17                  | 0.62     | 0.08                | 0.64       |
| (1,1990) | 1:92:A:ALA:HB1  | 1:91:A:GLY:H     | 17                  | 0.62     | 0.08                | 0.64       |
| (1,2582) | 1:60:A:VAL:HG11 | 1:57:A:VAL:HG12  | 17                  | 0.62     | 0.04                | 0.61       |
| (1,2582) | 1:60:A:VAL:HG12 | 1:57:A:VAL:HG12  | 17                  | 0.62     | 0.04                | 0.61       |
| (1,2582) | 1:60:A:VAL:HG13 | 1:57:A:VAL:HG12  | 17                  | 0.62     | 0.04                | 0.61       |
| (1,2582) | 1:60:A:VAL:HG12 | 1:57:A:VAL:HG13  | 17                  | 0.62     | 0.04                | 0.61       |
| (1,2582) | 1:60:A:VAL:HG11 | 1:57:A:VAL:HG11  | 17                  | 0.62     | 0.04                | 0.61       |
| (1,2582) | 1:60:A:VAL:HG13 | 1:57:A:VAL:HG13  | 17                  | 0.62     | 0.04                | 0.61       |
| (1,2582) | 1:60:A:VAL:HG11 | 1:57:A:VAL:HG13  | 17                  | 0.62     | 0.04                | 0.61       |
| (1,2582) | 1:60:A:VAL:HG12 | 1:57:A:VAL:HG11  | 17                  | 0.62     | 0.04                | 0.61       |
| (1,2582) | 1:60:A:VAL:HG13 | 1:57:A:VAL:HG11  | 17                  | 0.62     | 0.04                | 0.61       |
| (1,3362) | 1:56:A:LEU:HD22 | 1:56:A:LEU:HA    | 17                  | 0.62     | 0.02                | 0.62       |
| (1,3362) | 1:56:A:LEU:HD21 | 1:56:A:LEU:HA    | 17                  | 0.62     | 0.02                | 0.62       |
| (1,3362) | 1:56:A:LEU:HD23 | 1:56:A:LEU:HA    | 17                  | 0.62     | 0.02                | 0.62       |
| (3,112)  | 1:82:A:TRP:HA   | 1:117:A:LEU:HD13 | 17                  | 0.62     | 0.25                | 0.82       |
| (3,112)  | 1:82:A:TRP:HA   | 1:117:A:LEU:HD11 | 17                  | 0.62     | 0.25                | 0.82       |
| (3,112)  | 1:82:A:TRP:HA   | 1:117:A:LEU:HD12 | 17                  | 0.62     | 0.25                | 0.82       |
| (1,3870) | 1:85:A:LEU:HD22 | 1:87:A:GLY:H     | 17                  | 0.62     | 0.06                | 0.61       |
| (1,3870) | 1:85:A:LEU:HD21 | 1:87:A:GLY:H     | 17                  | 0.62     | 0.06                | 0.61       |
| (1,3870) | 1:85:A:LEU:HD23 | 1:87:A:GLY:H     | 17                  | 0.62     | 0.06                | 0.61       |
| (1,222)  | 1:102:A:CYS:H   | 1:95:A:VAL:HG12  | 17                  | 0.61     | 0.08                | 0.62       |
| (1,222)  | 1:102:A:CYS:H   | 1:95:A:VAL:HG11  | 17                  | 0.61     | 0.08                | 0.62       |
| (1,222)  | 1:102:A:CYS:H   | 1:95:A:VAL:HG13  | 17                  | 0.61     | 0.08                | 0.62       |
| (3,40)   | 1:55:A:ASP:H    | 1:52:A:ILE:HD12  | 17                  | 0.61     | 0.05                | 0.62       |
| (3,40)   | 1:55:A:ASP:H    | 1:52:A:ILE:HD13  | 17                  | 0.61     | 0.05                | 0.62       |
| (3,40)   | 1:55:A:ASP:H    | 1:52:A:ILE:HD11  | 17                  | 0.61     | 0.05                | 0.62       |
| (1,1420) | 1:97:A:LEU:HD22 | 1:56:A:LEU:HD23  | 17                  | 0.61     | 0.04                | 0.62       |
| (1,1420) | 1:97:A:LEU:HD23 | 1:56:A:LEU:HD23  | 17                  | 0.61     | 0.04                | 0.62       |
| (1,1420) | 1:97:A:LEU:HD23 | 1:56:A:LEU:HD22  | 17                  | 0.61     | 0.04                | 0.62       |
| (1,1420) | 1:97:A:LEU:HD21 | 1:56:A:LEU:HD21  | 17                  | 0.61     | 0.04                | 0.62       |
| (1,1420) | 1:97:A:LEU:HD21 | 1:56:A:LEU:HD23  | 17                  | 0.61     | 0.04                | 0.62       |
| (1,1420) | 1:97:A:LEU:HD23 | 1:56:A:LEU:HD21  | 17                  | 0.61     | 0.04                | 0.62       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1420) | 1:97:A:LEU:HD22  | 1:56:A:LEU:HD22  | 17                  | 0.61     | 0.04                | 0.62       |
| (1,1361) | 1:41:A:ALA:HA    | 1:32:A:ALA:HB3   | 17                  | 0.6      | 0.07                | 0.64       |
| (1,1361) | 1:41:A:ALA:HA    | 1:32:A:ALA:HB1   | 17                  | 0.6      | 0.07                | 0.64       |
| (1,1361) | 1:41:A:ALA:HA    | 1:32:A:ALA:HB2   | 17                  | 0.6      | 0.07                | 0.64       |
| (1,3947) | 1:71:A:LEU:HD11  | 1:61:A:ALA:H     | 17                  | 0.6      | 0.02                | 0.61       |
| (1,3947) | 1:71:A:LEU:HD13  | 1:61:A:ALA:H     | 17                  | 0.6      | 0.02                | 0.61       |
| (1,3947) | 1:71:A:LEU:HD12  | 1:61:A:ALA:H     | 17                  | 0.6      | 0.02                | 0.61       |
| (1,1502) | 1:52:A:ILE:HG13  | 1:54:A:GLN:HE21  | 17                  | 0.6      | 0.13                | 0.64       |
| (1,2664) | 1:97:A:LEU:HD13  | 1:60:A:VAL:HG12  | 17                  | 0.6      | 0.11                | 0.6        |
| (1,2664) | 1:97:A:LEU:HD12  | 1:60:A:VAL:HG13  | 17                  | 0.6      | 0.11                | 0.6        |
| (1,2664) | 1:97:A:LEU:HD13  | 1:60:A:VAL:HG11  | 17                  | 0.6      | 0.11                | 0.6        |
| (1,2664) | 1:97:A:LEU:HD13  | 1:60:A:VAL:HG13  | 17                  | 0.6      | 0.11                | 0.6        |
| (1,2664) | 1:97:A:LEU:HD11  | 1:60:A:VAL:HG13  | 17                  | 0.6      | 0.11                | 0.6        |
| (1,2664) | 1:97:A:LEU:HD12  | 1:60:A:VAL:HG11  | 17                  | 0.6      | 0.11                | 0.6        |
| (1,2664) | 1:97:A:LEU:HD11  | 1:60:A:VAL:HG12  | 17                  | 0.6      | 0.11                | 0.6        |
| (1,2664) | 1:97:A:LEU:HD11  | 1:60:A:VAL:HG11  | 17                  | 0.6      | 0.11                | 0.6        |
| (1,1998) | 1:116:A:GLN:HG3  | 1:116:A:GLN:HE21 | 17                  | 0.6      | 0.01                | 0.59       |
| (1,3799) | 1:105:A:LEU:HD13 | 1:111:A:GLU:H    | 17                  | 0.6      | 0.02                | 0.6        |
| (1,3799) | 1:105:A:LEU:HD11 | 1:111:A:GLU:H    | 17                  | 0.6      | 0.02                | 0.6        |
| (1,3799) | 1:105:A:LEU:HD12 | 1:111:A:GLU:H    | 17                  | 0.6      | 0.02                | 0.6        |
| (3,78)   | 1:77:A:LEU:HD22  | 1:77:A:LEU:H     | 17                  | 0.6      | 0.02                | 0.59       |
| (3,78)   | 1:77:A:LEU:HD23  | 1:77:A:LEU:H     | 17                  | 0.6      | 0.02                | 0.59       |
| (3,78)   | 1:77:A:LEU:HD21  | 1:77:A:LEU:H     | 17                  | 0.6      | 0.02                | 0.59       |
| (1,1601) | 1:75:A:LEU:HD21  | 1:31:A:LEU:HD13  | 17                  | 0.6      | 0.03                | 0.6        |
| (1,1601) | 1:75:A:LEU:HD23  | 1:31:A:LEU:HD13  | 17                  | 0.6      | 0.03                | 0.6        |
| (1,1601) | 1:75:A:LEU:HD21  | 1:31:A:LEU:HD12  | 17                  | 0.6      | 0.03                | 0.6        |
| (1,1601) | 1:75:A:LEU:HD23  | 1:31:A:LEU:HD12  | 17                  | 0.6      | 0.03                | 0.6        |
| (1,1601) | 1:75:A:LEU:HD22  | 1:31:A:LEU:HD11  | 17                  | 0.6      | 0.03                | 0.6        |
| (1,1601) | 1:75:A:LEU:HD22  | 1:31:A:LEU:HD13  | 17                  | 0.6      | 0.03                | 0.6        |
| (1,1601) | 1:75:A:LEU:HD22  | 1:31:A:LEU:HD12  | 17                  | 0.6      | 0.03                | 0.6        |
| (1,1601) | 1:75:A:LEU:HD23  | 1:31:A:LEU:HD11  | 17                  | 0.6      | 0.03                | 0.6        |
| (1,3484) | 1:32:A:ALA:H     | 1:31:A:LEU:HD11  | 17                  | 0.59     | 0.02                | 0.6        |
| (1,3484) | 1:32:A:ALA:H     | 1:31:A:LEU:HD13  | 17                  | 0.59     | 0.02                | 0.6        |
| (1,3484) | 1:32:A:ALA:H     | 1:31:A:LEU:HD12  | 17                  | 0.59     | 0.02                | 0.6        |
| (1,815)  | 1:50:A:ILE:HD13  | 1:50:A:ILE:HA    | 17                  | 0.59     | 0.16                | 0.65       |
| (1,815)  | 1:50:A:ILE:HD12  | 1:50:A:ILE:HA    | 17                  | 0.59     | 0.16                | 0.65       |
| (1,815)  | 1:50:A:ILE:HD11  | 1:50:A:ILE:HA    | 17                  | 0.59     | 0.16                | 0.65       |
| (1,3412) | 1:82:A:TRP:HZ3   | 1:117:A:LEU:HD12 | 17                  | 0.59     | 0.4                 | 0.26       |
| (1,3412) | 1:82:A:TRP:HZ3   | 1:117:A:LEU:HD11 | 17                  | 0.59     | 0.4                 | 0.26       |
| (1,3412) | 1:82:A:TRP:HZ3   | 1:117:A:LEU:HD13 | 17                  | 0.59     | 0.4                 | 0.26       |
| (3,98)   | 1:64:A:MET:HE1   | 1:63:A:GLU:HG3   | 17                  | 0.59     | 0.17                | 0.6        |
| (3,98)   | 1:64:A:MET:HE3   | 1:63:A:GLU:HG3   | 17                  | 0.59     | 0.17                | 0.6        |

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| Key      | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (3,98)   | 1:64:A:MET:HE2  | 1:63:A:GLU:HG3   | 17                  | 0.59     | 0.17                | 0.6        |
| (1,1360) | 1:32:A:ALA:HB3  | 1:31:A:LEU:H     | 17                  | 0.58     | 0.04                | 0.58       |
| (1,1360) | 1:32:A:ALA:HB1  | 1:31:A:LEU:H     | 17                  | 0.58     | 0.04                | 0.58       |
| (1,1360) | 1:32:A:ALA:HB2  | 1:31:A:LEU:H     | 17                  | 0.58     | 0.04                | 0.58       |
| (1,1369) | 1:39:A:PHE:HZ   | 1:28:A:ILE:HD13  | 17                  | 0.58     | 0.03                | 0.58       |
| (1,1369) | 1:39:A:PHE:HZ   | 1:28:A:ILE:HD11  | 17                  | 0.58     | 0.03                | 0.58       |
| (1,1369) | 1:39:A:PHE:HZ   | 1:28:A:ILE:HD12  | 17                  | 0.58     | 0.03                | 0.58       |
| (1,1482) | 1:64:A:MET:HE2  | 1:27:A:VAL:HA    | 17                  | 0.58     | 0.15                | 0.6        |
| (1,1482) | 1:64:A:MET:HE1  | 1:27:A:VAL:HA    | 17                  | 0.58     | 0.15                | 0.6        |
| (1,1482) | 1:64:A:MET:HE3  | 1:27:A:VAL:HA    | 17                  | 0.58     | 0.15                | 0.6        |
| (1,2864) | 1:78:A:TYR:HE2  | 1:78:A:TYR:HB3   | 17                  | 0.58     | 0.07                | 0.59       |
| (1,2864) | 1:78:A:TYR:HE1  | 1:78:A:TYR:HB3   | 17                  | 0.58     | 0.07                | 0.59       |
| (1,2669) | 1:75:A:LEU:HD21 | 1:78:A:TYR:HE2   | 17                  | 0.57     | 0.05                | 0.58       |
| (1,2669) | 1:75:A:LEU:HD21 | 1:78:A:TYR:HE1   | 17                  | 0.57     | 0.05                | 0.58       |
| (1,2669) | 1:75:A:LEU:HD22 | 1:78:A:TYR:HE2   | 17                  | 0.57     | 0.05                | 0.58       |
| (1,2669) | 1:75:A:LEU:HD22 | 1:78:A:TYR:HE1   | 17                  | 0.57     | 0.05                | 0.58       |
| (1,2669) | 1:75:A:LEU:HD23 | 1:78:A:TYR:HE1   | 17                  | 0.57     | 0.05                | 0.58       |
| (1,2669) | 1:75:A:LEU:HD23 | 1:78:A:TYR:HE2   | 17                  | 0.57     | 0.05                | 0.58       |
| (1,4082) | 1:22:A:ASN:HD21 | 1:22:A:ASN:HB3   | 17                  | 0.57     | 0.09                | 0.58       |
| (1,1069) | 1:48:A:LEU:HD13 | 1:52:A:ILE:HG12  | 17                  | 0.57     | 0.09                | 0.56       |
| (1,1069) | 1:48:A:LEU:HD12 | 1:52:A:ILE:HG12  | 17                  | 0.57     | 0.09                | 0.56       |
| (1,2954) | 1:71:A:LEU:HB2  | 1:75:A:LEU:HD11  | 17                  | 0.57     | 0.04                | 0.58       |
| (1,2954) | 1:71:A:LEU:HB2  | 1:75:A:LEU:HD12  | 17                  | 0.57     | 0.04                | 0.58       |
| (1,2954) | 1:71:A:LEU:HB2  | 1:75:A:LEU:HD13  | 17                  | 0.57     | 0.04                | 0.58       |
| (1,275)  | 1:85:A:LEU:HD22 | 1:87:A:GLY:H     | 17                  | 0.57     | 0.05                | 0.57       |
| (1,275)  | 1:85:A:LEU:HD21 | 1:87:A:GLY:H     | 17                  | 0.57     | 0.05                | 0.57       |
| (1,275)  | 1:85:A:LEU:HD23 | 1:87:A:GLY:H     | 17                  | 0.57     | 0.05                | 0.57       |
| (1,2962) | 1:97:A:LEU:HD22 | 1:56:A:LEU:HD23  | 17                  | 0.57     | 0.04                | 0.58       |
| (1,2962) | 1:97:A:LEU:HD23 | 1:56:A:LEU:HD23  | 17                  | 0.57     | 0.04                | 0.58       |
| (1,2962) | 1:97:A:LEU:HD23 | 1:56:A:LEU:HD22  | 17                  | 0.57     | 0.04                | 0.58       |
| (1,2962) | 1:97:A:LEU:HD21 | 1:56:A:LEU:HD21  | 17                  | 0.57     | 0.04                | 0.58       |
| (1,2962) | 1:97:A:LEU:HD21 | 1:56:A:LEU:HD23  | 17                  | 0.57     | 0.04                | 0.58       |
| (1,2962) | 1:97:A:LEU:HD23 | 1:56:A:LEU:HD21  | 17                  | 0.57     | 0.04                | 0.58       |
| (1,2962) | 1:97:A:LEU:HD22 | 1:56:A:LEU:HD22  | 17                  | 0.57     | 0.04                | 0.58       |
| (1,2572) | 1:125:A:GLN:H   | 1:124:A:VAL:HG21 | 17                  | 0.57     | 0.03                | 0.57       |
| (1,2572) | 1:125:A:GLN:H   | 1:124:A:VAL:HG22 | 17                  | 0.57     | 0.03                | 0.57       |
| (1,2572) | 1:125:A:GLN:H   | 1:124:A:VAL:HG23 | 17                  | 0.57     | 0.03                | 0.57       |
| (3,136)  | 1:82:A:TRP:HD1  | 1:82:A:TRP:H     | 17                  | 0.57     | 0.05                | 0.56       |
| (3,136)  | 1:81:A:SER:H    | 1:82:A:TRP:H     | 17                  | 0.57     | 0.05                | 0.56       |
| (1,4028) | 1:31:A:LEU:HD23 | 1:32:A:ALA:H     | 17                  | 0.56     | 0.02                | 0.57       |
| (1,4028) | 1:31:A:LEU:HD22 | 1:32:A:ALA:H     | 17                  | 0.56     | 0.02                | 0.57       |
| (1,4028) | 1:31:A:LEU:HD21 | 1:32:A:ALA:H     | 17                  | 0.56     | 0.02                | 0.57       |

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| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (3,62)   | 1:52:A:ILE:HG23  | 1:56:A:LEU:H    | 17                  | 0.56     | 0.2                 | 0.63       |
| (3,62)   | 1:52:A:ILE:HG21  | 1:56:A:LEU:H    | 17                  | 0.56     | 0.2                 | 0.63       |
| (3,62)   | 1:52:A:ILE:HG22  | 1:56:A:LEU:H    | 17                  | 0.56     | 0.2                 | 0.63       |
| (1,370)  | 1:71:A:LEU:HD11  | 1:61:A:ALA:H    | 17                  | 0.56     | 0.02                | 0.56       |
| (1,370)  | 1:71:A:LEU:HD13  | 1:61:A:ALA:H    | 17                  | 0.56     | 0.02                | 0.56       |
| (1,370)  | 1:71:A:LEU:HD12  | 1:61:A:ALA:H    | 17                  | 0.56     | 0.02                | 0.56       |
| (3,96)   | 1:110:A:VAL:HG21 | 1:109:A:HIS:HA  | 17                  | 0.56     | 0.02                | 0.56       |
| (3,96)   | 1:110:A:VAL:HG22 | 1:109:A:HIS:HA  | 17                  | 0.56     | 0.02                | 0.56       |
| (3,96)   | 1:110:A:VAL:HG23 | 1:109:A:HIS:HA  | 17                  | 0.56     | 0.02                | 0.56       |
| (1,4247) | 1:54:A:GLN:HE22  | 1:57:A:VAL:HG11 | 17                  | 0.56     | 0.16                | 0.51       |
| (1,4247) | 1:54:A:GLN:HE22  | 1:57:A:VAL:HG12 | 17                  | 0.56     | 0.16                | 0.51       |
| (1,4247) | 1:54:A:GLN:HE22  | 1:57:A:VAL:HG13 | 17                  | 0.56     | 0.16                | 0.51       |
| (3,97)   | 1:31:A:LEU:HD23  | 1:30:A:PHE:HB3  | 17                  | 0.56     | 0.04                | 0.56       |
| (3,97)   | 1:31:A:LEU:HD22  | 1:30:A:PHE:HB3  | 17                  | 0.56     | 0.04                | 0.56       |
| (3,97)   | 1:31:A:LEU:HD21  | 1:30:A:PHE:HB3  | 17                  | 0.56     | 0.04                | 0.56       |
| (1,2886) | 1:41:A:ALA:HA    | 1:32:A:ALA:HB3  | 17                  | 0.56     | 0.08                | 0.59       |
| (1,2886) | 1:41:A:ALA:HA    | 1:32:A:ALA:HB1  | 17                  | 0.56     | 0.08                | 0.59       |
| (1,2886) | 1:41:A:ALA:HA    | 1:32:A:ALA:HB2  | 17                  | 0.56     | 0.08                | 0.59       |
| (1,3810) | 1:105:A:LEU:HD13 | 1:106:A:ASP:H   | 17                  | 0.55     | 0.02                | 0.56       |
| (1,3810) | 1:105:A:LEU:HD11 | 1:106:A:ASP:H   | 17                  | 0.55     | 0.02                | 0.56       |
| (1,3810) | 1:105:A:LEU:HD12 | 1:106:A:ASP:H   | 17                  | 0.55     | 0.02                | 0.56       |
| (1,1839) | 1:95:A:VAL:HA    | 1:93:A:THR:HG21 | 17                  | 0.55     | 0.08                | 0.57       |
| (1,1839) | 1:95:A:VAL:HA    | 1:93:A:THR:HG22 | 17                  | 0.55     | 0.08                | 0.57       |
| (1,1839) | 1:95:A:VAL:HA    | 1:93:A:THR:HG23 | 17                  | 0.55     | 0.08                | 0.57       |
| (1,3171) | 1:75:A:LEU:HD21  | 1:31:A:LEU:HD13 | 17                  | 0.55     | 0.03                | 0.56       |
| (1,3171) | 1:75:A:LEU:HD23  | 1:31:A:LEU:HD13 | 17                  | 0.55     | 0.03                | 0.56       |
| (1,3171) | 1:75:A:LEU:HD21  | 1:31:A:LEU:HD12 | 17                  | 0.55     | 0.03                | 0.56       |
| (1,3171) | 1:75:A:LEU:HD23  | 1:31:A:LEU:HD12 | 17                  | 0.55     | 0.03                | 0.56       |
| (1,3171) | 1:75:A:LEU:HD22  | 1:31:A:LEU:HD11 | 17                  | 0.55     | 0.03                | 0.56       |
| (1,3171) | 1:75:A:LEU:HD22  | 1:31:A:LEU:HD13 | 17                  | 0.55     | 0.03                | 0.56       |
| (1,3171) | 1:75:A:LEU:HD22  | 1:31:A:LEU:HD12 | 17                  | 0.55     | 0.03                | 0.56       |
| (1,3171) | 1:75:A:LEU:HD23  | 1:31:A:LEU:HD11 | 17                  | 0.55     | 0.03                | 0.56       |
| (1,2585) | 1:92:A:ALA:HA    | 1:93:A:THR:HG21 | 17                  | 0.55     | 0.04                | 0.55       |
| (1,2585) | 1:92:A:ALA:HA    | 1:93:A:THR:HG23 | 17                  | 0.55     | 0.04                | 0.55       |
| (1,2585) | 1:92:A:ALA:HA    | 1:93:A:THR:HG22 | 17                  | 0.55     | 0.04                | 0.55       |
| (1,2397) | 1:50:A:ILE:HD13  | 1:50:A:ILE:HA   | 17                  | 0.55     | 0.16                | 0.61       |
| (1,2397) | 1:50:A:ILE:HD12  | 1:50:A:ILE:HA   | 17                  | 0.55     | 0.16                | 0.61       |
| (1,2397) | 1:50:A:ILE:HD11  | 1:50:A:ILE:HA   | 17                  | 0.55     | 0.16                | 0.61       |
| (1,1301) | 1:97:A:LEU:HD11  | 1:97:A:LEU:HA   | 17                  | 0.55     | 0.08                | 0.56       |
| (1,1301) | 1:97:A:LEU:HD13  | 1:97:A:LEU:HA   | 17                  | 0.55     | 0.08                | 0.56       |
| (1,1301) | 1:97:A:LEU:HD12  | 1:97:A:LEU:HA   | 17                  | 0.55     | 0.08                | 0.56       |
| (1,3045) | 1:52:A:ILE:HG13  | 1:54:A:GLN:HE21 | 17                  | 0.54     | 0.13                | 0.58       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1342) | 1:48:A:LEU:HD11 | 1:84:A:TYR:HE2  | 17                  | 0.54     | 0.16                | 0.6        |
| (1,1342) | 1:48:A:LEU:HD13 | 1:84:A:TYR:HE2  | 17                  | 0.54     | 0.16                | 0.6        |
| (1,1342) | 1:48:A:LEU:HD11 | 1:84:A:TYR:HE1  | 17                  | 0.54     | 0.16                | 0.6        |
| (1,1342) | 1:48:A:LEU:HD13 | 1:84:A:TYR:HE1  | 17                  | 0.54     | 0.16                | 0.6        |
| (1,1751) | 1:32:A:ALA:HB1  | 1:41:A:ALA:H    | 17                  | 0.54     | 0.09                | 0.55       |
| (1,1751) | 1:32:A:ALA:HB2  | 1:41:A:ALA:H    | 17                  | 0.54     | 0.09                | 0.55       |
| (1,1751) | 1:32:A:ALA:HB3  | 1:41:A:ALA:H    | 17                  | 0.54     | 0.09                | 0.55       |
| (1,4259) | 1:57:A:VAL:HG11 | 1:56:A:LEU:H    | 17                  | 0.54     | 0.07                | 0.56       |
| (1,4259) | 1:57:A:VAL:HG12 | 1:56:A:LEU:H    | 17                  | 0.54     | 0.07                | 0.56       |
| (1,4259) | 1:57:A:VAL:HG13 | 1:56:A:LEU:H    | 17                  | 0.54     | 0.07                | 0.56       |
| (1,2845) | 1:22:A:ASN:H    | 1:27:A:VAL:HG11 | 17                  | 0.53     | 0.08                | 0.54       |
| (1,2845) | 1:22:A:ASN:H    | 1:27:A:VAL:HG12 | 17                  | 0.53     | 0.08                | 0.54       |
| (1,2845) | 1:22:A:ASN:H    | 1:27:A:VAL:HG13 | 17                  | 0.53     | 0.08                | 0.54       |
| (1,1851) | 1:35:A:PHE:HE2  | 1:38:A:CYS:HB2  | 17                  | 0.53     | 0.07                | 0.52       |
| (1,1851) | 1:35:A:PHE:HE1  | 1:38:A:CYS:HB2  | 17                  | 0.53     | 0.07                | 0.52       |
| (1,2309) | 1:39:A:PHE:HB3  | 1:39:A:PHE:HE2  | 17                  | 0.53     | 0.05                | 0.55       |
| (1,2309) | 1:39:A:PHE:HB3  | 1:39:A:PHE:HE1  | 17                  | 0.53     | 0.05                | 0.55       |
| (1,3957) | 1:58:A:ASP:H    | 1:57:A:VAL:HG12 | 17                  | 0.53     | 0.05                | 0.53       |
| (1,3957) | 1:58:A:ASP:H    | 1:57:A:VAL:HG13 | 17                  | 0.53     | 0.05                | 0.53       |
| (1,3957) | 1:58:A:ASP:H    | 1:57:A:VAL:HG11 | 17                  | 0.53     | 0.05                | 0.53       |
| (1,2885) | 1:32:A:ALA:HB3  | 1:31:A:LEU:H    | 17                  | 0.53     | 0.04                | 0.53       |
| (1,2885) | 1:32:A:ALA:HB1  | 1:31:A:LEU:H    | 17                  | 0.53     | 0.04                | 0.53       |
| (1,2885) | 1:32:A:ALA:HB2  | 1:31:A:LEU:H    | 17                  | 0.53     | 0.04                | 0.53       |
| (1,2248) | 1:57:A:VAL:HG21 | 1:57:A:VAL:HA   | 17                  | 0.53     | 0.02                | 0.52       |
| (1,2248) | 1:57:A:VAL:HG23 | 1:57:A:VAL:HA   | 17                  | 0.53     | 0.02                | 0.52       |
| (1,2248) | 1:57:A:VAL:HG22 | 1:57:A:VAL:HA   | 17                  | 0.53     | 0.02                | 0.52       |
| (1,3782) | 1:120:A:ALA:HB1 | 1:119:A:GLU:H   | 17                  | 0.53     | 0.05                | 0.53       |
| (1,3782) | 1:120:A:ALA:HB2 | 1:119:A:GLU:H   | 17                  | 0.53     | 0.05                | 0.53       |
| (1,3782) | 1:120:A:ALA:HB3 | 1:119:A:GLU:H   | 17                  | 0.53     | 0.05                | 0.53       |
| (1,1343) | 1:78:A:TYR:HE2  | 1:48:A:LEU:HD11 | 17                  | 0.53     | 0.07                | 0.54       |
| (1,1343) | 1:78:A:TYR:HE1  | 1:48:A:LEU:HD13 | 17                  | 0.53     | 0.07                | 0.54       |
| (1,1343) | 1:78:A:TYR:HE1  | 1:48:A:LEU:HD11 | 17                  | 0.53     | 0.07                | 0.54       |
| (1,1343) | 1:78:A:TYR:HE2  | 1:48:A:LEU:HD13 | 17                  | 0.53     | 0.07                | 0.54       |
| (1,1343) | 1:78:A:TYR:HE2  | 1:48:A:LEU:HD12 | 17                  | 0.53     | 0.07                | 0.54       |
| (1,1343) | 1:78:A:TYR:HE1  | 1:48:A:LEU:HD12 | 17                  | 0.53     | 0.07                | 0.54       |
| (1,2608) | 1:48:A:LEU:HD13 | 1:52:A:ILE:HG12 | 17                  | 0.53     | 0.1                 | 0.51       |
| (1,2608) | 1:48:A:LEU:HD12 | 1:52:A:ILE:HG12 | 17                  | 0.53     | 0.1                 | 0.51       |
| (1,1682) | 1:41:A:ALA:HB2  | 1:33:A:GLU:H    | 17                  | 0.53     | 0.06                | 0.54       |
| (1,1682) | 1:41:A:ALA:HB3  | 1:33:A:GLU:H    | 17                  | 0.53     | 0.06                | 0.54       |
| (1,1682) | 1:41:A:ALA:HB1  | 1:33:A:GLU:H    | 17                  | 0.53     | 0.06                | 0.54       |
| (1,3023) | 1:64:A:MET:HE2  | 1:27:A:VAL:HA   | 17                  | 0.52     | 0.15                | 0.55       |
| (1,3023) | 1:64:A:MET:HE1  | 1:27:A:VAL:HA   | 17                  | 0.52     | 0.15                | 0.55       |

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| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,3023) | 1:64:A:MET:HE3   | 1:27:A:VAL:HA   | 17                  | 0.52     | 0.15                | 0.55       |
| (3,105)  | 1:64:A:MET:H     | 1:66:A:LEU:HD22 | 17                  | 0.52     | 0.15                | 0.57       |
| (3,105)  | 1:64:A:MET:H     | 1:66:A:LEU:HD21 | 17                  | 0.52     | 0.15                | 0.57       |
| (3,105)  | 1:64:A:MET:H     | 1:66:A:LEU:HD23 | 17                  | 0.52     | 0.15                | 0.57       |
| (1,2305) | 1:45:A:ALA:HB2   | 1:44:A:GLU:HA   | 17                  | 0.52     | 0.06                | 0.51       |
| (1,2305) | 1:45:A:ALA:HB3   | 1:44:A:GLU:HA   | 17                  | 0.52     | 0.06                | 0.51       |
| (1,2305) | 1:45:A:ALA:HB1   | 1:44:A:GLU:HA   | 17                  | 0.52     | 0.06                | 0.51       |
| (1,2897) | 1:39:A:PHE:HZ    | 1:28:A:ILE:HD13 | 17                  | 0.52     | 0.03                | 0.53       |
| (1,2897) | 1:39:A:PHE:HZ    | 1:28:A:ILE:HD11 | 17                  | 0.52     | 0.03                | 0.53       |
| (1,2897) | 1:39:A:PHE:HZ    | 1:28:A:ILE:HD12 | 17                  | 0.52     | 0.03                | 0.53       |
| (1,1867) | 1:53:A:PHE:HA    | 1:31:A:LEU:HD13 | 17                  | 0.52     | 0.01                | 0.52       |
| (1,1867) | 1:53:A:PHE:HA    | 1:31:A:LEU:HD12 | 17                  | 0.52     | 0.01                | 0.52       |
| (1,1867) | 1:53:A:PHE:HA    | 1:31:A:LEU:HD11 | 17                  | 0.52     | 0.01                | 0.52       |
| (1,1740) | 1:77:A:LEU:HD13  | 1:78:A:TYR:H    | 17                  | 0.52     | 0.01                | 0.52       |
| (1,1740) | 1:77:A:LEU:HD11  | 1:78:A:TYR:H    | 17                  | 0.52     | 0.01                | 0.52       |
| (1,1740) | 1:77:A:LEU:HD12  | 1:78:A:TYR:H    | 17                  | 0.52     | 0.01                | 0.52       |
| (1,1336) | 1:85:A:LEU:HD22  | 1:84:A:TYR:HD1  | 17                  | 0.52     | 0.04                | 0.51       |
| (1,1336) | 1:85:A:LEU:HD23  | 1:84:A:TYR:HD2  | 17                  | 0.52     | 0.04                | 0.51       |
| (1,1336) | 1:85:A:LEU:HD21  | 1:84:A:TYR:HD2  | 17                  | 0.52     | 0.04                | 0.51       |
| (1,1336) | 1:85:A:LEU:HD22  | 1:84:A:TYR:HD2  | 17                  | 0.52     | 0.04                | 0.51       |
| (1,1336) | 1:85:A:LEU:HD21  | 1:84:A:TYR:HD1  | 17                  | 0.52     | 0.04                | 0.51       |
| (1,3366) | 1:72:A:ARG:HA    | 1:56:A:LEU:HD21 | 17                  | 0.52     | 0.02                | 0.52       |
| (1,3366) | 1:72:A:ARG:HA    | 1:56:A:LEU:HD23 | 17                  | 0.52     | 0.02                | 0.52       |
| (1,3366) | 1:72:A:ARG:HA    | 1:56:A:LEU:HD22 | 17                  | 0.52     | 0.02                | 0.52       |
| (1,467)  | 1:31:A:LEU:HD23  | 1:32:A:ALA:H    | 17                  | 0.52     | 0.01                | 0.52       |
| (1,467)  | 1:31:A:LEU:HD22  | 1:32:A:ALA:H    | 17                  | 0.52     | 0.01                | 0.52       |
| (1,467)  | 1:31:A:LEU:HD21  | 1:32:A:ALA:H    | 17                  | 0.52     | 0.01                | 0.52       |
| (1,204)  | 1:105:A:LEU:HD13 | 1:106:A:ASP:H   | 17                  | 0.51     | 0.02                | 0.52       |
| (1,204)  | 1:105:A:LEU:HD11 | 1:106:A:ASP:H   | 17                  | 0.51     | 0.02                | 0.52       |
| (1,204)  | 1:105:A:LEU:HD12 | 1:106:A:ASP:H   | 17                  | 0.51     | 0.02                | 0.52       |
| (1,2577) | 1:60:A:VAL:HG12  | 1:59:A:ARG:HA   | 17                  | 0.51     | 0.04                | 0.52       |
| (1,2577) | 1:60:A:VAL:HG13  | 1:59:A:ARG:HA   | 17                  | 0.51     | 0.04                | 0.52       |
| (1,2577) | 1:60:A:VAL:HG11  | 1:59:A:ARG:HA   | 17                  | 0.51     | 0.04                | 0.52       |
| (1,2147) | 1:85:A:LEU:HA    | 1:85:A:LEU:HD13 | 17                  | 0.51     | 0.03                | 0.5        |
| (1,2147) | 1:85:A:LEU:HA    | 1:85:A:LEU:HD11 | 17                  | 0.51     | 0.03                | 0.5        |
| (1,2147) | 1:85:A:LEU:HA    | 1:85:A:LEU:HD12 | 17                  | 0.51     | 0.03                | 0.5        |
| (1,4164) | 1:32:A:ALA:HB1   | 1:41:A:ALA:H    | 17                  | 0.51     | 0.09                | 0.53       |
| (1,4164) | 1:32:A:ALA:HB2   | 1:41:A:ALA:H    | 17                  | 0.51     | 0.09                | 0.53       |
| (1,4164) | 1:32:A:ALA:HB3   | 1:41:A:ALA:H    | 17                  | 0.51     | 0.09                | 0.53       |
| (1,1372) | 1:28:A:ILE:HD13  | 1:31:A:LEU:HB3  | 17                  | 0.51     | 0.03                | 0.51       |
| (1,1372) | 1:28:A:ILE:HD11  | 1:31:A:LEU:HB3  | 17                  | 0.51     | 0.03                | 0.51       |
| (1,1372) | 1:28:A:ILE:HD12  | 1:31:A:LEU:HB3  | 17                  | 0.51     | 0.03                | 0.51       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,576)  | 1:50:A:ILE:HD11 | 1:50:A:ILE:H    | 17                  | 0.51     | 0.12                | 0.45       |
| (1,576)  | 1:50:A:ILE:HD12 | 1:50:A:ILE:H    | 17                  | 0.51     | 0.12                | 0.45       |
| (1,576)  | 1:50:A:ILE:HD13 | 1:50:A:ILE:H    | 17                  | 0.51     | 0.12                | 0.45       |
| (3,99)   | 1:72:A:ARG:HG3  | 1:75:A:LEU:HD11 | 17                  | 0.51     | 0.05                | 0.51       |
| (3,99)   | 1:72:A:ARG:HG3  | 1:75:A:LEU:HD12 | 17                  | 0.51     | 0.05                | 0.51       |
| (3,99)   | 1:72:A:ARG:HG3  | 1:75:A:LEU:HD13 | 17                  | 0.51     | 0.05                | 0.51       |
| (1,4171) | 1:48:A:LEU:HD23 | 1:49:A:LYS:H    | 17                  | 0.5      | 0.1                 | 0.53       |
| (1,4171) | 1:48:A:LEU:HD21 | 1:49:A:LYS:H    | 17                  | 0.5      | 0.1                 | 0.53       |
| (1,4171) | 1:48:A:LEU:HD22 | 1:49:A:LYS:H    | 17                  | 0.5      | 0.1                 | 0.53       |
| (1,2817) | 1:97:A:LEU:HD11 | 1:97:A:LEU:HA   | 17                  | 0.5      | 0.08                | 0.51       |
| (1,2817) | 1:97:A:LEU:HD13 | 1:97:A:LEU:HA   | 17                  | 0.5      | 0.08                | 0.51       |
| (1,2817) | 1:97:A:LEU:HD12 | 1:97:A:LEU:HA   | 17                  | 0.5      | 0.08                | 0.51       |
| (1,3302) | 1:83:A:ARG:HB2  | 1:86:A:TYR:HD2  | 17                  | 0.5      | 0.11                | 0.5        |
| (1,3302) | 1:83:A:ARG:HB2  | 1:86:A:TYR:HD1  | 17                  | 0.5      | 0.11                | 0.5        |
| (1,697)  | 1:57:A:VAL:HG11 | 1:56:A:LEU:H    | 17                  | 0.5      | 0.07                | 0.52       |
| (1,697)  | 1:57:A:VAL:HG12 | 1:56:A:LEU:H    | 17                  | 0.5      | 0.07                | 0.52       |
| (1,697)  | 1:57:A:VAL:HG13 | 1:56:A:LEU:H    | 17                  | 0.5      | 0.07                | 0.52       |
| (1,3822) | 1:93:A:THR:HG23 | 1:103:A:GLY:H   | 17                  | 0.49     | 0.06                | 0.49       |
| (1,3822) | 1:93:A:THR:HG21 | 1:103:A:GLY:H   | 17                  | 0.49     | 0.06                | 0.49       |
| (1,3822) | 1:93:A:THR:HG22 | 1:103:A:GLY:H   | 17                  | 0.49     | 0.06                | 0.49       |
| (1,3452) | 1:95:A:VAL:HA   | 1:93:A:THR:HG21 | 17                  | 0.49     | 0.08                | 0.51       |
| (1,3452) | 1:95:A:VAL:HA   | 1:93:A:THR:HG22 | 17                  | 0.49     | 0.08                | 0.51       |
| (1,3452) | 1:95:A:VAL:HA   | 1:93:A:THR:HG23 | 17                  | 0.49     | 0.08                | 0.51       |
| (3,132)  | 1:113:A:ALA:HB2 | 1:112:A:HIS:H   | 17                  | 0.49     | 0.04                | 0.5        |
| (3,132)  | 1:113:A:ALA:HB1 | 1:112:A:HIS:H   | 17                  | 0.49     | 0.04                | 0.5        |
| (3,132)  | 1:113:A:ALA:HB3 | 1:112:A:HIS:H   | 17                  | 0.49     | 0.04                | 0.5        |
| (1,169)  | 1:120:A:ALA:HB1 | 1:119:A:GLU:H   | 17                  | 0.49     | 0.05                | 0.5        |
| (1,169)  | 1:120:A:ALA:HB2 | 1:119:A:GLU:H   | 17                  | 0.49     | 0.05                | 0.5        |
| (1,169)  | 1:120:A:ALA:HB3 | 1:119:A:GLU:H   | 17                  | 0.49     | 0.05                | 0.5        |
| (1,1838) | 1:93:A:THR:HA   | 1:93:A:THR:HG22 | 17                  | 0.49     | 0.02                | 0.49       |
| (1,1838) | 1:93:A:THR:HA   | 1:93:A:THR:HG23 | 17                  | 0.49     | 0.02                | 0.49       |
| (1,1838) | 1:93:A:THR:HA   | 1:93:A:THR:HG21 | 17                  | 0.49     | 0.02                | 0.49       |
| (1,389)  | 1:58:A:ASP:H    | 1:57:A:VAL:HG12 | 17                  | 0.49     | 0.05                | 0.49       |
| (1,389)  | 1:58:A:ASP:H    | 1:57:A:VAL:HG13 | 17                  | 0.49     | 0.05                | 0.49       |
| (1,389)  | 1:58:A:ASP:H    | 1:57:A:VAL:HG11 | 17                  | 0.49     | 0.05                | 0.49       |
| (1,2592) | 1:69:A:THR:HG22 | 1:70:A:GLN:H    | 17                  | 0.49     | 0.01                | 0.49       |
| (1,2592) | 1:69:A:THR:HG21 | 1:70:A:GLN:H    | 17                  | 0.49     | 0.01                | 0.49       |
| (1,2592) | 1:69:A:THR:HG23 | 1:70:A:GLN:H    | 17                  | 0.49     | 0.01                | 0.49       |
| (1,3116) | 1:57:A:VAL:HG23 | 1:53:A:PHE:HE2  | 17                  | 0.49     | 0.03                | 0.49       |
| (1,3116) | 1:57:A:VAL:HG22 | 1:53:A:PHE:HE2  | 17                  | 0.49     | 0.03                | 0.49       |
| (1,3116) | 1:57:A:VAL:HG23 | 1:53:A:PHE:HE1  | 17                  | 0.49     | 0.03                | 0.49       |
| (1,3116) | 1:57:A:VAL:HG21 | 1:53:A:PHE:HE1  | 17                  | 0.49     | 0.03                | 0.49       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,3116) | 1:57:A:VAL:HG21 | 1:53:A:PHE:HE2  | 17                  | 0.49     | 0.03                | 0.49       |
| (1,3116) | 1:57:A:VAL:HG22 | 1:53:A:PHE:HE1  | 17                  | 0.49     | 0.03                | 0.49       |
| (1,2865) | 1:78:A:TYR:HE2  | 1:48:A:LEU:HD11 | 17                  | 0.49     | 0.08                | 0.5        |
| (1,2865) | 1:78:A:TYR:HE1  | 1:48:A:LEU:HD13 | 17                  | 0.49     | 0.08                | 0.5        |
| (1,2865) | 1:78:A:TYR:HE1  | 1:48:A:LEU:HD11 | 17                  | 0.49     | 0.08                | 0.5        |
| (1,2865) | 1:78:A:TYR:HE2  | 1:48:A:LEU:HD13 | 17                  | 0.49     | 0.08                | 0.5        |
| (1,2865) | 1:78:A:TYR:HE2  | 1:48:A:LEU:HD12 | 17                  | 0.49     | 0.08                | 0.5        |
| (1,2865) | 1:78:A:TYR:HE1  | 1:48:A:LEU:HD12 | 17                  | 0.49     | 0.08                | 0.5        |
| (1,3742) | 1:28:A:ILE:H    | 1:29:A:ALA:HB2  | 17                  | 0.49     | 0.06                | 0.46       |
| (1,3742) | 1:28:A:ILE:H    | 1:29:A:ALA:HB3  | 17                  | 0.49     | 0.06                | 0.46       |
| (1,3742) | 1:28:A:ILE:H    | 1:29:A:ALA:HB1  | 17                  | 0.49     | 0.06                | 0.46       |
| (1,1155) | 1:53:A:PHE:HB3  | 1:53:A:PHE:HE2  | 17                  | 0.48     | 0.02                | 0.48       |
| (1,1155) | 1:53:A:PHE:HB3  | 1:53:A:PHE:HE1  | 17                  | 0.48     | 0.02                | 0.48       |
| (1,3368) | 1:31:A:LEU:HD13 | 1:31:A:LEU:HA   | 17                  | 0.48     | 0.03                | 0.48       |
| (1,3368) | 1:31:A:LEU:HD12 | 1:31:A:LEU:HA   | 17                  | 0.48     | 0.03                | 0.48       |
| (1,3368) | 1:31:A:LEU:HD11 | 1:31:A:LEU:HA   | 17                  | 0.48     | 0.03                | 0.48       |
| (1,1305) | 1:97:A:LEU:HD22 | 1:52:A:ILE:HB   | 17                  | 0.48     | 0.04                | 0.47       |
| (1,1305) | 1:97:A:LEU:HD23 | 1:52:A:ILE:HB   | 17                  | 0.48     | 0.04                | 0.47       |
| (1,1305) | 1:97:A:LEU:HD21 | 1:52:A:ILE:HB   | 17                  | 0.48     | 0.04                | 0.47       |
| (1,2581) | 1:71:A:LEU:HD12 | 1:60:A:VAL:HG11 | 17                  | 0.47     | 0.04                | 0.49       |
| (1,2581) | 1:71:A:LEU:HD11 | 1:60:A:VAL:HG12 | 17                  | 0.47     | 0.04                | 0.49       |
| (1,2581) | 1:71:A:LEU:HD11 | 1:60:A:VAL:HG11 | 17                  | 0.47     | 0.04                | 0.49       |
| (1,2581) | 1:71:A:LEU:HD13 | 1:60:A:VAL:HG13 | 17                  | 0.47     | 0.04                | 0.49       |
| (1,2581) | 1:71:A:LEU:HD12 | 1:60:A:VAL:HG12 | 17                  | 0.47     | 0.04                | 0.49       |
| (1,2581) | 1:71:A:LEU:HD11 | 1:60:A:VAL:HG13 | 17                  | 0.47     | 0.04                | 0.49       |
| (1,2581) | 1:71:A:LEU:HD13 | 1:60:A:VAL:HG11 | 17                  | 0.47     | 0.04                | 0.49       |
| (1,2581) | 1:71:A:LEU:HD13 | 1:60:A:VAL:HG12 | 17                  | 0.47     | 0.04                | 0.49       |
| (1,3256) | 1:41:A:ALA:HB2  | 1:33:A:GLU:H    | 17                  | 0.47     | 0.06                | 0.48       |
| (1,3256) | 1:41:A:ALA:HB3  | 1:33:A:GLU:H    | 17                  | 0.47     | 0.06                | 0.48       |
| (1,3256) | 1:41:A:ALA:HB1  | 1:33:A:GLU:H    | 17                  | 0.47     | 0.06                | 0.48       |
| (1,604)  | 1:32:A:ALA:HB1  | 1:41:A:ALA:H    | 17                  | 0.47     | 0.09                | 0.49       |
| (1,604)  | 1:32:A:ALA:HB2  | 1:41:A:ALA:H    | 17                  | 0.47     | 0.09                | 0.49       |
| (1,604)  | 1:32:A:ALA:HB3  | 1:41:A:ALA:H    | 17                  | 0.47     | 0.09                | 0.49       |
| (1,3329) | 1:77:A:LEU:HD13 | 1:78:A:TYR:H    | 17                  | 0.47     | 0.01                | 0.47       |
| (1,3329) | 1:77:A:LEU:HD11 | 1:78:A:TYR:H    | 17                  | 0.47     | 0.01                | 0.47       |
| (1,3329) | 1:77:A:LEU:HD12 | 1:78:A:TYR:H    | 17                  | 0.47     | 0.01                | 0.47       |
| (1,1507) | 1:78:A:TYR:HE1  | 1:28:A:ILE:HG21 | 17                  | 0.47     | 0.05                | 0.46       |
| (1,1507) | 1:78:A:TYR:HE2  | 1:28:A:ILE:HG23 | 17                  | 0.47     | 0.05                | 0.46       |
| (1,1507) | 1:78:A:TYR:HE2  | 1:28:A:ILE:HG22 | 17                  | 0.47     | 0.05                | 0.46       |
| (1,1507) | 1:78:A:TYR:HE1  | 1:28:A:ILE:HG22 | 17                  | 0.47     | 0.05                | 0.46       |
| (1,1507) | 1:78:A:TYR:HE2  | 1:28:A:ILE:HG21 | 17                  | 0.47     | 0.05                | 0.46       |
| (1,2578) | 1:57:A:VAL:HA   | 1:60:A:VAL:HG11 | 17                  | 0.47     | 0.03                | 0.48       |

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| Key      | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,2578) | 1:57:A:VAL:HA   | 1:60:A:VAL:HG12  | 17                  | 0.47     | 0.03                | 0.48       |
| (1,2578) | 1:57:A:VAL:HA   | 1:60:A:VAL:HG13  | 17                  | 0.47     | 0.03                | 0.48       |
| (1,942)  | 1:93:A:THR:HB   | 1:95:A:VAL:HG12  | 17                  | 0.47     | 0.07                | 0.45       |
| (1,942)  | 1:93:A:THR:HB   | 1:95:A:VAL:HG11  | 17                  | 0.47     | 0.07                | 0.45       |
| (1,942)  | 1:93:A:THR:HB   | 1:95:A:VAL:HG13  | 17                  | 0.47     | 0.07                | 0.45       |
| (1,2854) | 1:85:A:LEU:HD22 | 1:84:A:TYR:HD1   | 17                  | 0.47     | 0.04                | 0.46       |
| (1,2854) | 1:85:A:LEU:HD23 | 1:84:A:TYR:HD2   | 17                  | 0.47     | 0.04                | 0.46       |
| (1,2854) | 1:85:A:LEU:HD21 | 1:84:A:TYR:HD2   | 17                  | 0.47     | 0.04                | 0.46       |
| (1,2854) | 1:85:A:LEU:HD22 | 1:84:A:TYR:HD2   | 17                  | 0.47     | 0.04                | 0.46       |
| (1,2854) | 1:85:A:LEU:HD21 | 1:84:A:TYR:HD1   | 17                  | 0.47     | 0.04                | 0.46       |
| (1,1950) | 1:105:A:LEU:HB2 | 1:110:A:VAL:HG13 | 17                  | 0.47     | 0.02                | 0.46       |
| (1,1950) | 1:105:A:LEU:HB2 | 1:110:A:VAL:HG11 | 17                  | 0.47     | 0.02                | 0.46       |
| (1,1950) | 1:105:A:LEU:HB2 | 1:110:A:VAL:HG12 | 17                  | 0.47     | 0.02                | 0.46       |
| (1,3483) | 1:53:A:PHE:HA   | 1:31:A:LEU:HD13  | 17                  | 0.47     | 0.01                | 0.47       |
| (1,3483) | 1:53:A:PHE:HA   | 1:31:A:LEU:HD12  | 17                  | 0.47     | 0.01                | 0.47       |
| (1,3483) | 1:53:A:PHE:HA   | 1:31:A:LEU:HD11  | 17                  | 0.47     | 0.01                | 0.47       |
| (1,1075) | 1:31:A:LEU:HD13 | 1:31:A:LEU:HA    | 17                  | 0.47     | 0.03                | 0.47       |
| (1,1075) | 1:31:A:LEU:HD12 | 1:31:A:LEU:HA    | 17                  | 0.47     | 0.03                | 0.47       |
| (1,1075) | 1:31:A:LEU:HD11 | 1:31:A:LEU:HA    | 17                  | 0.47     | 0.03                | 0.47       |
| (1,1043) | 1:78:A:TYR:HE2  | 1:28:A:ILE:HD13  | 17                  | 0.47     | 0.04                | 0.45       |
| (1,1043) | 1:78:A:TYR:HE1  | 1:28:A:ILE:HD13  | 17                  | 0.47     | 0.04                | 0.45       |
| (1,1043) | 1:78:A:TYR:HE1  | 1:28:A:ILE:HD11  | 17                  | 0.47     | 0.04                | 0.45       |
| (1,1043) | 1:78:A:TYR:HE2  | 1:28:A:ILE:HD11  | 17                  | 0.47     | 0.04                | 0.45       |
| (1,1043) | 1:78:A:TYR:HE2  | 1:28:A:ILE:HD12  | 17                  | 0.47     | 0.04                | 0.45       |
| (1,1043) | 1:78:A:TYR:HE1  | 1:28:A:ILE:HD12  | 17                  | 0.47     | 0.04                | 0.45       |
| (1,2150) | 1:105:A:LEU:H   | 1:105:A:LEU:HD11 | 17                  | 0.47     | 0.01                | 0.47       |
| (1,2150) | 1:105:A:LEU:H   | 1:105:A:LEU:HD12 | 17                  | 0.47     | 0.01                | 0.47       |
| (1,2150) | 1:105:A:LEU:H   | 1:105:A:LEU:HD13 | 17                  | 0.47     | 0.01                | 0.47       |
| (1,610)  | 1:48:A:LEU:HD23 | 1:49:A:LYS:H     | 17                  | 0.46     | 0.1                 | 0.49       |
| (1,610)  | 1:48:A:LEU:HD21 | 1:49:A:LYS:H     | 17                  | 0.46     | 0.1                 | 0.49       |
| (1,610)  | 1:48:A:LEU:HD22 | 1:49:A:LYS:H     | 17                  | 0.46     | 0.1                 | 0.49       |
| (1,2900) | 1:28:A:ILE:HD13 | 1:31:A:LEU:HB3   | 17                  | 0.46     | 0.03                | 0.46       |
| (1,2900) | 1:28:A:ILE:HD11 | 1:31:A:LEU:HB3   | 17                  | 0.46     | 0.03                | 0.46       |
| (1,2900) | 1:28:A:ILE:HD12 | 1:31:A:LEU:HB3   | 17                  | 0.46     | 0.03                | 0.46       |
| (1,1790) | 1:90:A:PRO:HA   | 1:92:A:ALA:HB3   | 17                  | 0.46     | 0.07                | 0.45       |
| (1,1790) | 1:90:A:PRO:HA   | 1:92:A:ALA:HB2   | 17                  | 0.46     | 0.07                | 0.45       |
| (1,1790) | 1:90:A:PRO:HA   | 1:92:A:ALA:HB1   | 17                  | 0.46     | 0.07                | 0.45       |
| (1,3463) | 1:35:A:PHE:HE2  | 1:38:A:CYS:HB2   | 17                  | 0.46     | 0.07                | 0.45       |
| (1,3463) | 1:35:A:PHE:HE1  | 1:38:A:CYS:HB2   | 17                  | 0.46     | 0.07                | 0.45       |
| (1,3554) | 1:66:A:LEU:HB2  | 1:66:A:LEU:HD22  | 17                  | 0.46     | 0.04                | 0.45       |
| (1,3554) | 1:66:A:LEU:HB2  | 1:66:A:LEU:HD21  | 17                  | 0.46     | 0.04                | 0.45       |
| (1,3554) | 1:66:A:LEU:HB2  | 1:66:A:LEU:HD23  | 17                  | 0.46     | 0.04                | 0.45       |

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| Key      | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,2423) | 1:64:A:MET:HA   | 1:64:A:MET:HE3   | 17                  | 0.46     | 0.11                | 0.44       |
| (1,2423) | 1:64:A:MET:HA   | 1:64:A:MET:HE2   | 17                  | 0.46     | 0.11                | 0.44       |
| (1,2423) | 1:64:A:MET:HA   | 1:64:A:MET:HE1   | 17                  | 0.46     | 0.11                | 0.44       |
| (1,1853) | 1:86:A:TYR:HE2  | 1:85:A:LEU:HD13  | 17                  | 0.46     | 0.03                | 0.45       |
| (1,1853) | 1:86:A:TYR:HE1  | 1:85:A:LEU:HD13  | 17                  | 0.46     | 0.03                | 0.45       |
| (1,1853) | 1:86:A:TYR:HE2  | 1:85:A:LEU:HD11  | 17                  | 0.46     | 0.03                | 0.45       |
| (1,1853) | 1:86:A:TYR:HE2  | 1:85:A:LEU:HD12  | 17                  | 0.46     | 0.03                | 0.45       |
| (1,1853) | 1:86:A:TYR:HE1  | 1:85:A:LEU:HD11  | 17                  | 0.46     | 0.03                | 0.45       |
| (1,1853) | 1:86:A:TYR:HE1  | 1:85:A:LEU:HD12  | 17                  | 0.46     | 0.03                | 0.45       |
| (1,2146) | 1:104:A:GLU:HB3 | 1:93:A:THR:HG23  | 17                  | 0.46     | 0.05                | 0.44       |
| (1,2146) | 1:104:A:GLU:HB3 | 1:93:A:THR:HG21  | 17                  | 0.46     | 0.05                | 0.44       |
| (1,2146) | 1:104:A:GLU:HB3 | 1:93:A:THR:HG22  | 17                  | 0.46     | 0.05                | 0.44       |
| (1,217)  | 1:93:A:THR:HG23 | 1:103:A:GLY:H    | 17                  | 0.46     | 0.06                | 0.45       |
| (1,217)  | 1:93:A:THR:HG21 | 1:103:A:GLY:H    | 17                  | 0.46     | 0.06                | 0.45       |
| (1,217)  | 1:93:A:THR:HG22 | 1:103:A:GLY:H    | 17                  | 0.46     | 0.06                | 0.45       |
| (1,1308) | 1:97:A:LEU:HD21 | 1:35:A:PHE:HD2   | 17                  | 0.45     | 0.12                | 0.43       |
| (1,1308) | 1:97:A:LEU:HD22 | 1:35:A:PHE:HD1   | 17                  | 0.45     | 0.12                | 0.43       |
| (1,1308) | 1:97:A:LEU:HD22 | 1:35:A:PHE:HD2   | 17                  | 0.45     | 0.12                | 0.43       |
| (1,1308) | 1:97:A:LEU:HD23 | 1:35:A:PHE:HD2   | 17                  | 0.45     | 0.12                | 0.43       |
| (1,1308) | 1:97:A:LEU:HD23 | 1:35:A:PHE:HD1   | 17                  | 0.45     | 0.12                | 0.43       |
| (1,1308) | 1:97:A:LEU:HD21 | 1:35:A:PHE:HD1   | 17                  | 0.45     | 0.12                | 0.43       |
| (1,1679) | 1:92:A:ALA:HB3  | 1:91:A:GLY:H     | 17                  | 0.45     | 0.08                | 0.47       |
| (1,1679) | 1:92:A:ALA:HB2  | 1:91:A:GLY:H     | 17                  | 0.45     | 0.08                | 0.47       |
| (1,1679) | 1:92:A:ALA:HB1  | 1:91:A:GLY:H     | 17                  | 0.45     | 0.08                | 0.47       |
| (1,2028) | 1:97:A:LEU:HD23 | 1:97:A:LEU:H     | 17                  | 0.45     | 0.22                | 0.3        |
| (1,2028) | 1:97:A:LEU:HD21 | 1:97:A:LEU:H     | 17                  | 0.45     | 0.22                | 0.3        |
| (1,2028) | 1:97:A:LEU:HD22 | 1:97:A:LEU:H     | 17                  | 0.45     | 0.22                | 0.3        |
| (1,3451) | 1:93:A:THR:HA   | 1:93:A:THR:HG22  | 17                  | 0.45     | 0.02                | 0.45       |
| (1,3451) | 1:93:A:THR:HA   | 1:93:A:THR:HG23  | 17                  | 0.45     | 0.02                | 0.45       |
| (1,3451) | 1:93:A:THR:HA   | 1:93:A:THR:HG21  | 17                  | 0.45     | 0.02                | 0.45       |
| (1,3601) | 1:113:A:ALA:HB2 | 1:111:A:GLU:H    | 17                  | 0.45     | 0.05                | 0.44       |
| (1,3601) | 1:113:A:ALA:HB1 | 1:111:A:GLU:H    | 17                  | 0.45     | 0.05                | 0.44       |
| (1,3601) | 1:113:A:ALA:HB3 | 1:111:A:GLU:H    | 17                  | 0.45     | 0.05                | 0.44       |
| (1,1309) | 1:97:A:LEU:HD23 | 1:97:A:LEU:H     | 17                  | 0.45     | 0.22                | 0.3        |
| (1,1309) | 1:97:A:LEU:HD21 | 1:97:A:LEU:H     | 17                  | 0.45     | 0.22                | 0.3        |
| (1,1309) | 1:97:A:LEU:HD22 | 1:97:A:LEU:H     | 17                  | 0.45     | 0.22                | 0.3        |
| (1,1702) | 1:116:A:GLN:HG3 | 1:116:A:GLN:HE21 | 17                  | 0.45     | 0.02                | 0.44       |
| (1,126)  | 1:28:A:ILE:H    | 1:29:A:ALA:HB2   | 17                  | 0.45     | 0.06                | 0.42       |
| (1,126)  | 1:28:A:ILE:H    | 1:29:A:ALA:HB3   | 17                  | 0.45     | 0.06                | 0.42       |
| (1,126)  | 1:28:A:ILE:H    | 1:29:A:ALA:HB1   | 17                  | 0.45     | 0.06                | 0.42       |
| (1,1450) | 1:54:A:GLN:HE22 | 1:54:A:GLN:HG2   | 17                  | 0.45     | 0.13                | 0.39       |
| (3,18)   | 1:58:A:ASP:HB3  | 1:60:A:VAL:HG12  | 17                  | 0.45     | 0.15                | 0.43       |

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| Key      | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (3,18)   | 1:58:A:ASP:HB3  | 1:60:A:VAL:HG13  | 17                  | 0.45     | 0.15                | 0.43       |
| (3,18)   | 1:58:A:ASP:HB3  | 1:60:A:VAL:HG11  | 17                  | 0.45     | 0.15                | 0.43       |
| (1,1076) | 1:30:A:PHE:HD1  | 1:31:A:LEU:HD12  | 17                  | 0.44     | 0.02                | 0.44       |
| (1,1076) | 1:30:A:PHE:HD2  | 1:31:A:LEU:HD12  | 17                  | 0.44     | 0.02                | 0.44       |
| (1,1076) | 1:30:A:PHE:HD2  | 1:31:A:LEU:HD11  | 17                  | 0.44     | 0.02                | 0.44       |
| (1,1076) | 1:30:A:PHE:HD1  | 1:31:A:LEU:HD11  | 17                  | 0.44     | 0.02                | 0.44       |
| (1,1076) | 1:30:A:PHE:HD2  | 1:31:A:LEU:HD13  | 17                  | 0.44     | 0.02                | 0.44       |
| (1,1076) | 1:30:A:PHE:HD1  | 1:31:A:LEU:HD13  | 17                  | 0.44     | 0.02                | 0.44       |
| (1,3373) | 1:88:A:VAL:HA   | 1:93:A:THR:HG22  | 17                  | 0.44     | 0.05                | 0.46       |
| (1,3373) | 1:88:A:VAL:HA   | 1:93:A:THR:HG23  | 17                  | 0.44     | 0.05                | 0.46       |
| (1,3373) | 1:88:A:VAL:HA   | 1:93:A:THR:HG21  | 17                  | 0.44     | 0.05                | 0.46       |
| (1,2006) | 1:78:A:TYR:HE2  | 1:48:A:LEU:HD11  | 17                  | 0.44     | 0.07                | 0.46       |
| (1,2006) | 1:78:A:TYR:HE1  | 1:48:A:LEU:HD13  | 17                  | 0.44     | 0.07                | 0.46       |
| (1,2006) | 1:78:A:TYR:HE1  | 1:48:A:LEU:HD11  | 17                  | 0.44     | 0.07                | 0.46       |
| (1,2006) | 1:78:A:TYR:HE2  | 1:48:A:LEU:HD13  | 17                  | 0.44     | 0.07                | 0.46       |
| (1,2006) | 1:78:A:TYR:HE2  | 1:48:A:LEU:HD12  | 17                  | 0.44     | 0.07                | 0.46       |
| (1,2006) | 1:78:A:TYR:HE1  | 1:48:A:LEU:HD12  | 17                  | 0.44     | 0.07                | 0.46       |
| (1,3051) | 1:78:A:TYR:HE1  | 1:28:A:ILE:HG21  | 17                  | 0.43     | 0.05                | 0.43       |
| (1,3051) | 1:78:A:TYR:HE2  | 1:28:A:ILE:HG23  | 17                  | 0.43     | 0.05                | 0.43       |
| (1,3051) | 1:78:A:TYR:HE2  | 1:28:A:ILE:HG22  | 17                  | 0.43     | 0.05                | 0.43       |
| (1,3051) | 1:78:A:TYR:HE1  | 1:28:A:ILE:HG22  | 17                  | 0.43     | 0.05                | 0.43       |
| (1,3051) | 1:78:A:TYR:HE2  | 1:28:A:ILE:HG21  | 17                  | 0.43     | 0.05                | 0.43       |
| (1,3594) | 1:105:A:LEU:HB2 | 1:110:A:VAL:HG13 | 17                  | 0.43     | 0.01                | 0.43       |
| (1,3594) | 1:105:A:LEU:HB2 | 1:110:A:VAL:HG11 | 17                  | 0.43     | 0.01                | 0.43       |
| (1,3594) | 1:105:A:LEU:HB2 | 1:110:A:VAL:HG12 | 17                  | 0.43     | 0.01                | 0.43       |
| (1,2194) | 1:50:A:ILE:HD12 | 1:80:A:SER:H     | 17                  | 0.43     | 0.07                | 0.44       |
| (1,2194) | 1:50:A:ILE:HD13 | 1:80:A:SER:H     | 17                  | 0.43     | 0.07                | 0.44       |
| (1,2194) | 1:50:A:ILE:HD11 | 1:80:A:SER:H     | 17                  | 0.43     | 0.07                | 0.44       |
| (3,50)   | 1:31:A:LEU:HD21 | 1:97:A:LEU:HD21  | 17                  | 0.43     | 0.03                | 0.44       |
| (3,50)   | 1:31:A:LEU:HD23 | 1:97:A:LEU:HD22  | 17                  | 0.43     | 0.03                | 0.44       |
| (3,50)   | 1:31:A:LEU:HD23 | 1:97:A:LEU:HD23  | 17                  | 0.43     | 0.03                | 0.44       |
| (3,50)   | 1:31:A:LEU:HD22 | 1:97:A:LEU:HD23  | 17                  | 0.43     | 0.03                | 0.44       |
| (3,50)   | 1:31:A:LEU:HD22 | 1:97:A:LEU:HD22  | 17                  | 0.43     | 0.03                | 0.44       |
| (3,50)   | 1:31:A:LEU:HD21 | 1:97:A:LEU:HD22  | 17                  | 0.43     | 0.03                | 0.44       |
| (3,50)   | 1:31:A:LEU:HD23 | 1:97:A:LEU:HD21  | 17                  | 0.43     | 0.03                | 0.44       |
| (3,50)   | 1:31:A:LEU:HD22 | 1:97:A:LEU:HD21  | 17                  | 0.43     | 0.03                | 0.44       |
| (1,789)  | 1:50:A:ILE:HG13 | 1:50:A:ILE:HG21  | 17                  | 0.43     | 0.04                | 0.44       |
| (1,789)  | 1:50:A:ILE:HG13 | 1:50:A:ILE:HG23  | 17                  | 0.43     | 0.04                | 0.44       |
| (1,789)  | 1:50:A:ILE:HG13 | 1:50:A:ILE:HG22  | 17                  | 0.43     | 0.04                | 0.44       |
| (1,3834) | 1:95:A:VAL:HG23 | 1:100:A:ASN:H    | 17                  | 0.43     | 0.03                | 0.43       |
| (1,3834) | 1:95:A:VAL:HG22 | 1:100:A:ASN:H    | 17                  | 0.43     | 0.03                | 0.43       |
| (1,3834) | 1:95:A:VAL:HG21 | 1:100:A:ASN:H    | 17                  | 0.43     | 0.03                | 0.43       |

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| Key      | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (3,152)  | 1:27:A:VAL:H    | 1:74:A:ALA:HB1   | 17                  | 0.43     | 0.1                 | 0.42       |
| (3,152)  | 1:27:A:VAL:H    | 1:74:A:ALA:HB2   | 17                  | 0.43     | 0.1                 | 0.42       |
| (3,152)  | 1:27:A:VAL:H    | 1:74:A:ALA:HB3   | 17                  | 0.43     | 0.1                 | 0.42       |
| (3,152)  | 1:27:A:VAL:H    | 1:29:A:ALA:HB2   | 17                  | 0.43     | 0.1                 | 0.42       |
| (1,3342) | 1:92:A:ALA:HB2  | 1:88:A:VAL:H     | 17                  | 0.43     | 0.06                | 0.45       |
| (1,3342) | 1:92:A:ALA:HB1  | 1:88:A:VAL:H     | 17                  | 0.43     | 0.06                | 0.45       |
| (1,3342) | 1:92:A:ALA:HB3  | 1:88:A:VAL:H     | 17                  | 0.43     | 0.06                | 0.45       |
| (1,3405) | 1:55:A:ASP:HB2  | 1:56:A:LEU:HD22  | 17                  | 0.43     | 0.06                | 0.46       |
| (1,3405) | 1:55:A:ASP:HB2  | 1:56:A:LEU:HD21  | 17                  | 0.43     | 0.06                | 0.46       |
| (1,3405) | 1:55:A:ASP:HB2  | 1:56:A:LEU:HD23  | 17                  | 0.43     | 0.06                | 0.46       |
| (1,2271) | 1:113:A:ALA:HB2 | 1:112:A:HIS:HD2  | 17                  | 0.43     | 0.03                | 0.43       |
| (1,2271) | 1:113:A:ALA:HB1 | 1:112:A:HIS:HD2  | 17                  | 0.43     | 0.03                | 0.43       |
| (1,2271) | 1:113:A:ALA:HB3 | 1:112:A:HIS:HD2  | 17                  | 0.43     | 0.03                | 0.43       |
| (1,3570) | 1:90:A:PRO:HA   | 1:105:A:LEU:HD11 | 17                  | 0.43     | 0.07                | 0.41       |
| (1,3570) | 1:90:A:PRO:HA   | 1:105:A:LEU:HD12 | 17                  | 0.43     | 0.07                | 0.41       |
| (1,3570) | 1:90:A:PRO:HA   | 1:105:A:LEU:HD13 | 17                  | 0.43     | 0.07                | 0.41       |
| (1,2568) | 1:78:A:TYR:HE2  | 1:28:A:ILE:HD13  | 17                  | 0.43     | 0.04                | 0.42       |
| (1,2568) | 1:78:A:TYR:HE1  | 1:28:A:ILE:HD13  | 17                  | 0.43     | 0.04                | 0.42       |
| (1,2568) | 1:78:A:TYR:HE1  | 1:28:A:ILE:HD11  | 17                  | 0.43     | 0.04                | 0.42       |
| (1,2568) | 1:78:A:TYR:HE2  | 1:28:A:ILE:HD11  | 17                  | 0.43     | 0.04                | 0.42       |
| (1,2568) | 1:78:A:TYR:HE2  | 1:28:A:ILE:HD12  | 17                  | 0.43     | 0.04                | 0.42       |
| (1,2568) | 1:78:A:TYR:HE1  | 1:28:A:ILE:HD12  | 17                  | 0.43     | 0.04                | 0.42       |
| (1,2678) | 1:53:A:PHE:HB3  | 1:53:A:PHE:HE2   | 17                  | 0.43     | 0.02                | 0.42       |
| (1,2678) | 1:53:A:PHE:HB3  | 1:53:A:PHE:HE1   | 17                  | 0.43     | 0.02                | 0.42       |
| (1,3231) | 1:27:A:VAL:HG22 | 1:27:A:VAL:HA    | 17                  | 0.43     | 0.01                | 0.42       |
| (1,3231) | 1:27:A:VAL:HG23 | 1:27:A:VAL:HA    | 17                  | 0.43     | 0.01                | 0.42       |
| (1,3231) | 1:27:A:VAL:HG21 | 1:27:A:VAL:HA    | 17                  | 0.43     | 0.01                | 0.42       |
| (1,2827) | 1:97:A:LEU:HD22 | 1:52:A:ILE:HB    | 17                  | 0.42     | 0.04                | 0.42       |
| (1,2827) | 1:97:A:LEU:HD23 | 1:52:A:ILE:HB    | 17                  | 0.42     | 0.04                | 0.42       |
| (1,2827) | 1:97:A:LEU:HD21 | 1:52:A:ILE:HB    | 17                  | 0.42     | 0.04                | 0.42       |
| (1,3923) | 1:71:A:LEU:HD13 | 1:72:A:ARG:H     | 17                  | 0.42     | 0.01                | 0.43       |
| (1,3923) | 1:71:A:LEU:HD12 | 1:72:A:ARG:H     | 17                  | 0.42     | 0.01                | 0.43       |
| (1,3923) | 1:71:A:LEU:HD11 | 1:72:A:ARG:H     | 17                  | 0.42     | 0.01                | 0.43       |
| (1,2831) | 1:97:A:LEU:HD21 | 1:35:A:PHE:HD2   | 17                  | 0.42     | 0.12                | 0.4        |
| (1,2831) | 1:97:A:LEU:HD22 | 1:35:A:PHE:HD1   | 17                  | 0.42     | 0.12                | 0.4        |
| (1,2831) | 1:97:A:LEU:HD22 | 1:35:A:PHE:HD2   | 17                  | 0.42     | 0.12                | 0.4        |
| (1,2831) | 1:97:A:LEU:HD23 | 1:35:A:PHE:HD2   | 17                  | 0.42     | 0.12                | 0.4        |
| (1,2831) | 1:97:A:LEU:HD23 | 1:35:A:PHE:HD1   | 17                  | 0.42     | 0.12                | 0.4        |
| (1,2831) | 1:97:A:LEU:HD21 | 1:35:A:PHE:HD1   | 17                  | 0.42     | 0.12                | 0.4        |
| (1,3199) | 1:113:A:ALA:HB2 | 1:112:A:HIS:HB2  | 17                  | 0.42     | 0.04                | 0.42       |
| (1,3199) | 1:113:A:ALA:HB1 | 1:112:A:HIS:HB2  | 17                  | 0.42     | 0.04                | 0.42       |
| (1,3199) | 1:113:A:ALA:HB3 | 1:112:A:HIS:HB2  | 17                  | 0.42     | 0.04                | 0.42       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,3644) | 1:53:A:PHE:H     | 1:53:A:PHE:HD1   | 17                  | 0.42     | 0.03                | 0.42       |
| (1,3644) | 1:53:A:PHE:H     | 1:53:A:PHE:HD2   | 17                  | 0.42     | 0.03                | 0.42       |
| (1,3861) | 1:110:A:VAL:HG22 | 1:91:A:GLY:H     | 17                  | 0.42     | 0.14                | 0.44       |
| (1,3861) | 1:110:A:VAL:HG23 | 1:91:A:GLY:H     | 17                  | 0.42     | 0.14                | 0.44       |
| (1,3861) | 1:110:A:VAL:HG21 | 1:91:A:GLY:H     | 17                  | 0.42     | 0.14                | 0.44       |
| (1,2991) | 1:54:A:GLN:HE22  | 1:54:A:GLN:HG2   | 17                  | 0.42     | 0.13                | 0.36       |
| (1,2212) | 1:110:A:VAL:HG23 | 1:114:A:ARG:H    | 17                  | 0.42     | 0.04                | 0.42       |
| (1,2212) | 1:110:A:VAL:HG21 | 1:114:A:ARG:H    | 17                  | 0.42     | 0.04                | 0.42       |
| (1,2212) | 1:110:A:VAL:HG22 | 1:114:A:ARG:H    | 17                  | 0.42     | 0.04                | 0.42       |
| (1,2405) | 1:29:A:ALA:H     | 1:28:A:ILE:HD12  | 17                  | 0.42     | 0.03                | 0.41       |
| (1,2405) | 1:29:A:ALA:H     | 1:28:A:ILE:HD13  | 17                  | 0.42     | 0.03                | 0.41       |
| (1,2405) | 1:29:A:ALA:H     | 1:28:A:ILE:HD11  | 17                  | 0.42     | 0.03                | 0.41       |
| (1,3078) | 1:54:A:GLN:HB3   | 1:57:A:VAL:HG11  | 17                  | 0.42     | 0.04                | 0.41       |
| (1,3078) | 1:54:A:GLN:HB3   | 1:57:A:VAL:HG12  | 17                  | 0.42     | 0.04                | 0.41       |
| (1,3078) | 1:54:A:GLN:HB3   | 1:57:A:VAL:HG13  | 17                  | 0.42     | 0.04                | 0.41       |
| (1,2872) | 1:129:A:ALA:HB2  | 1:129:A:ALA:HA   | 17                  | 0.41     | 0.04                | 0.42       |
| (1,2872) | 1:129:A:ALA:HB3  | 1:129:A:ALA:HA   | 17                  | 0.41     | 0.04                | 0.42       |
| (1,2872) | 1:129:A:ALA:HB1  | 1:129:A:ALA:HA   | 17                  | 0.41     | 0.04                | 0.42       |
| (1,3323) | 1:66:A:LEU:HD22  | 1:66:A:LEU:H     | 17                  | 0.41     | 0.03                | 0.42       |
| (1,3323) | 1:66:A:LEU:HD21  | 1:66:A:LEU:H     | 17                  | 0.41     | 0.03                | 0.42       |
| (1,3323) | 1:66:A:LEU:HD23  | 1:66:A:LEU:H     | 17                  | 0.41     | 0.03                | 0.42       |
| (1,2832) | 1:97:A:LEU:HD23  | 1:97:A:LEU:H     | 17                  | 0.41     | 0.22                | 0.26       |
| (1,2832) | 1:97:A:LEU:HD21  | 1:97:A:LEU:H     | 17                  | 0.41     | 0.22                | 0.26       |
| (1,2832) | 1:97:A:LEU:HD22  | 1:97:A:LEU:H     | 17                  | 0.41     | 0.22                | 0.26       |
| (1,3070) | 1:55:A:ASP:H     | 1:54:A:GLN:HB2   | 17                  | 0.41     | 0.03                | 0.41       |
| (3,72)   | 1:117:A:LEU:HG   | 1:117:A:LEU:H    | 17                  | 0.41     | 0.1                 | 0.47       |
| (1,4138) | 1:31:A:LEU:H     | 1:28:A:ILE:HD12  | 17                  | 0.41     | 0.03                | 0.41       |
| (1,4138) | 1:31:A:LEU:H     | 1:28:A:ILE:HD13  | 17                  | 0.41     | 0.03                | 0.41       |
| (1,4138) | 1:31:A:LEU:H     | 1:28:A:ILE:HD11  | 17                  | 0.41     | 0.03                | 0.41       |
| (1,3386) | 1:90:A:PRO:HA    | 1:92:A:ALA:HB3   | 17                  | 0.41     | 0.07                | 0.39       |
| (1,3386) | 1:90:A:PRO:HA    | 1:92:A:ALA:HB2   | 17                  | 0.41     | 0.07                | 0.39       |
| (1,3386) | 1:90:A:PRO:HA    | 1:92:A:ALA:HB1   | 17                  | 0.41     | 0.07                | 0.39       |
| (1,2785) | 1:50:A:ILE:HG22  | 1:51:A:GLY:HA3   | 17                  | 0.41     | 0.03                | 0.42       |
| (1,2785) | 1:50:A:ILE:HG21  | 1:51:A:GLY:HA3   | 17                  | 0.41     | 0.03                | 0.42       |
| (1,2785) | 1:50:A:ILE:HG23  | 1:51:A:GLY:HA3   | 17                  | 0.41     | 0.03                | 0.42       |
| (1,3002) | 1:57:A:VAL:HG12  | 1:60:A:VAL:HB    | 17                  | 0.41     | 0.06                | 0.4        |
| (1,3002) | 1:57:A:VAL:HG13  | 1:60:A:VAL:HB    | 17                  | 0.41     | 0.06                | 0.4        |
| (1,3002) | 1:57:A:VAL:HG11  | 1:60:A:VAL:HB    | 17                  | 0.41     | 0.06                | 0.4        |
| (1,3286) | 1:116:A:GLN:HG3  | 1:116:A:GLN:HE21 | 17                  | 0.41     | 0.01                | 0.4        |
| (1,2484) | 1:93:A:THR:HB    | 1:95:A:VAL:HG12  | 17                  | 0.41     | 0.07                | 0.39       |
| (1,2484) | 1:93:A:THR:HB    | 1:95:A:VAL:HG11  | 17                  | 0.41     | 0.07                | 0.39       |
| (1,2484) | 1:93:A:THR:HB    | 1:95:A:VAL:HG13  | 17                  | 0.41     | 0.07                | 0.39       |

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| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,2890) | 1:33:A:GLU:HB3   | 1:32:A:ALA:HB2  | 17                  | 0.41     | 0.05                | 0.4        |
| (1,2890) | 1:33:A:GLU:HB3   | 1:32:A:ALA:HB3  | 17                  | 0.41     | 0.05                | 0.4        |
| (1,2890) | 1:33:A:GLU:HB3   | 1:32:A:ALA:HB1  | 17                  | 0.41     | 0.05                | 0.4        |
| (1,3081) | 1:97:A:LEU:HD11  | 1:55:A:ASP:HA   | 17                  | 0.41     | 0.08                | 0.42       |
| (1,3081) | 1:97:A:LEU:HD13  | 1:55:A:ASP:HA   | 17                  | 0.41     | 0.08                | 0.42       |
| (1,3081) | 1:97:A:LEU:HD12  | 1:55:A:ASP:HA   | 17                  | 0.41     | 0.08                | 0.42       |
| (1,1545) | 1:56:A:LEU:HD11  | 1:60:A:VAL:HB   | 17                  | 0.41     | 0.07                | 0.4        |
| (1,1545) | 1:56:A:LEU:HD12  | 1:60:A:VAL:HB   | 17                  | 0.41     | 0.07                | 0.4        |
| (1,1545) | 1:56:A:LEU:HD13  | 1:60:A:VAL:HB   | 17                  | 0.41     | 0.07                | 0.4        |
| (1,3578) | 1:105:A:LEU:HD13 | 1:109:A:HIS:HA  | 17                  | 0.4      | 0.02                | 0.4        |
| (1,3578) | 1:105:A:LEU:HD11 | 1:109:A:HIS:HA  | 17                  | 0.4      | 0.02                | 0.4        |
| (1,3578) | 1:105:A:LEU:HD12 | 1:109:A:HIS:HA  | 17                  | 0.4      | 0.02                | 0.4        |
| (1,3482) | 1:71:A:LEU:HB2   | 1:31:A:LEU:HD12 | 17                  | 0.4      | 0.02                | 0.41       |
| (1,3482) | 1:71:A:LEU:HB2   | 1:31:A:LEU:HD11 | 17                  | 0.4      | 0.02                | 0.41       |
| (1,3482) | 1:71:A:LEU:HB2   | 1:31:A:LEU:HD13 | 17                  | 0.4      | 0.02                | 0.41       |
| (1,3253) | 1:92:A:ALA:HB3   | 1:91:A:GLY:H    | 17                  | 0.4      | 0.08                | 0.42       |
| (1,3253) | 1:92:A:ALA:HB2   | 1:91:A:GLY:H    | 17                  | 0.4      | 0.08                | 0.42       |
| (1,3253) | 1:92:A:ALA:HB1   | 1:91:A:GLY:H    | 17                  | 0.4      | 0.08                | 0.42       |
| (3,69)   | 1:57:A:VAL:HA    | 1:71:A:LEU:HB2  | 17                  | 0.4      | 0.05                | 0.39       |
| (3,147)  | 1:71:A:LEU:H     | 1:66:A:LEU:HD23 | 17                  | 0.4      | 0.04                | 0.39       |
| (3,147)  | 1:71:A:LEU:H     | 1:66:A:LEU:HD22 | 17                  | 0.4      | 0.04                | 0.39       |
| (3,147)  | 1:71:A:LEU:H     | 1:66:A:LEU:HD21 | 17                  | 0.4      | 0.04                | 0.39       |
| (3,139)  | 1:66:A:LEU:HD23  | 1:70:A:GLN:H    | 17                  | 0.4      | 0.03                | 0.39       |
| (3,139)  | 1:66:A:LEU:HD22  | 1:70:A:GLN:H    | 17                  | 0.4      | 0.03                | 0.39       |
| (3,139)  | 1:66:A:LEU:HD21  | 1:70:A:GLN:H    | 17                  | 0.4      | 0.03                | 0.39       |
| (1,3464) | 1:86:A:TYR:HE2   | 1:85:A:LEU:HD13 | 17                  | 0.4      | 0.02                | 0.39       |
| (1,3464) | 1:86:A:TYR:HE1   | 1:85:A:LEU:HD13 | 17                  | 0.4      | 0.02                | 0.39       |
| (1,3464) | 1:86:A:TYR:HE2   | 1:85:A:LEU:HD11 | 17                  | 0.4      | 0.02                | 0.39       |
| (1,3464) | 1:86:A:TYR:HE2   | 1:85:A:LEU:HD12 | 17                  | 0.4      | 0.02                | 0.39       |
| (1,3464) | 1:86:A:TYR:HE1   | 1:85:A:LEU:HD11 | 17                  | 0.4      | 0.02                | 0.39       |
| (1,3464) | 1:86:A:TYR:HE1   | 1:85:A:LEU:HD12 | 17                  | 0.4      | 0.02                | 0.39       |
| (1,825)  | 1:45:A:ALA:HB2   | 1:78:A:TYR:HB3  | 17                  | 0.4      | 0.03                | 0.39       |
| (1,825)  | 1:45:A:ALA:HB1   | 1:78:A:TYR:HB3  | 17                  | 0.4      | 0.03                | 0.39       |
| (1,825)  | 1:45:A:ALA:HB3   | 1:78:A:TYR:HB3  | 17                  | 0.4      | 0.03                | 0.39       |
| (1,3972) | 1:53:A:PHE:H     | 1:56:A:LEU:HB3  | 17                  | 0.4      | 0.06                | 0.39       |
| (1,2614) | 1:30:A:PHE:HD1   | 1:31:A:LEU:HD12 | 17                  | 0.4      | 0.02                | 0.4        |
| (1,2614) | 1:30:A:PHE:HD2   | 1:31:A:LEU:HD12 | 17                  | 0.4      | 0.02                | 0.4        |
| (1,2614) | 1:30:A:PHE:HD2   | 1:31:A:LEU:HD11 | 17                  | 0.4      | 0.02                | 0.4        |
| (1,2614) | 1:30:A:PHE:HD1   | 1:31:A:LEU:HD11 | 17                  | 0.4      | 0.02                | 0.4        |
| (1,2614) | 1:30:A:PHE:HD2   | 1:31:A:LEU:HD13 | 17                  | 0.4      | 0.02                | 0.4        |
| (1,2614) | 1:30:A:PHE:HD1   | 1:31:A:LEU:HD13 | 17                  | 0.4      | 0.02                | 0.4        |
| (1,2190) | 1:61:A:ALA:HB2   | 1:62:A:GLY:HA2  | 17                  | 0.39     | 0.13                | 0.36       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2190) | 1:61:A:ALA:HB3   | 1:62:A:GLY:HA2   | 17                  | 0.39     | 0.13                | 0.36       |
| (1,2190) | 1:61:A:ALA:HB1   | 1:62:A:GLY:HA2   | 17                  | 0.39     | 0.13                | 0.36       |
| (1,3196) | 1:64:A:MET:HB2   | 1:64:A:MET:HA    | 17                  | 0.39     | 0.06                | 0.41       |
| (1,2370) | 1:50:A:ILE:HG13  | 1:50:A:ILE:HG21  | 17                  | 0.39     | 0.04                | 0.4        |
| (1,2370) | 1:50:A:ILE:HG13  | 1:50:A:ILE:HG23  | 17                  | 0.39     | 0.04                | 0.4        |
| (1,2370) | 1:50:A:ILE:HG13  | 1:50:A:ILE:HG22  | 17                  | 0.39     | 0.04                | 0.4        |
| (1,1405) | 1:102:A:CYS:H    | 1:95:A:VAL:HG12  | 17                  | 0.39     | 0.08                | 0.39       |
| (1,1405) | 1:102:A:CYS:H    | 1:95:A:VAL:HG11  | 17                  | 0.39     | 0.08                | 0.39       |
| (1,1405) | 1:102:A:CYS:H    | 1:95:A:VAL:HG13  | 17                  | 0.39     | 0.08                | 0.39       |
| (1,2940) | 1:99:A:GLY:HA3   | 1:95:A:VAL:HG13  | 17                  | 0.39     | 0.04                | 0.39       |
| (1,2940) | 1:99:A:GLY:HA3   | 1:95:A:VAL:HG12  | 17                  | 0.39     | 0.04                | 0.39       |
| (1,2940) | 1:99:A:GLY:HA3   | 1:95:A:VAL:HG11  | 17                  | 0.39     | 0.04                | 0.39       |
| (1,3052) | 1:39:A:PHE:HZ    | 1:52:A:ILE:HG22  | 17                  | 0.39     | 0.13                | 0.46       |
| (1,3052) | 1:39:A:PHE:HZ    | 1:52:A:ILE:HG23  | 17                  | 0.39     | 0.13                | 0.46       |
| (1,3052) | 1:39:A:PHE:HZ    | 1:52:A:ILE:HG21  | 17                  | 0.39     | 0.13                | 0.46       |
| (1,2256) | 1:101:A:PRO:HB2  | 1:105:A:LEU:HD21 | 17                  | 0.38     | 0.02                | 0.39       |
| (1,2256) | 1:101:A:PRO:HB2  | 1:105:A:LEU:HD23 | 17                  | 0.38     | 0.02                | 0.39       |
| (1,2256) | 1:101:A:PRO:HB2  | 1:105:A:LEU:HD22 | 17                  | 0.38     | 0.02                | 0.39       |
| (1,228)  | 1:95:A:VAL:HG23  | 1:100:A:ASN:H    | 17                  | 0.38     | 0.03                | 0.38       |
| (1,228)  | 1:95:A:VAL:HG22  | 1:100:A:ASN:H    | 17                  | 0.38     | 0.03                | 0.38       |
| (1,228)  | 1:95:A:VAL:HG21  | 1:100:A:ASN:H    | 17                  | 0.38     | 0.03                | 0.38       |
| (1,3101) | 1:56:A:LEU:HD13  | 1:53:A:PHE:HA    | 17                  | 0.38     | 0.02                | 0.39       |
| (1,3101) | 1:56:A:LEU:HD11  | 1:53:A:PHE:HA    | 17                  | 0.38     | 0.02                | 0.39       |
| (1,3101) | 1:56:A:LEU:HD12  | 1:53:A:PHE:HA    | 17                  | 0.38     | 0.02                | 0.39       |
| (1,338)  | 1:71:A:LEU:HD13  | 1:72:A:ARG:H     | 17                  | 0.38     | 0.01                | 0.38       |
| (1,338)  | 1:71:A:LEU:HD12  | 1:72:A:ARG:H     | 17                  | 0.38     | 0.01                | 0.38       |
| (1,338)  | 1:71:A:LEU:HD11  | 1:72:A:ARG:H     | 17                  | 0.38     | 0.01                | 0.38       |
| (1,32)   | 1:53:A:PHE:H     | 1:53:A:PHE:HD1   | 17                  | 0.38     | 0.03                | 0.38       |
| (1,32)   | 1:53:A:PHE:H     | 1:53:A:PHE:HD2   | 17                  | 0.38     | 0.03                | 0.38       |
| (1,2196) | 1:107:A:GLU:HA   | 1:110:A:VAL:HG11 | 17                  | 0.38     | 0.02                | 0.38       |
| (1,2196) | 1:107:A:GLU:HA   | 1:110:A:VAL:HG12 | 17                  | 0.38     | 0.02                | 0.38       |
| (1,2196) | 1:107:A:GLU:HA   | 1:110:A:VAL:HG13 | 17                  | 0.38     | 0.02                | 0.38       |
| (1,1516) | 1:31:A:LEU:HD11  | 1:28:A:ILE:HG21  | 17                  | 0.38     | 0.05                | 0.39       |
| (1,1516) | 1:31:A:LEU:HD11  | 1:28:A:ILE:HG23  | 17                  | 0.38     | 0.05                | 0.39       |
| (1,1516) | 1:31:A:LEU:HD13  | 1:28:A:ILE:HG22  | 17                  | 0.38     | 0.05                | 0.39       |
| (1,1516) | 1:31:A:LEU:HD11  | 1:28:A:ILE:HG22  | 17                  | 0.38     | 0.05                | 0.39       |
| (1,1516) | 1:31:A:LEU:HD13  | 1:28:A:ILE:HG23  | 17                  | 0.38     | 0.05                | 0.39       |
| (1,1516) | 1:31:A:LEU:HD12  | 1:28:A:ILE:HG22  | 17                  | 0.38     | 0.05                | 0.39       |
| (1,1516) | 1:31:A:LEU:HD13  | 1:28:A:ILE:HG21  | 17                  | 0.38     | 0.05                | 0.39       |
| (1,263)  | 1:110:A:VAL:HG22 | 1:91:A:GLY:H     | 17                  | 0.38     | 0.14                | 0.39       |
| (1,263)  | 1:110:A:VAL:HG23 | 1:91:A:GLY:H     | 17                  | 0.38     | 0.14                | 0.39       |
| (1,263)  | 1:110:A:VAL:HG21 | 1:91:A:GLY:H     | 17                  | 0.38     | 0.14                | 0.39       |

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| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1481) | 1:64:A:MET:HE2   | 1:30:A:PHE:HA   | 17                  | 0.38     | 0.08                | 0.39       |
| (1,1481) | 1:64:A:MET:HE1   | 1:30:A:PHE:HA   | 17                  | 0.38     | 0.08                | 0.39       |
| (1,1481) | 1:64:A:MET:HE3   | 1:30:A:PHE:HA   | 17                  | 0.38     | 0.08                | 0.39       |
| (1,3612) | 1:120:A:ALA:HB2  | 1:120:A:ALA:HA  | 17                  | 0.38     | 0.04                | 0.39       |
| (1,3612) | 1:120:A:ALA:HB3  | 1:120:A:ALA:HA  | 17                  | 0.38     | 0.04                | 0.39       |
| (1,3612) | 1:120:A:ALA:HB1  | 1:120:A:ALA:HA  | 17                  | 0.38     | 0.04                | 0.39       |
| (1,2841) | 1:110:A:VAL:HG11 | 1:109:A:HIS:H   | 17                  | 0.37     | 0.02                | 0.38       |
| (1,2841) | 1:110:A:VAL:HG12 | 1:109:A:HIS:H   | 17                  | 0.37     | 0.02                | 0.38       |
| (1,2841) | 1:110:A:VAL:HG13 | 1:109:A:HIS:H   | 17                  | 0.37     | 0.02                | 0.38       |
| (1,3067) | 1:52:A:ILE:HG23  | 1:53:A:PHE:HB3  | 17                  | 0.37     | 0.09                | 0.38       |
| (1,3067) | 1:52:A:ILE:HG21  | 1:53:A:PHE:HB3  | 17                  | 0.37     | 0.09                | 0.38       |
| (1,3067) | 1:52:A:ILE:HG22  | 1:53:A:PHE:HB3  | 17                  | 0.37     | 0.09                | 0.38       |
| (1,1322) | 1:28:A:ILE:H     | 1:27:A:VAL:HG13 | 17                  | 0.37     | 0.02                | 0.37       |
| (1,1322) | 1:28:A:ILE:H     | 1:27:A:VAL:HG11 | 17                  | 0.37     | 0.02                | 0.37       |
| (1,1322) | 1:28:A:ILE:H     | 1:27:A:VAL:HG12 | 17                  | 0.37     | 0.02                | 0.37       |
| (1,788)  | 1:52:A:ILE:HD12  | 1:56:A:LEU:H    | 17                  | 0.37     | 0.06                | 0.35       |
| (1,788)  | 1:52:A:ILE:HD13  | 1:56:A:LEU:H    | 17                  | 0.37     | 0.06                | 0.35       |
| (1,788)  | 1:52:A:ILE:HD11  | 1:56:A:LEU:H    | 17                  | 0.37     | 0.06                | 0.35       |
| (1,2873) | 1:126:A:ALA:HA   | 1:126:A:ALA:HB3 | 17                  | 0.37     | 0.05                | 0.37       |
| (1,2873) | 1:126:A:ALA:HA   | 1:126:A:ALA:HB2 | 17                  | 0.37     | 0.05                | 0.37       |
| (1,2873) | 1:126:A:ALA:HA   | 1:126:A:ALA:HB1 | 17                  | 0.37     | 0.05                | 0.37       |
| (1,2163) | 1:78:A:TYR:HA    | 1:78:A:TYR:HD2  | 17                  | 0.37     | 0.04                | 0.36       |
| (1,2163) | 1:78:A:TYR:HA    | 1:78:A:TYR:HD1  | 17                  | 0.37     | 0.04                | 0.36       |
| (1,1484) | 1:57:A:VAL:HA    | 1:71:A:LEU:HD11 | 17                  | 0.37     | 0.03                | 0.36       |
| (1,1484) | 1:57:A:VAL:HA    | 1:71:A:LEU:HD13 | 17                  | 0.37     | 0.03                | 0.36       |
| (1,1484) | 1:57:A:VAL:HA    | 1:71:A:LEU:HD12 | 17                  | 0.37     | 0.03                | 0.36       |
| (1,1398) | 1:88:A:VAL:HG23  | 1:85:A:LEU:H    | 17                  | 0.36     | 0.04                | 0.36       |
| (1,1398) | 1:88:A:VAL:HG22  | 1:85:A:LEU:H    | 17                  | 0.36     | 0.04                | 0.36       |
| (1,1398) | 1:88:A:VAL:HG21  | 1:85:A:LEU:H    | 17                  | 0.36     | 0.04                | 0.36       |
| (1,575)  | 1:31:A:LEU:H     | 1:28:A:ILE:HD12 | 17                  | 0.36     | 0.02                | 0.37       |
| (1,575)  | 1:31:A:LEU:H     | 1:28:A:ILE:HD13 | 17                  | 0.36     | 0.02                | 0.37       |
| (1,575)  | 1:31:A:LEU:H     | 1:28:A:ILE:HD11 | 17                  | 0.36     | 0.02                | 0.37       |
| (1,1490) | 1:78:A:TYR:HH    | 1:45:A:ALA:HB3  | 17                  | 0.36     | 0.07                | 0.36       |
| (1,1490) | 1:78:A:TYR:HH    | 1:45:A:ALA:HB2  | 17                  | 0.36     | 0.07                | 0.36       |
| (1,1490) | 1:78:A:TYR:HH    | 1:45:A:ALA:HB1  | 17                  | 0.36     | 0.07                | 0.36       |
| (1,2863) | 1:78:A:TYR:HE2   | 1:84:A:TYR:HD2  | 17                  | 0.36     | 0.08                | 0.34       |
| (1,2863) | 1:78:A:TYR:HE1   | 1:84:A:TYR:HD2  | 17                  | 0.36     | 0.08                | 0.34       |
| (1,2863) | 1:78:A:TYR:HE1   | 1:84:A:TYR:HD1  | 17                  | 0.36     | 0.08                | 0.34       |
| (1,2863) | 1:78:A:TYR:HE2   | 1:84:A:TYR:HD1  | 17                  | 0.36     | 0.08                | 0.34       |
| (1,2877) | 1:61:A:ALA:HB2   | 1:61:A:ALA:HA   | 17                  | 0.36     | 0.07                | 0.39       |
| (1,2877) | 1:61:A:ALA:HB3   | 1:61:A:ALA:HA   | 17                  | 0.36     | 0.07                | 0.39       |
| (1,2877) | 1:61:A:ALA:HB1   | 1:61:A:ALA:HA   | 17                  | 0.36     | 0.07                | 0.39       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (3,110)  | 1:105:A:LEU:HG   | 1:110:A:VAL:HG21 | 17                  | 0.36     | 0.01                | 0.36       |
| (3,110)  | 1:105:A:LEU:HG   | 1:110:A:VAL:HG22 | 17                  | 0.36     | 0.01                | 0.36       |
| (3,110)  | 1:105:A:LEU:HG   | 1:110:A:VAL:HG23 | 17                  | 0.36     | 0.01                | 0.36       |
| (1,2230) | 1:28:A:ILE:H     | 1:28:A:ILE:HG22  | 17                  | 0.36     | 0.03                | 0.35       |
| (1,2230) | 1:28:A:ILE:H     | 1:28:A:ILE:HG21  | 17                  | 0.36     | 0.03                | 0.35       |
| (1,2230) | 1:28:A:ILE:H     | 1:28:A:ILE:HG23  | 17                  | 0.36     | 0.03                | 0.35       |
| (1,2870) | 1:133:A:ALA:HA   | 1:133:A:ALA:HB1  | 17                  | 0.35     | 0.01                | 0.35       |
| (1,2870) | 1:133:A:ALA:HA   | 1:133:A:ALA:HB3  | 17                  | 0.35     | 0.01                | 0.35       |
| (1,2870) | 1:133:A:ALA:HA   | 1:133:A:ALA:HB2  | 17                  | 0.35     | 0.01                | 0.35       |
| (1,979)  | 1:122:A:ALA:HA   | 1:122:A:ALA:HB1  | 17                  | 0.35     | 0.01                | 0.35       |
| (1,979)  | 1:122:A:ALA:HA   | 1:122:A:ALA:HB2  | 17                  | 0.35     | 0.01                | 0.35       |
| (1,979)  | 1:122:A:ALA:HA   | 1:122:A:ALA:HB3  | 17                  | 0.35     | 0.01                | 0.35       |
| (1,3103) | 1:56:A:LEU:HD11  | 1:60:A:VAL:HB    | 17                  | 0.35     | 0.07                | 0.34       |
| (1,3103) | 1:56:A:LEU:HD12  | 1:60:A:VAL:HB    | 17                  | 0.35     | 0.07                | 0.34       |
| (1,3103) | 1:56:A:LEU:HD13  | 1:60:A:VAL:HB    | 17                  | 0.35     | 0.07                | 0.34       |
| (1,3092) | 1:55:A:ASP:HA    | 1:56:A:LEU:HB3   | 17                  | 0.35     | 0.02                | 0.35       |
| (1,3161) | 1:82:A:TRP:HH2   | 1:120:A:ALA:HB3  | 17                  | 0.35     | 0.05                | 0.35       |
| (1,3161) | 1:82:A:TRP:HH2   | 1:120:A:ALA:HB1  | 17                  | 0.35     | 0.05                | 0.35       |
| (1,3161) | 1:82:A:TRP:HH2   | 1:120:A:ALA:HB2  | 17                  | 0.35     | 0.05                | 0.35       |
| (1,3319) | 1:66:A:LEU:HD21  | 1:27:A:VAL:HG12  | 17                  | 0.35     | 0.04                | 0.34       |
| (1,3319) | 1:66:A:LEU:HD23  | 1:27:A:VAL:HG13  | 17                  | 0.35     | 0.04                | 0.34       |
| (1,3319) | 1:66:A:LEU:HD21  | 1:27:A:VAL:HG13  | 17                  | 0.35     | 0.04                | 0.34       |
| (1,3319) | 1:66:A:LEU:HD22  | 1:27:A:VAL:HG12  | 17                  | 0.35     | 0.04                | 0.34       |
| (1,3319) | 1:66:A:LEU:HD21  | 1:27:A:VAL:HG11  | 17                  | 0.35     | 0.04                | 0.34       |
| (1,3319) | 1:66:A:LEU:HD23  | 1:27:A:VAL:HG12  | 17                  | 0.35     | 0.04                | 0.34       |
| (1,3319) | 1:66:A:LEU:HD22  | 1:27:A:VAL:HG11  | 17                  | 0.35     | 0.04                | 0.34       |
| (1,3077) | 1:54:A:GLN:HB2   | 1:57:A:VAL:HG11  | 17                  | 0.35     | 0.04                | 0.34       |
| (1,3077) | 1:54:A:GLN:HB2   | 1:57:A:VAL:HG12  | 17                  | 0.35     | 0.04                | 0.34       |
| (1,3077) | 1:54:A:GLN:HB2   | 1:57:A:VAL:HG13  | 17                  | 0.35     | 0.04                | 0.34       |
| (1,3590) | 1:110:A:VAL:HG21 | 1:109:A:HIS:HB2  | 17                  | 0.34     | 0.01                | 0.35       |
| (1,3590) | 1:110:A:VAL:HG22 | 1:109:A:HIS:HB2  | 17                  | 0.34     | 0.01                | 0.35       |
| (1,3590) | 1:110:A:VAL:HG23 | 1:109:A:HIS:HB2  | 17                  | 0.34     | 0.01                | 0.35       |
| (1,410)  | 1:53:A:PHE:H     | 1:56:A:LEU:HB3   | 17                  | 0.34     | 0.06                | 0.34       |
| (1,2412) | 1:45:A:ALA:HB2   | 1:78:A:TYR:HB3   | 17                  | 0.34     | 0.03                | 0.34       |
| (1,2412) | 1:45:A:ALA:HB1   | 1:78:A:TYR:HB3   | 17                  | 0.34     | 0.03                | 0.34       |
| (1,2412) | 1:45:A:ALA:HB3   | 1:78:A:TYR:HB3   | 17                  | 0.34     | 0.03                | 0.34       |
| (1,3115) | 1:58:A:ASP:HA    | 1:57:A:VAL:HG21  | 17                  | 0.34     | 0.04                | 0.35       |
| (1,3115) | 1:58:A:ASP:HA    | 1:57:A:VAL:HG23  | 17                  | 0.34     | 0.04                | 0.35       |
| (1,3115) | 1:58:A:ASP:HA    | 1:57:A:VAL:HG22  | 17                  | 0.34     | 0.04                | 0.35       |
| (1,1061) | 1:21:A:LEU:HD23  | 1:27:A:VAL:HG11  | 17                  | 0.34     | 0.05                | 0.35       |
| (1,1061) | 1:21:A:LEU:HD23  | 1:27:A:VAL:HG12  | 17                  | 0.34     | 0.05                | 0.35       |
| (1,1061) | 1:21:A:LEU:HD21  | 1:27:A:VAL:HG12  | 17                  | 0.34     | 0.05                | 0.35       |

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| Key      | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,1061) | 1:21:A:LEU:HD22 | 1:27:A:VAL:HG12  | 17                  | 0.34     | 0.05                | 0.35       |
| (1,1061) | 1:21:A:LEU:HD22 | 1:27:A:VAL:HG11  | 17                  | 0.34     | 0.05                | 0.35       |
| (1,1061) | 1:21:A:LEU:HD23 | 1:27:A:VAL:HG13  | 17                  | 0.34     | 0.05                | 0.35       |
| (1,1061) | 1:21:A:LEU:HD21 | 1:27:A:VAL:HG13  | 17                  | 0.34     | 0.05                | 0.35       |
| (1,2851) | 1:50:A:ILE:HG21 | 1:50:A:ILE:HA    | 17                  | 0.34     | 0.07                | 0.37       |
| (1,2851) | 1:50:A:ILE:HG23 | 1:50:A:ILE:HA    | 17                  | 0.34     | 0.07                | 0.37       |
| (1,2851) | 1:50:A:ILE:HG22 | 1:50:A:ILE:HA    | 17                  | 0.34     | 0.07                | 0.37       |
| (1,909)  | 1:53:A:PHE:HE1  | 1:72:A:ARG:HG3   | 17                  | 0.34     | 0.02                | 0.34       |
| (1,909)  | 1:53:A:PHE:HE2  | 1:72:A:ARG:HG3   | 17                  | 0.34     | 0.02                | 0.34       |
| (1,2720) | 1:86:A:TYR:HB3  | 1:117:A:LEU:HD13 | 17                  | 0.34     | 0.05                | 0.37       |
| (1,2720) | 1:86:A:TYR:HB3  | 1:117:A:LEU:HD11 | 17                  | 0.34     | 0.05                | 0.37       |
| (1,2720) | 1:86:A:TYR:HB3  | 1:117:A:LEU:HD12 | 17                  | 0.34     | 0.05                | 0.37       |
| (1,1408) | 1:57:A:VAL:HG21 | 1:57:A:VAL:HB    | 17                  | 0.34     | 0.03                | 0.34       |
| (1,1408) | 1:57:A:VAL:HG23 | 1:57:A:VAL:HB    | 17                  | 0.34     | 0.03                | 0.34       |
| (1,1408) | 1:57:A:VAL:HG22 | 1:57:A:VAL:HB    | 17                  | 0.34     | 0.03                | 0.34       |
| (1,1400) | 1:95:A:VAL:HG23 | 1:99:A:GLY:H     | 17                  | 0.34     | 0.06                | 0.34       |
| (1,1400) | 1:95:A:VAL:HG22 | 1:99:A:GLY:H     | 17                  | 0.34     | 0.06                | 0.34       |
| (1,1400) | 1:95:A:VAL:HG21 | 1:99:A:GLY:H     | 17                  | 0.34     | 0.06                | 0.34       |
| (1,2830) | 1:39:A:PHE:HZ   | 1:97:A:LEU:HD22  | 17                  | 0.33     | 0.02                | 0.33       |
| (1,2830) | 1:39:A:PHE:HZ   | 1:97:A:LEU:HD23  | 17                  | 0.33     | 0.02                | 0.33       |
| (1,2830) | 1:39:A:PHE:HZ   | 1:97:A:LEU:HD21  | 17                  | 0.33     | 0.02                | 0.33       |
| (1,1741) | 1:55:A:ASP:HB2  | 1:56:A:LEU:HD22  | 17                  | 0.33     | 0.06                | 0.36       |
| (1,1741) | 1:55:A:ASP:HB2  | 1:56:A:LEU:HD21  | 17                  | 0.33     | 0.06                | 0.36       |
| (1,1741) | 1:55:A:ASP:HB2  | 1:56:A:LEU:HD23  | 17                  | 0.33     | 0.06                | 0.36       |
| (1,3061) | 1:31:A:LEU:HD11 | 1:28:A:ILE:HG21  | 17                  | 0.33     | 0.05                | 0.35       |
| (1,3061) | 1:31:A:LEU:HD11 | 1:28:A:ILE:HG23  | 17                  | 0.33     | 0.05                | 0.35       |
| (1,3061) | 1:31:A:LEU:HD13 | 1:28:A:ILE:HG22  | 17                  | 0.33     | 0.05                | 0.35       |
| (1,3061) | 1:31:A:LEU:HD11 | 1:28:A:ILE:HG22  | 17                  | 0.33     | 0.05                | 0.35       |
| (1,3061) | 1:31:A:LEU:HD13 | 1:28:A:ILE:HG23  | 17                  | 0.33     | 0.05                | 0.35       |
| (1,3061) | 1:31:A:LEU:HD12 | 1:28:A:ILE:HG22  | 17                  | 0.33     | 0.05                | 0.35       |
| (1,3061) | 1:31:A:LEU:HD13 | 1:28:A:ILE:HG21  | 17                  | 0.33     | 0.05                | 0.35       |
| (1,1124) | 1:97:A:LEU:HD12 | 1:57:A:VAL:H     | 17                  | 0.33     | 0.04                | 0.35       |
| (1,1124) | 1:97:A:LEU:HD11 | 1:57:A:VAL:H     | 17                  | 0.33     | 0.04                | 0.35       |
| (1,1124) | 1:97:A:LEU:HD13 | 1:57:A:VAL:H     | 17                  | 0.33     | 0.04                | 0.35       |
| (1,3027) | 1:57:A:VAL:HA   | 1:71:A:LEU:HD11  | 17                  | 0.33     | 0.03                | 0.33       |
| (1,3027) | 1:57:A:VAL:HA   | 1:71:A:LEU:HD13  | 17                  | 0.33     | 0.03                | 0.33       |
| (1,3027) | 1:57:A:VAL:HA   | 1:71:A:LEU:HD12  | 17                  | 0.33     | 0.03                | 0.33       |
| (1,1656) | 1:31:A:LEU:HB2  | 1:39:A:PHE:HE2   | 17                  | 0.33     | 0.04                | 0.32       |
| (1,1656) | 1:31:A:LEU:HB2  | 1:39:A:PHE:HE1   | 17                  | 0.33     | 0.04                | 0.32       |
| (1,2842) | 1:28:A:ILE:H    | 1:27:A:VAL:HG13  | 17                  | 0.33     | 0.02                | 0.33       |
| (1,2842) | 1:28:A:ILE:H    | 1:27:A:VAL:HG11  | 17                  | 0.33     | 0.02                | 0.33       |
| (1,2842) | 1:28:A:ILE:H    | 1:27:A:VAL:HG12  | 17                  | 0.33     | 0.02                | 0.33       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,3606) | 1:117:A:LEU:HA   | 1:82:A:TRP:HZ2   | 17                  | 0.33     | 0.04                | 0.32       |
| (1,3738) | 1:103:A:GLY:HA3  | 1:104:A:GLU:H    | 17                  | 0.33     | 0.02                | 0.33       |
| (1,4300) | 1:92:A:ALA:H     | 1:105:A:LEU:HD21 | 17                  | 0.33     | 0.07                | 0.32       |
| (1,4300) | 1:92:A:ALA:H     | 1:105:A:LEU:HD23 | 17                  | 0.33     | 0.07                | 0.32       |
| (1,4300) | 1:92:A:ALA:H     | 1:105:A:LEU:HD22 | 17                  | 0.33     | 0.07                | 0.32       |
| (1,1231) | 1:97:A:LEU:HD13  | 1:59:A:ARG:HD3   | 17                  | 0.33     | 0.06                | 0.33       |
| (1,1231) | 1:97:A:LEU:HD11  | 1:59:A:ARG:HD3   | 17                  | 0.33     | 0.06                | 0.33       |
| (1,1231) | 1:97:A:LEU:HD12  | 1:59:A:ARG:HD3   | 17                  | 0.33     | 0.06                | 0.33       |
| (1,3022) | 1:64:A:MET:HE2   | 1:30:A:PHE:HA    | 17                  | 0.33     | 0.08                | 0.34       |
| (1,3022) | 1:64:A:MET:HE1   | 1:30:A:PHE:HA    | 17                  | 0.33     | 0.08                | 0.34       |
| (1,3022) | 1:64:A:MET:HE3   | 1:30:A:PHE:HA    | 17                  | 0.33     | 0.08                | 0.34       |
| (1,3198) | 1:114:A:ARG:HA   | 1:113:A:ALA:HB1  | 17                  | 0.33     | 0.03                | 0.33       |
| (1,3198) | 1:114:A:ARG:HA   | 1:113:A:ALA:HB3  | 17                  | 0.33     | 0.03                | 0.33       |
| (1,3198) | 1:114:A:ARG:HA   | 1:113:A:ALA:HB2  | 17                  | 0.33     | 0.03                | 0.33       |
| (1,2513) | 1:122:A:ALA:HA   | 1:122:A:ALA:HB1  | 17                  | 0.33     | 0.01                | 0.33       |
| (1,2513) | 1:122:A:ALA:HA   | 1:122:A:ALA:HB2  | 17                  | 0.33     | 0.01                | 0.33       |
| (1,2513) | 1:122:A:ALA:HA   | 1:122:A:ALA:HB3  | 17                  | 0.33     | 0.01                | 0.33       |
| (1,1686) | 1:85:A:LEU:HD13  | 1:85:A:LEU:HD22  | 17                  | 0.32     | 0.07                | 0.32       |
| (1,1686) | 1:85:A:LEU:HD11  | 1:85:A:LEU:HD22  | 17                  | 0.32     | 0.07                | 0.32       |
| (1,1686) | 1:85:A:LEU:HD13  | 1:85:A:LEU:HD23  | 17                  | 0.32     | 0.07                | 0.32       |
| (1,1686) | 1:85:A:LEU:HD12  | 1:85:A:LEU:HD21  | 17                  | 0.32     | 0.07                | 0.32       |
| (1,1686) | 1:85:A:LEU:HD11  | 1:85:A:LEU:HD21  | 17                  | 0.32     | 0.07                | 0.32       |
| (1,1686) | 1:85:A:LEU:HD11  | 1:85:A:LEU:HD23  | 17                  | 0.32     | 0.07                | 0.32       |
| (1,1686) | 1:85:A:LEU:HD13  | 1:85:A:LEU:HD21  | 17                  | 0.32     | 0.07                | 0.32       |
| (1,1686) | 1:85:A:LEU:HD12  | 1:85:A:LEU:HD23  | 17                  | 0.32     | 0.07                | 0.32       |
| (1,1686) | 1:85:A:LEU:HD12  | 1:85:A:LEU:HD22  | 17                  | 0.32     | 0.07                | 0.32       |
| (1,1879) | 1:124:A:VAL:HG13 | 1:124:A:VAL:HG23 | 17                  | 0.32     | 0.02                | 0.32       |
| (1,1879) | 1:124:A:VAL:HG12 | 1:124:A:VAL:HG21 | 17                  | 0.32     | 0.02                | 0.32       |
| (1,1879) | 1:124:A:VAL:HG11 | 1:124:A:VAL:HG22 | 17                  | 0.32     | 0.02                | 0.32       |
| (1,1879) | 1:124:A:VAL:HG13 | 1:124:A:VAL:HG21 | 17                  | 0.32     | 0.02                | 0.32       |
| (1,1879) | 1:124:A:VAL:HG11 | 1:124:A:VAL:HG21 | 17                  | 0.32     | 0.02                | 0.32       |
| (1,1879) | 1:124:A:VAL:HG11 | 1:124:A:VAL:HG23 | 17                  | 0.32     | 0.02                | 0.32       |
| (1,1879) | 1:124:A:VAL:HG12 | 1:124:A:VAL:HG22 | 17                  | 0.32     | 0.02                | 0.32       |
| (1,1879) | 1:124:A:VAL:HG12 | 1:124:A:VAL:HG23 | 17                  | 0.32     | 0.02                | 0.32       |
| (1,2350) | 1:110:A:VAL:HG21 | 1:110:A:VAL:HA   | 17                  | 0.32     | 0.01                | 0.32       |
| (1,2350) | 1:110:A:VAL:HG22 | 1:110:A:VAL:HA   | 17                  | 0.32     | 0.01                | 0.32       |
| (1,2350) | 1:110:A:VAL:HG23 | 1:110:A:VAL:HA   | 17                  | 0.32     | 0.01                | 0.32       |
| (1,3564) | 1:105:A:LEU:HB3  | 1:104:A:GLU:HG2  | 17                  | 0.32     | 0.02                | 0.32       |
| (1,3678) | 1:95:A:VAL:H     | 1:96:A:ASP:H     | 17                  | 0.32     | 0.05                | 0.32       |
| (1,2369) | 1:52:A:ILE:HD12  | 1:56:A:LEU:H     | 17                  | 0.32     | 0.06                | 0.3        |
| (1,2369) | 1:52:A:ILE:HD13  | 1:56:A:LEU:H     | 17                  | 0.32     | 0.06                | 0.3        |
| (1,2369) | 1:52:A:ILE:HD11  | 1:56:A:LEU:H     | 17                  | 0.32     | 0.06                | 0.3        |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,3402) | 1:58:A:ASP:H     | 1:55:A:ASP:HA    | 17                  | 0.32     | 0.02                | 0.32       |
| (1,4210) | 1:110:A:VAL:HG12 | 1:113:A:ALA:H    | 17                  | 0.32     | 0.01                | 0.32       |
| (1,4210) | 1:110:A:VAL:HG13 | 1:113:A:ALA:H    | 17                  | 0.32     | 0.01                | 0.32       |
| (1,4210) | 1:110:A:VAL:HG11 | 1:113:A:ALA:H    | 17                  | 0.32     | 0.01                | 0.32       |
| (1,2694) | 1:73:A:SER:HB2   | 1:74:A:ALA:H     | 17                  | 0.32     | 0.09                | 0.38       |
| (1,3427) | 1:117:A:LEU:HA   | 1:117:A:LEU:H    | 17                  | 0.32     | 0.02                | 0.33       |
| (1,2418) | 1:113:A:ALA:HB2  | 1:110:A:VAL:HG12 | 17                  | 0.32     | 0.03                | 0.32       |
| (1,2418) | 1:113:A:ALA:HB2  | 1:110:A:VAL:HG13 | 17                  | 0.32     | 0.03                | 0.32       |
| (1,2418) | 1:113:A:ALA:HB1  | 1:110:A:VAL:HG11 | 17                  | 0.32     | 0.03                | 0.32       |
| (1,2418) | 1:113:A:ALA:HB2  | 1:110:A:VAL:HG11 | 17                  | 0.32     | 0.03                | 0.32       |
| (1,2418) | 1:113:A:ALA:HB3  | 1:110:A:VAL:HG12 | 17                  | 0.32     | 0.03                | 0.32       |
| (1,2418) | 1:113:A:ALA:HB1  | 1:110:A:VAL:HG13 | 17                  | 0.32     | 0.03                | 0.32       |
| (1,2418) | 1:113:A:ALA:HB1  | 1:110:A:VAL:HG12 | 17                  | 0.32     | 0.03                | 0.32       |
| (1,2418) | 1:113:A:ALA:HB3  | 1:110:A:VAL:HG11 | 17                  | 0.32     | 0.03                | 0.32       |
| (1,1110) | 1:77:A:LEU:HD22  | 1:77:A:LEU:HB2   | 17                  | 0.32     | 0.01                | 0.32       |
| (1,1110) | 1:77:A:LEU:HD23  | 1:77:A:LEU:HB2   | 17                  | 0.32     | 0.01                | 0.32       |
| (1,1110) | 1:77:A:LEU:HD21  | 1:77:A:LEU:HB2   | 17                  | 0.32     | 0.01                | 0.32       |
| (1,2931) | 1:88:A:VAL:HG23  | 1:85:A:LEU:H     | 17                  | 0.32     | 0.04                | 0.32       |
| (1,2931) | 1:88:A:VAL:HG22  | 1:85:A:LEU:H     | 17                  | 0.32     | 0.04                | 0.32       |
| (1,2931) | 1:88:A:VAL:HG21  | 1:85:A:LEU:H     | 17                  | 0.32     | 0.04                | 0.32       |
| (1,1304) | 1:97:A:LEU:HD21  | 1:56:A:LEU:HA    | 17                  | 0.32     | 0.03                | 0.32       |
| (1,1304) | 1:97:A:LEU:HD22  | 1:56:A:LEU:HA    | 17                  | 0.32     | 0.03                | 0.32       |
| (1,1304) | 1:97:A:LEU:HD23  | 1:56:A:LEU:HA    | 17                  | 0.32     | 0.03                | 0.32       |
| (1,3584) | 1:110:A:VAL:HA   | 1:105:A:LEU:HD22 | 17                  | 0.32     | 0.01                | 0.32       |
| (1,3584) | 1:110:A:VAL:HA   | 1:105:A:LEU:HD21 | 17                  | 0.32     | 0.01                | 0.32       |
| (1,3584) | 1:110:A:VAL:HA   | 1:105:A:LEU:HD23 | 17                  | 0.32     | 0.01                | 0.32       |
| (1,1375) | 1:110:A:VAL:HG13 | 1:91:A:GLY:HA2   | 17                  | 0.31     | 0.02                | 0.32       |
| (1,1375) | 1:110:A:VAL:HG11 | 1:91:A:GLY:HA2   | 17                  | 0.31     | 0.02                | 0.32       |
| (1,1375) | 1:110:A:VAL:HG12 | 1:91:A:GLY:HA2   | 17                  | 0.31     | 0.02                | 0.32       |
| (1,1870) | 1:86:A:TYR:HE2   | 1:85:A:LEU:HD22  | 17                  | 0.31     | 0.02                | 0.31       |
| (1,1870) | 1:86:A:TYR:HE1   | 1:85:A:LEU:HD22  | 17                  | 0.31     | 0.02                | 0.31       |
| (1,1870) | 1:86:A:TYR:HE1   | 1:85:A:LEU:HD23  | 17                  | 0.31     | 0.02                | 0.31       |
| (1,1870) | 1:86:A:TYR:HE2   | 1:85:A:LEU:HD21  | 17                  | 0.31     | 0.02                | 0.31       |
| (1,1870) | 1:86:A:TYR:HE1   | 1:85:A:LEU:HD21  | 17                  | 0.31     | 0.02                | 0.31       |
| (1,2942) | 1:57:A:VAL:HG21  | 1:57:A:VAL:HB    | 17                  | 0.31     | 0.03                | 0.32       |
| (1,2942) | 1:57:A:VAL:HG23  | 1:57:A:VAL:HB    | 17                  | 0.31     | 0.03                | 0.32       |
| (1,2942) | 1:57:A:VAL:HG22  | 1:57:A:VAL:HB    | 17                  | 0.31     | 0.03                | 0.32       |
| (1,3114) | 1:57:A:VAL:HG22  | 1:57:A:VAL:HG11  | 17                  | 0.31     | 0.03                | 0.32       |
| (1,3114) | 1:57:A:VAL:HG21  | 1:57:A:VAL:HG11  | 17                  | 0.31     | 0.03                | 0.32       |
| (1,3114) | 1:57:A:VAL:HG23  | 1:57:A:VAL:HG11  | 17                  | 0.31     | 0.03                | 0.32       |
| (1,3114) | 1:57:A:VAL:HG21  | 1:57:A:VAL:HG12  | 17                  | 0.31     | 0.03                | 0.32       |
| (1,3114) | 1:57:A:VAL:HG23  | 1:57:A:VAL:HG13  | 17                  | 0.31     | 0.03                | 0.32       |

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| Key      | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,3114) | 1:57:A:VAL:HG22 | 1:57:A:VAL:HG12  | 17                  | 0.31     | 0.03                | 0.32       |
| (1,3114) | 1:57:A:VAL:HG23 | 1:57:A:VAL:HG12  | 17                  | 0.31     | 0.03                | 0.32       |
| (1,3114) | 1:57:A:VAL:HG22 | 1:57:A:VAL:HG13  | 17                  | 0.31     | 0.03                | 0.32       |
| (1,4342) | 1:38:A:CYS:H    | 1:95:A:VAL:HG11  | 17                  | 0.31     | 0.09                | 0.31       |
| (1,4342) | 1:38:A:CYS:H    | 1:95:A:VAL:HG12  | 17                  | 0.31     | 0.09                | 0.31       |
| (1,4342) | 1:38:A:CYS:H    | 1:95:A:VAL:HG13  | 17                  | 0.31     | 0.09                | 0.31       |
| (1,2597) | 1:21:A:LEU:HD23 | 1:27:A:VAL:HG11  | 17                  | 0.31     | 0.05                | 0.32       |
| (1,2597) | 1:21:A:LEU:HD23 | 1:27:A:VAL:HG12  | 17                  | 0.31     | 0.05                | 0.32       |
| (1,2597) | 1:21:A:LEU:HD21 | 1:27:A:VAL:HG12  | 17                  | 0.31     | 0.05                | 0.32       |
| (1,2597) | 1:21:A:LEU:HD22 | 1:27:A:VAL:HG12  | 17                  | 0.31     | 0.05                | 0.32       |
| (1,2597) | 1:21:A:LEU:HD22 | 1:27:A:VAL:HG11  | 17                  | 0.31     | 0.05                | 0.32       |
| (1,2597) | 1:21:A:LEU:HD23 | 1:27:A:VAL:HG13  | 17                  | 0.31     | 0.05                | 0.32       |
| (1,2597) | 1:21:A:LEU:HD21 | 1:27:A:VAL:HG13  | 17                  | 0.31     | 0.05                | 0.32       |
| (1,2344) | 1:104:A:GLU:HG2 | 1:105:A:LEU:HD21 | 17                  | 0.31     | 0.03                | 0.3        |
| (1,2344) | 1:104:A:GLU:HG2 | 1:105:A:LEU:HD23 | 17                  | 0.31     | 0.03                | 0.3        |
| (1,2344) | 1:104:A:GLU:HG2 | 1:105:A:LEU:HD22 | 17                  | 0.31     | 0.03                | 0.3        |
| (1,3733) | 1:27:A:VAL:HG13 | 1:26:A:GLU:H     | 17                  | 0.31     | 0.07                | 0.3        |
| (1,3733) | 1:27:A:VAL:HG12 | 1:26:A:GLU:H     | 17                  | 0.31     | 0.07                | 0.3        |
| (1,3733) | 1:27:A:VAL:HG11 | 1:26:A:GLU:H     | 17                  | 0.31     | 0.07                | 0.3        |
| (1,2036) | 1:97:A:LEU:HD21 | 1:97:A:LEU:HB2   | 17                  | 0.31     | 0.03                | 0.32       |
| (1,2036) | 1:97:A:LEU:HD22 | 1:97:A:LEU:HB2   | 17                  | 0.31     | 0.03                | 0.32       |
| (1,2036) | 1:97:A:LEU:HD23 | 1:97:A:LEU:HB2   | 17                  | 0.31     | 0.03                | 0.32       |
| (1,3036) | 1:78:A:TYR:HH   | 1:45:A:ALA:HB3   | 17                  | 0.31     | 0.07                | 0.3        |
| (1,3036) | 1:78:A:TYR:HH   | 1:45:A:ALA:HB2   | 17                  | 0.31     | 0.07                | 0.3        |
| (1,3036) | 1:78:A:TYR:HH   | 1:45:A:ALA:HB1   | 17                  | 0.31     | 0.07                | 0.3        |
| (1,4255) | 1:75:A:LEU:HD23 | 1:54:A:GLN:H     | 17                  | 0.31     | 0.02                | 0.3        |
| (1,4255) | 1:75:A:LEU:HD22 | 1:54:A:GLN:H     | 17                  | 0.31     | 0.02                | 0.3        |
| (1,4255) | 1:75:A:LEU:HD21 | 1:54:A:GLN:H     | 17                  | 0.31     | 0.02                | 0.3        |
| (3,143)  | 1:25:A:LYS:H    | 1:77:A:LEU:HD22  | 17                  | 0.31     | 0.1                 | 0.31       |
| (3,143)  | 1:25:A:LYS:H    | 1:77:A:LEU:HD23  | 17                  | 0.31     | 0.1                 | 0.31       |
| (3,143)  | 1:25:A:LYS:H    | 1:77:A:LEU:HD21  | 17                  | 0.31     | 0.1                 | 0.31       |
| (1,2331) | 1:54:A:GLN:HG2  | 1:55:A:ASP:HA    | 17                  | 0.31     | 0.02                | 0.31       |
| (3,135)  | 1:123:A:ARG:HB3 | 1:120:A:ALA:HA   | 17                  | 0.3      | 0.07                | 0.31       |
| (1,1903) | 1:122:A:ALA:HB3 | 1:121:A:LYS:HE3  | 17                  | 0.3      | 0.02                | 0.3        |
| (1,1903) | 1:122:A:ALA:HB1 | 1:121:A:LYS:HE3  | 17                  | 0.3      | 0.02                | 0.3        |
| (1,1903) | 1:122:A:ALA:HB2 | 1:121:A:LYS:HE3  | 17                  | 0.3      | 0.02                | 0.3        |
| (1,3732) | 1:21:A:LEU:HD12 | 1:30:A:PHE:H     | 17                  | 0.3      | 0.07                | 0.34       |
| (1,3732) | 1:21:A:LEU:HD13 | 1:30:A:PHE:H     | 17                  | 0.3      | 0.07                | 0.34       |
| (1,3732) | 1:21:A:LEU:HD11 | 1:30:A:PHE:H     | 17                  | 0.3      | 0.07                | 0.34       |
| (1,3266) | 1:85:A:LEU:HD13 | 1:85:A:LEU:HD22  | 17                  | 0.3      | 0.07                | 0.29       |
| (1,3266) | 1:85:A:LEU:HD11 | 1:85:A:LEU:HD22  | 17                  | 0.3      | 0.07                | 0.29       |
| (1,3266) | 1:85:A:LEU:HD13 | 1:85:A:LEU:HD23  | 17                  | 0.3      | 0.07                | 0.29       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,3266) | 1:85:A:LEU:HD12  | 1:85:A:LEU:HD21  | 17                  | 0.3      | 0.07                | 0.29       |
| (1,3266) | 1:85:A:LEU:HD11  | 1:85:A:LEU:HD21  | 17                  | 0.3      | 0.07                | 0.29       |
| (1,3266) | 1:85:A:LEU:HD11  | 1:85:A:LEU:HD23  | 17                  | 0.3      | 0.07                | 0.29       |
| (1,3266) | 1:85:A:LEU:HD13  | 1:85:A:LEU:HD21  | 17                  | 0.3      | 0.07                | 0.29       |
| (1,3266) | 1:85:A:LEU:HD12  | 1:85:A:LEU:HD23  | 17                  | 0.3      | 0.07                | 0.29       |
| (1,3266) | 1:85:A:LEU:HD12  | 1:85:A:LEU:HD22  | 17                  | 0.3      | 0.07                | 0.29       |
| (1,3495) | 1:54:A:GLN:H     | 1:75:A:LEU:HD13  | 17                  | 0.3      | 0.02                | 0.3        |
| (1,3495) | 1:54:A:GLN:H     | 1:75:A:LEU:HD11  | 17                  | 0.3      | 0.02                | 0.3        |
| (1,3495) | 1:54:A:GLN:H     | 1:75:A:LEU:HD12  | 17                  | 0.3      | 0.02                | 0.3        |
| (1,3189) | 1:110:A:VAL:HA   | 1:105:A:LEU:HD13 | 17                  | 0.3      | 0.01                | 0.3        |
| (1,3189) | 1:110:A:VAL:HA   | 1:105:A:LEU:HD11 | 17                  | 0.3      | 0.01                | 0.3        |
| (1,3189) | 1:110:A:VAL:HA   | 1:105:A:LEU:HD12 | 17                  | 0.3      | 0.01                | 0.3        |
| (1,3505) | 1:124:A:VAL:HG13 | 1:124:A:VAL:HG23 | 17                  | 0.3      | 0.02                | 0.3        |
| (1,3505) | 1:124:A:VAL:HG12 | 1:124:A:VAL:HG21 | 17                  | 0.3      | 0.02                | 0.3        |
| (1,3505) | 1:124:A:VAL:HG11 | 1:124:A:VAL:HG22 | 17                  | 0.3      | 0.02                | 0.3        |
| (1,3505) | 1:124:A:VAL:HG13 | 1:124:A:VAL:HG21 | 17                  | 0.3      | 0.02                | 0.3        |
| (1,3505) | 1:124:A:VAL:HG11 | 1:124:A:VAL:HG21 | 17                  | 0.3      | 0.02                | 0.3        |
| (1,3505) | 1:124:A:VAL:HG11 | 1:124:A:VAL:HG23 | 17                  | 0.3      | 0.02                | 0.3        |
| (1,3505) | 1:124:A:VAL:HG12 | 1:124:A:VAL:HG22 | 17                  | 0.3      | 0.02                | 0.3        |
| (1,3505) | 1:124:A:VAL:HG12 | 1:124:A:VAL:HG23 | 17                  | 0.3      | 0.02                | 0.3        |
| (1,4114) | 1:65:A:ASN:H     | 1:65:A:ASN:HD21  | 17                  | 0.3      | 0.06                | 0.29       |
| (1,3728) | 1:29:A:ALA:HA    | 1:30:A:PHE:H     | 17                  | 0.3      | 0.02                | 0.3        |
| (1,2367) | 1:52:A:ILE:H     | 1:52:A:ILE:HD13  | 17                  | 0.3      | 0.1                 | 0.33       |
| (1,2367) | 1:52:A:ILE:H     | 1:52:A:ILE:HD11  | 17                  | 0.3      | 0.1                 | 0.33       |
| (1,2367) | 1:52:A:ILE:H     | 1:52:A:ILE:HD12  | 17                  | 0.3      | 0.1                 | 0.33       |
| (1,1048) | 1:124:A:VAL:HG21 | 1:120:A:ALA:HA   | 17                  | 0.3      | 0.02                | 0.29       |
| (1,1048) | 1:124:A:VAL:HG22 | 1:120:A:ALA:HA   | 17                  | 0.3      | 0.02                | 0.29       |
| (1,1048) | 1:124:A:VAL:HG23 | 1:120:A:ALA:HA   | 17                  | 0.3      | 0.02                | 0.29       |
| (1,1307) | 1:97:A:LEU:HD21  | 1:97:A:LEU:HB2   | 17                  | 0.3      | 0.03                | 0.31       |
| (1,1307) | 1:97:A:LEU:HD22  | 1:97:A:LEU:HB2   | 17                  | 0.3      | 0.03                | 0.31       |
| (1,1307) | 1:97:A:LEU:HD23  | 1:97:A:LEU:HB2   | 17                  | 0.3      | 0.03                | 0.31       |
| (1,3741) | 1:28:A:ILE:HG13  | 1:28:A:ILE:H     | 17                  | 0.3      | 0.01                | 0.3        |
| (1,3889) | 1:100:A:ASN:HB3  | 1:100:A:ASN:HD21 | 17                  | 0.3      | 0.01                | 0.29       |
| (1,2753) | 1:97:A:LEU:HD13  | 1:59:A:ARG:HD3   | 17                  | 0.3      | 0.06                | 0.3        |
| (1,2753) | 1:97:A:LEU:HD11  | 1:59:A:ARG:HD3   | 17                  | 0.3      | 0.06                | 0.3        |
| (1,2753) | 1:97:A:LEU:HD12  | 1:59:A:ARG:HD3   | 17                  | 0.3      | 0.06                | 0.3        |
| (1,1955) | 1:92:A:ALA:HB1   | 1:113:A:ALA:HB3  | 17                  | 0.29     | 0.1                 | 0.31       |
| (1,1955) | 1:92:A:ALA:HB3   | 1:113:A:ALA:HB3  | 17                  | 0.29     | 0.1                 | 0.31       |
| (1,1955) | 1:92:A:ALA:HB3   | 1:113:A:ALA:HB1  | 17                  | 0.29     | 0.1                 | 0.31       |
| (1,1955) | 1:92:A:ALA:HB2   | 1:113:A:ALA:HB1  | 17                  | 0.29     | 0.1                 | 0.31       |
| (1,1955) | 1:92:A:ALA:HB2   | 1:113:A:ALA:HB2  | 17                  | 0.29     | 0.1                 | 0.31       |
| (1,1955) | 1:92:A:ALA:HB1   | 1:113:A:ALA:HB1  | 17                  | 0.29     | 0.1                 | 0.31       |

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| Key      | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,1955) | 1:92:A:ALA:HB1  | 1:113:A:ALA:HB2  | 17                  | 0.29     | 0.1                 | 0.31       |
| (1,4230) | 1:128:A:ARG:HA  | 1:128:A:ARG:H    | 17                  | 0.29     | 0.02                | 0.29       |
| (1,3264) | 1:121:A:LYS:HG2 | 1:121:A:LYS:H    | 17                  | 0.29     | 0.05                | 0.31       |
| (1,2098) | 1:21:A:LEU:HD23 | 1:27:A:VAL:HG11  | 17                  | 0.29     | 0.05                | 0.3        |
| (1,2098) | 1:21:A:LEU:HD23 | 1:27:A:VAL:HG12  | 17                  | 0.29     | 0.05                | 0.3        |
| (1,2098) | 1:21:A:LEU:HD21 | 1:27:A:VAL:HG12  | 17                  | 0.29     | 0.05                | 0.3        |
| (1,2098) | 1:21:A:LEU:HD22 | 1:27:A:VAL:HG12  | 17                  | 0.29     | 0.05                | 0.3        |
| (1,2098) | 1:21:A:LEU:HD22 | 1:27:A:VAL:HG11  | 17                  | 0.29     | 0.05                | 0.3        |
| (1,2098) | 1:21:A:LEU:HD23 | 1:27:A:VAL:HG13  | 17                  | 0.29     | 0.05                | 0.3        |
| (1,2098) | 1:21:A:LEU:HD21 | 1:27:A:VAL:HG13  | 17                  | 0.29     | 0.05                | 0.3        |
| (1,2650) | 1:77:A:LEU:HD22 | 1:77:A:LEU:HB2   | 17                  | 0.29     | 0.01                | 0.29       |
| (1,2650) | 1:77:A:LEU:HD23 | 1:77:A:LEU:HB2   | 17                  | 0.29     | 0.01                | 0.29       |
| (1,2650) | 1:77:A:LEU:HD21 | 1:77:A:LEU:HB2   | 17                  | 0.29     | 0.01                | 0.29       |
| (1,2468) | 1:53:A:PHE:HE1  | 1:72:A:ARG:HG3   | 17                  | 0.29     | 0.02                | 0.29       |
| (1,2468) | 1:53:A:PHE:HE2  | 1:72:A:ARG:HG3   | 17                  | 0.29     | 0.02                | 0.29       |
| (1,2502) | 1:42:A:GLU:HA   | 1:43:A:GLY:H     | 17                  | 0.29     | 0.03                | 0.29       |
| (1,532)  | 1:116:A:GLN:HG3 | 1:116:A:GLN:HE21 | 17                  | 0.29     | 0.01                | 0.29       |
| (1,1060) | 1:74:A:ALA:HB1  | 1:27:A:VAL:HG13  | 17                  | 0.29     | 0.03                | 0.3        |
| (1,1060) | 1:74:A:ALA:HB1  | 1:27:A:VAL:HG11  | 17                  | 0.29     | 0.03                | 0.3        |
| (1,1060) | 1:74:A:ALA:HB2  | 1:27:A:VAL:HG11  | 17                  | 0.29     | 0.03                | 0.3        |
| (1,1060) | 1:74:A:ALA:HB3  | 1:27:A:VAL:HG11  | 17                  | 0.29     | 0.03                | 0.3        |
| (1,1060) | 1:74:A:ALA:HB3  | 1:27:A:VAL:HG13  | 17                  | 0.29     | 0.03                | 0.3        |
| (1,1060) | 1:74:A:ALA:HB3  | 1:27:A:VAL:HG12  | 17                  | 0.29     | 0.03                | 0.3        |
| (3,16)   | 1:90:A:PRO:HA   | 1:110:A:VAL:HG12 | 17                  | 0.29     | 0.07                | 0.28       |
| (3,16)   | 1:90:A:PRO:HA   | 1:110:A:VAL:HG13 | 17                  | 0.29     | 0.07                | 0.28       |
| (3,16)   | 1:90:A:PRO:HA   | 1:110:A:VAL:HG11 | 17                  | 0.29     | 0.07                | 0.28       |
| (1,1945) | 1:105:A:LEU:HB3 | 1:110:A:VAL:HG21 | 17                  | 0.29     | 0.02                | 0.29       |
| (1,1945) | 1:105:A:LEU:HB3 | 1:110:A:VAL:HG22 | 17                  | 0.29     | 0.02                | 0.29       |
| (1,1945) | 1:105:A:LEU:HB3 | 1:110:A:VAL:HG23 | 17                  | 0.29     | 0.02                | 0.29       |
| (1,1485) | 1:71:A:LEU:HD13 | 1:72:A:ARG:HA    | 17                  | 0.29     | 0.02                | 0.29       |
| (1,1485) | 1:71:A:LEU:HD12 | 1:72:A:ARG:HA    | 17                  | 0.29     | 0.02                | 0.29       |
| (1,1485) | 1:71:A:LEU:HD11 | 1:72:A:ARG:HA    | 17                  | 0.29     | 0.02                | 0.29       |
| (1,1081) | 1:71:A:LEU:HD12 | 1:57:A:VAL:H     | 17                  | 0.29     | 0.05                | 0.27       |
| (1,1081) | 1:71:A:LEU:HD11 | 1:57:A:VAL:H     | 17                  | 0.29     | 0.05                | 0.27       |
| (1,1081) | 1:71:A:LEU:HD13 | 1:57:A:VAL:H     | 17                  | 0.29     | 0.05                | 0.27       |
| (1,3178) | 1:116:A:GLN:HA  | 1:116:A:GLN:H    | 17                  | 0.29     | 0.01                | 0.29       |
| (1,1521) | 1:30:A:PHE:HB3  | 1:29:A:ALA:HB1   | 17                  | 0.29     | 0.03                | 0.28       |
| (1,1521) | 1:30:A:PHE:HB3  | 1:29:A:ALA:HB2   | 17                  | 0.29     | 0.03                | 0.28       |
| (1,1521) | 1:30:A:PHE:HB3  | 1:29:A:ALA:HB3   | 17                  | 0.29     | 0.03                | 0.28       |
| (1,1062) | 1:27:A:VAL:HG23 | 1:27:A:VAL:HG13  | 17                  | 0.28     | 0.03                | 0.28       |
| (1,1062) | 1:27:A:VAL:HG21 | 1:27:A:VAL:HG11  | 17                  | 0.28     | 0.03                | 0.28       |
| (1,1062) | 1:27:A:VAL:HG23 | 1:27:A:VAL:HG11  | 17                  | 0.28     | 0.03                | 0.28       |

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| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1062) | 1:27:A:VAL:HG21  | 1:27:A:VAL:HG13 | 17                  | 0.28     | 0.03                | 0.28       |
| (1,1062) | 1:27:A:VAL:HG22  | 1:27:A:VAL:HG13 | 17                  | 0.28     | 0.03                | 0.28       |
| (1,1062) | 1:27:A:VAL:HG21  | 1:27:A:VAL:HG12 | 17                  | 0.28     | 0.03                | 0.28       |
| (1,1737) | 1:77:A:LEU:HG    | 1:77:A:LEU:HD12 | 17                  | 0.28     | 0.02                | 0.28       |
| (1,1737) | 1:77:A:LEU:HG    | 1:77:A:LEU:HD13 | 17                  | 0.28     | 0.02                | 0.28       |
| (1,1737) | 1:77:A:LEU:HG    | 1:77:A:LEU:HD11 | 17                  | 0.28     | 0.02                | 0.28       |
| (1,2675) | 1:85:A:LEU:HB2   | 1:86:A:TYR:HD2  | 17                  | 0.28     | 0.04                | 0.28       |
| (1,2675) | 1:85:A:LEU:HB2   | 1:86:A:TYR:HD1  | 17                  | 0.28     | 0.04                | 0.28       |
| (1,643)  | 1:110:A:VAL:HG12 | 1:113:A:ALA:H   | 17                  | 0.28     | 0.01                | 0.28       |
| (1,643)  | 1:110:A:VAL:HG13 | 1:113:A:ALA:H   | 17                  | 0.28     | 0.01                | 0.28       |
| (1,643)  | 1:110:A:VAL:HG11 | 1:113:A:ALA:H   | 17                  | 0.28     | 0.01                | 0.28       |
| (1,1994) | 1:91:A:GLY:HA2   | 1:91:A:GLY:H    | 17                  | 0.28     | 0.02                | 0.28       |
| (1,3421) | 1:53:A:PHE:HA    | 1:75:A:LEU:HD23 | 17                  | 0.28     | 0.01                | 0.28       |
| (1,3421) | 1:53:A:PHE:HA    | 1:75:A:LEU:HD22 | 17                  | 0.28     | 0.01                | 0.28       |
| (1,3421) | 1:53:A:PHE:HA    | 1:75:A:LEU:HD21 | 17                  | 0.28     | 0.01                | 0.28       |
| (1,4280) | 1:112:A:HIS:HA   | 1:116:A:GLN:H   | 17                  | 0.28     | 0.02                | 0.28       |
| (1,2824) | 1:97:A:LEU:HD21  | 1:56:A:LEU:HA   | 17                  | 0.28     | 0.03                | 0.28       |
| (1,2824) | 1:97:A:LEU:HD22  | 1:56:A:LEU:HA   | 17                  | 0.28     | 0.03                | 0.28       |
| (1,2824) | 1:97:A:LEU:HD23  | 1:56:A:LEU:HA   | 17                  | 0.28     | 0.03                | 0.28       |
| (1,1082) | 1:71:A:LEU:HD13  | 1:72:A:ARG:H    | 17                  | 0.28     | 0.01                | 0.28       |
| (1,1082) | 1:71:A:LEU:HD12  | 1:72:A:ARG:H    | 17                  | 0.28     | 0.01                | 0.28       |
| (1,1082) | 1:71:A:LEU:HD11  | 1:72:A:ARG:H    | 17                  | 0.28     | 0.01                | 0.28       |
| (1,3345) | 1:29:A:ALA:HA    | 1:29:A:ALA:HB3  | 17                  | 0.28     | 0.03                | 0.27       |
| (1,3345) | 1:29:A:ALA:HA    | 1:29:A:ALA:HB1  | 17                  | 0.28     | 0.03                | 0.27       |
| (1,3345) | 1:29:A:ALA:HA    | 1:29:A:ALA:HB2  | 17                  | 0.28     | 0.03                | 0.27       |
| (1,2909) | 1:110:A:VAL:HG13 | 1:91:A:GLY:HA2  | 17                  | 0.28     | 0.02                | 0.28       |
| (1,2909) | 1:110:A:VAL:HG11 | 1:91:A:GLY:HA2  | 17                  | 0.28     | 0.02                | 0.28       |
| (1,2909) | 1:110:A:VAL:HG12 | 1:91:A:GLY:HA2  | 17                  | 0.28     | 0.02                | 0.28       |
| (1,4140) | 1:118:A:GLU:HA   | 1:118:A:GLU:H   | 17                  | 0.28     | 0.02                | 0.27       |
| (1,2662) | 1:97:A:LEU:HD12  | 1:57:A:VAL:H    | 17                  | 0.28     | 0.04                | 0.29       |
| (1,2662) | 1:97:A:LEU:HD11  | 1:57:A:VAL:H    | 17                  | 0.28     | 0.04                | 0.29       |
| (1,2662) | 1:97:A:LEU:HD13  | 1:57:A:VAL:H    | 17                  | 0.28     | 0.04                | 0.29       |
| (1,3123) | 1:59:A:ARG:HB2   | 1:59:A:ARG:HA   | 17                  | 0.28     | 0.02                | 0.28       |
| (1,819)  | 1:28:A:ILE:HD11  | 1:74:A:ALA:HA   | 17                  | 0.27     | 0.02                | 0.27       |
| (1,819)  | 1:28:A:ILE:HD12  | 1:74:A:ALA:HA   | 17                  | 0.27     | 0.02                | 0.27       |
| (1,819)  | 1:28:A:ILE:HD13  | 1:74:A:ALA:HA   | 17                  | 0.27     | 0.02                | 0.27       |
| (1,3223) | 1:84:A:TYR:HE2   | 1:79:A:THR:HA   | 17                  | 0.27     | 0.04                | 0.28       |
| (1,3223) | 1:84:A:TYR:HE1   | 1:79:A:THR:HA   | 17                  | 0.27     | 0.04                | 0.28       |
| (1,3228) | 1:31:A:LEU:HB2   | 1:39:A:PHE:HE2  | 17                  | 0.27     | 0.04                | 0.26       |
| (1,3228) | 1:31:A:LEU:HB2   | 1:39:A:PHE:HE1  | 17                  | 0.27     | 0.04                | 0.26       |
| (1,1865) | 1:45:A:ALA:HB1   | 1:44:A:GLU:HB3  | 17                  | 0.27     | 0.07                | 0.26       |
| (1,1865) | 1:45:A:ALA:HB3   | 1:44:A:GLU:HB3  | 17                  | 0.27     | 0.07                | 0.26       |

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| Key      | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,1865) | 1:45:A:ALA:HB2  | 1:44:A:GLU:HB3   | 17                  | 0.27     | 0.07                | 0.26       |
| (1,1746) | 1:71:A:LEU:HD23 | 1:74:A:ALA:H     | 17                  | 0.27     | 0.04                | 0.29       |
| (1,1746) | 1:71:A:LEU:HD22 | 1:74:A:ALA:H     | 17                  | 0.27     | 0.04                | 0.29       |
| (1,1746) | 1:71:A:LEU:HD21 | 1:74:A:ALA:H     | 17                  | 0.27     | 0.04                | 0.29       |
| (1,850)  | 1:86:A:TYR:HB2  | 1:117:A:LEU:HB3  | 17                  | 0.27     | 0.01                | 0.27       |
| (1,895)  | 1:129:A:ALA:HB2 | 1:129:A:ALA:HA   | 17                  | 0.27     | 0.04                | 0.28       |
| (1,895)  | 1:129:A:ALA:HB3 | 1:129:A:ALA:HA   | 17                  | 0.27     | 0.04                | 0.28       |
| (1,895)  | 1:129:A:ALA:HB1 | 1:129:A:ALA:HA   | 17                  | 0.27     | 0.04                | 0.28       |
| (1,1752) | 1:41:A:ALA:HB2  | 1:28:A:ILE:HG22  | 17                  | 0.27     | 0.03                | 0.27       |
| (1,1752) | 1:41:A:ALA:HB3  | 1:28:A:ILE:HG21  | 17                  | 0.27     | 0.03                | 0.27       |
| (1,1752) | 1:41:A:ALA:HB3  | 1:28:A:ILE:HG23  | 17                  | 0.27     | 0.03                | 0.27       |
| (1,1752) | 1:41:A:ALA:HB1  | 1:28:A:ILE:HG23  | 17                  | 0.27     | 0.03                | 0.27       |
| (1,1752) | 1:41:A:ALA:HB2  | 1:28:A:ILE:HG23  | 17                  | 0.27     | 0.03                | 0.27       |
| (1,1752) | 1:41:A:ALA:HB1  | 1:28:A:ILE:HG21  | 17                  | 0.27     | 0.03                | 0.27       |
| (1,1752) | 1:41:A:ALA:HB3  | 1:28:A:ILE:HG22  | 17                  | 0.27     | 0.03                | 0.27       |
| (1,1940) | 1:111:A:GLU:HB2 | 1:109:A:HIS:HA   | 17                  | 0.27     | 0.01                | 0.27       |
| (1,1811) | 1:86:A:TYR:H    | 1:117:A:LEU:HD13 | 17                  | 0.27     | 0.09                | 0.23       |
| (1,1811) | 1:86:A:TYR:H    | 1:117:A:LEU:HD11 | 17                  | 0.27     | 0.09                | 0.23       |
| (1,1811) | 1:86:A:TYR:H    | 1:117:A:LEU:HD12 | 17                  | 0.27     | 0.09                | 0.23       |
| (1,2679) | 1:53:A:PHE:HA   | 1:53:A:PHE:HE1   | 17                  | 0.27     | 0.02                | 0.27       |
| (1,2679) | 1:53:A:PHE:HA   | 1:53:A:PHE:HE2   | 17                  | 0.27     | 0.02                | 0.27       |
| (1,2829) | 1:97:A:LEU:HD21 | 1:97:A:LEU:HB2   | 17                  | 0.27     | 0.03                | 0.28       |
| (1,2829) | 1:97:A:LEU:HD22 | 1:97:A:LEU:HB2   | 17                  | 0.27     | 0.03                | 0.28       |
| (1,2829) | 1:97:A:LEU:HD23 | 1:97:A:LEU:HB2   | 17                  | 0.27     | 0.03                | 0.28       |
| (1,116)  | 1:21:A:LEU:HD12 | 1:30:A:PHE:H     | 17                  | 0.27     | 0.07                | 0.3        |
| (1,116)  | 1:21:A:LEU:HD13 | 1:30:A:PHE:H     | 17                  | 0.27     | 0.07                | 0.3        |
| (1,116)  | 1:21:A:LEU:HD11 | 1:30:A:PHE:H     | 17                  | 0.27     | 0.07                | 0.3        |
| (1,3668) | 1:84:A:TYR:H    | 1:84:A:TYR:HD1   | 17                  | 0.27     | 0.07                | 0.25       |
| (1,3668) | 1:84:A:TYR:H    | 1:84:A:TYR:HD2   | 17                  | 0.27     | 0.07                | 0.25       |
| (1,3491) | 1:86:A:TYR:HE2  | 1:85:A:LEU:HD22  | 17                  | 0.27     | 0.01                | 0.27       |
| (1,3491) | 1:86:A:TYR:HE1  | 1:85:A:LEU:HD22  | 17                  | 0.27     | 0.01                | 0.27       |
| (1,3491) | 1:86:A:TYR:HE1  | 1:85:A:LEU:HD23  | 17                  | 0.27     | 0.01                | 0.27       |
| (1,3491) | 1:86:A:TYR:HE2  | 1:85:A:LEU:HD21  | 17                  | 0.27     | 0.01                | 0.27       |
| (1,3491) | 1:86:A:TYR:HE1  | 1:85:A:LEU:HD21  | 17                  | 0.27     | 0.01                | 0.27       |
| (3,109)  | 1:92:A:ALA:H    | 1:110:A:VAL:HB   | 17                  | 0.27     | 0.05                | 0.27       |
| (1,3565) | 1:105:A:LEU:HB3 | 1:105:A:LEU:HA   | 17                  | 0.27     | 0.01                | 0.27       |
| (1,3604) | 1:97:A:LEU:HB2  | 1:97:A:LEU:HA    | 17                  | 0.27     | 0.01                | 0.27       |
| (1,3531) | 1:65:A:ASN:H    | 1:65:A:ASN:HA    | 17                  | 0.27     | 0.05                | 0.29       |
| (1,1723) | 1:68:A:LYS:HD3  | 1:57:A:VAL:HG13  | 17                  | 0.26     | 0.02                | 0.27       |
| (1,1723) | 1:68:A:LYS:HD3  | 1:57:A:VAL:HG11  | 17                  | 0.26     | 0.02                | 0.27       |
| (1,1723) | 1:68:A:LYS:HD3  | 1:57:A:VAL:HG12  | 17                  | 0.26     | 0.02                | 0.27       |
| (1,4141) | 1:98:A:ASP:HB2  | 1:100:A:ASN:HD21 | 17                  | 0.26     | 0.03                | 0.28       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (3,15)   | 1:85:A:LEU:HB3   | 1:82:A:TRP:HA    | 17                  | 0.26     | 0.02                | 0.26       |
| (1,300)  | 1:100:A:ASN:HB3  | 1:100:A:ASN:HD21 | 17                  | 0.26     | 0.02                | 0.26       |
| (1,2346) | 1:105:A:LEU:HD13 | 1:107:A:GLU:HA   | 17                  | 0.26     | 0.04                | 0.26       |
| (1,2346) | 1:105:A:LEU:HD11 | 1:107:A:GLU:HA   | 17                  | 0.26     | 0.04                | 0.26       |
| (1,2346) | 1:105:A:LEU:HD12 | 1:107:A:GLU:HA   | 17                  | 0.26     | 0.04                | 0.26       |
| (1,125)  | 1:28:A:ILE:HG13  | 1:28:A:ILE:H     | 17                  | 0.26     | 0.01                | 0.26       |
| (1,2598) | 1:27:A:VAL:HG23  | 1:27:A:VAL:HG13  | 17                  | 0.26     | 0.03                | 0.26       |
| (1,2598) | 1:27:A:VAL:HG21  | 1:27:A:VAL:HG11  | 17                  | 0.26     | 0.03                | 0.26       |
| (1,2598) | 1:27:A:VAL:HG23  | 1:27:A:VAL:HG11  | 17                  | 0.26     | 0.03                | 0.26       |
| (1,2598) | 1:27:A:VAL:HG21  | 1:27:A:VAL:HG13  | 17                  | 0.26     | 0.03                | 0.26       |
| (1,2598) | 1:27:A:VAL:HG22  | 1:27:A:VAL:HG13  | 17                  | 0.26     | 0.03                | 0.26       |
| (1,2598) | 1:27:A:VAL:HG21  | 1:27:A:VAL:HG12  | 17                  | 0.26     | 0.03                | 0.26       |
| (1,4310) | 1:64:A:MET:HA    | 1:65:A:ASN:H     | 17                  | 0.26     | 0.03                | 0.25       |
| (1,894)  | 1:133:A:ALA:HA   | 1:133:A:ALA:HB1  | 17                  | 0.26     | 0.01                | 0.26       |
| (1,894)  | 1:133:A:ALA:HA   | 1:133:A:ALA:HB3  | 17                  | 0.26     | 0.01                | 0.26       |
| (1,894)  | 1:133:A:ALA:HA   | 1:133:A:ALA:HB2  | 17                  | 0.26     | 0.01                | 0.26       |
| (1,691)  | 1:75:A:LEU:HD23  | 1:54:A:GLN:H     | 17                  | 0.26     | 0.02                | 0.25       |
| (1,691)  | 1:75:A:LEU:HD22  | 1:54:A:GLN:H     | 17                  | 0.26     | 0.02                | 0.25       |
| (1,691)  | 1:75:A:LEU:HD21  | 1:54:A:GLN:H     | 17                  | 0.26     | 0.02                | 0.25       |
| (1,2596) | 1:74:A:ALA:HB1   | 1:27:A:VAL:HG13  | 17                  | 0.26     | 0.03                | 0.26       |
| (1,2596) | 1:74:A:ALA:HB1   | 1:27:A:VAL:HG11  | 17                  | 0.26     | 0.03                | 0.26       |
| (1,2596) | 1:74:A:ALA:HB2   | 1:27:A:VAL:HG11  | 17                  | 0.26     | 0.03                | 0.26       |
| (1,2596) | 1:74:A:ALA:HB3   | 1:27:A:VAL:HG11  | 17                  | 0.26     | 0.03                | 0.26       |
| (1,2596) | 1:74:A:ALA:HB3   | 1:27:A:VAL:HG13  | 17                  | 0.26     | 0.03                | 0.26       |
| (1,2596) | 1:74:A:ALA:HB3   | 1:27:A:VAL:HG12  | 17                  | 0.26     | 0.03                | 0.26       |
| (1,552)  | 1:65:A:ASN:H     | 1:65:A:ASN:HD21  | 17                  | 0.26     | 0.06                | 0.25       |
| (1,3326) | 1:77:A:LEU:HG    | 1:77:A:LEU:HD12  | 17                  | 0.26     | 0.02                | 0.26       |
| (1,3326) | 1:77:A:LEU:HG    | 1:77:A:LEU:HD13  | 17                  | 0.26     | 0.02                | 0.26       |
| (1,3326) | 1:77:A:LEU:HG    | 1:77:A:LEU:HD11  | 17                  | 0.26     | 0.02                | 0.26       |
| (1,2576) | 1:124:A:VAL:HG21 | 1:120:A:ALA:HA   | 17                  | 0.26     | 0.03                | 0.25       |
| (1,2576) | 1:124:A:VAL:HG22 | 1:120:A:ALA:HA   | 17                  | 0.26     | 0.03                | 0.25       |
| (1,2576) | 1:124:A:VAL:HG23 | 1:120:A:ALA:HA   | 17                  | 0.26     | 0.03                | 0.25       |
| (1,1799) | 1:71:A:LEU:HA    | 1:74:A:ALA:HB3   | 17                  | 0.25     | 0.05                | 0.25       |
| (1,1799) | 1:71:A:LEU:HA    | 1:74:A:ALA:HB1   | 17                  | 0.25     | 0.05                | 0.25       |
| (1,1799) | 1:71:A:LEU:HA    | 1:74:A:ALA:HB2   | 17                  | 0.25     | 0.05                | 0.25       |
| (1,1904) | 1:74:A:ALA:HB2   | 1:28:A:ILE:HA    | 17                  | 0.25     | 0.01                | 0.26       |
| (1,1904) | 1:74:A:ALA:HB3   | 1:28:A:ILE:HA    | 17                  | 0.25     | 0.01                | 0.26       |
| (1,1904) | 1:74:A:ALA:HB1   | 1:28:A:ILE:HA    | 17                  | 0.25     | 0.01                | 0.26       |
| (1,3588) | 1:105:A:LEU:HB3  | 1:110:A:VAL:HG21 | 17                  | 0.25     | 0.02                | 0.25       |
| (1,3588) | 1:105:A:LEU:HB3  | 1:110:A:VAL:HG22 | 17                  | 0.25     | 0.02                | 0.25       |
| (1,3588) | 1:105:A:LEU:HB3  | 1:110:A:VAL:HG23 | 17                  | 0.25     | 0.02                | 0.25       |
| (1,2945) | 1:110:A:VAL:HB   | 1:110:A:VAL:HG12 | 17                  | 0.25     | 0.02                | 0.25       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2945) | 1:110:A:VAL:HB   | 1:110:A:VAL:HG13 | 17                  | 0.25     | 0.02                | 0.25       |
| (1,2945) | 1:110:A:VAL:HB   | 1:110:A:VAL:HG11 | 17                  | 0.25     | 0.02                | 0.25       |
| (1,3180) | 1:111:A:GLU:HG2  | 1:111:A:GLU:HA   | 17                  | 0.25     | 0.04                | 0.26       |
| (1,3132) | 1:68:A:LYS:HB2   | 1:53:A:PHE:HE2   | 17                  | 0.25     | 0.04                | 0.24       |
| (1,3132) | 1:68:A:LYS:HB2   | 1:53:A:PHE:HE1   | 17                  | 0.25     | 0.04                | 0.24       |
| (1,3401) | 1:86:A:TYR:HE2   | 1:86:A:TYR:HA    | 17                  | 0.25     | 0.07                | 0.22       |
| (1,3401) | 1:86:A:TYR:HE1   | 1:86:A:TYR:HA    | 17                  | 0.25     | 0.07                | 0.22       |
| (1,2358) | 1:107:A:GLU:HA   | 1:111:A:GLU:H    | 17                  | 0.25     | 0.03                | 0.25       |
| (1,3716) | 1:35:A:PHE:HE2   | 1:35:A:PHE:H     | 17                  | 0.25     | 0.02                | 0.25       |
| (1,3716) | 1:35:A:PHE:HE1   | 1:35:A:PHE:H     | 17                  | 0.25     | 0.02                | 0.25       |
| (1,3816) | 1:105:A:LEU:H    | 1:105:A:LEU:HD21 | 17                  | 0.25     | 0.02                | 0.25       |
| (1,3816) | 1:105:A:LEU:H    | 1:105:A:LEU:HD23 | 17                  | 0.25     | 0.02                | 0.25       |
| (1,3816) | 1:105:A:LEU:H    | 1:105:A:LEU:HD22 | 17                  | 0.25     | 0.02                | 0.25       |
| (1,3534) | 1:122:A:ALA:HB3  | 1:121:A:LYS:HE3  | 17                  | 0.25     | 0.02                | 0.25       |
| (1,3534) | 1:122:A:ALA:HB1  | 1:121:A:LYS:HE3  | 17                  | 0.25     | 0.02                | 0.25       |
| (1,3534) | 1:122:A:ALA:HB2  | 1:121:A:LYS:HE3  | 17                  | 0.25     | 0.02                | 0.25       |
| (1,1947) | 1:93:A:THR:HB    | 1:88:A:VAL:HG13  | 17                  | 0.25     | 0.04                | 0.24       |
| (1,1947) | 1:93:A:THR:HB    | 1:88:A:VAL:HG12  | 17                  | 0.25     | 0.04                | 0.24       |
| (1,1947) | 1:93:A:THR:HB    | 1:88:A:VAL:HG11  | 17                  | 0.25     | 0.04                | 0.24       |
| (1,1613) | 1:124:A:VAL:HG21 | 1:121:A:LYS:HA   | 17                  | 0.25     | 0.05                | 0.26       |
| (1,1613) | 1:124:A:VAL:HG22 | 1:121:A:LYS:HA   | 17                  | 0.25     | 0.05                | 0.26       |
| (1,1613) | 1:124:A:VAL:HG23 | 1:121:A:LYS:HA   | 17                  | 0.25     | 0.05                | 0.26       |
| (1,3513) | 1:72:A:ARG:HG3   | 1:73:A:SER:HB3   | 17                  | 0.25     | 0.08                | 0.3        |
| (1,3773) | 1:123:A:ARG:HA   | 1:124:A:VAL:H    | 17                  | 0.25     | 0.01                | 0.25       |
| (1,2989) | 1:42:A:GLU:HA    | 1:42:A:GLU:HB2   | 17                  | 0.25     | 0.03                | 0.25       |
| (1,1618) | 1:109:A:HIS:HB2  | 1:110:A:VAL:HG11 | 17                  | 0.24     | 0.01                | 0.25       |
| (1,1618) | 1:109:A:HIS:HB2  | 1:110:A:VAL:HG12 | 17                  | 0.24     | 0.01                | 0.25       |
| (1,1618) | 1:109:A:HIS:HB2  | 1:110:A:VAL:HG13 | 17                  | 0.24     | 0.01                | 0.25       |
| (1,2547) | 1:11:A:SER:HA    | 1:12:A:GLN:HG3   | 17                  | 0.24     | 0.08                | 0.25       |
| (1,3503) | 1:27:A:VAL:HG22  | 1:31:A:LEU:H     | 17                  | 0.24     | 0.02                | 0.24       |
| (1,3503) | 1:27:A:VAL:HG23  | 1:31:A:LEU:H     | 17                  | 0.24     | 0.02                | 0.24       |
| (1,3503) | 1:27:A:VAL:HG21  | 1:31:A:LEU:H     | 17                  | 0.24     | 0.02                | 0.24       |
| (1,3776) | 1:121:A:LYS:HA   | 1:122:A:ALA:H    | 17                  | 0.24     | 0.02                | 0.24       |
| (1,3358) | 1:28:A:ILE:HB    | 1:29:A:ALA:HA    | 17                  | 0.24     | 0.01                | 0.24       |
| (1,1331) | 1:78:A:TYR:HE2   | 1:84:A:TYR:HD2   | 17                  | 0.24     | 0.08                | 0.21       |
| (1,1331) | 1:78:A:TYR:HE1   | 1:84:A:TYR:HD2   | 17                  | 0.24     | 0.08                | 0.21       |
| (1,1331) | 1:78:A:TYR:HE1   | 1:84:A:TYR:HD1   | 17                  | 0.24     | 0.08                | 0.21       |
| (1,1331) | 1:78:A:TYR:HE2   | 1:84:A:TYR:HD1   | 17                  | 0.24     | 0.08                | 0.21       |
| (1,3592) | 1:109:A:HIS:HB2  | 1:110:A:VAL:HG11 | 17                  | 0.24     | 0.01                | 0.24       |
| (1,3592) | 1:109:A:HIS:HB2  | 1:110:A:VAL:HG12 | 17                  | 0.24     | 0.01                | 0.24       |
| (1,3592) | 1:109:A:HIS:HB2  | 1:110:A:VAL:HG13 | 17                  | 0.24     | 0.01                | 0.24       |
| (1,1210) | 1:86:A:TYR:HB3   | 1:86:A:TYR:H     | 17                  | 0.24     | 0.01                | 0.24       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2622) | 1:71:A:LEU:HD12  | 1:57:A:VAL:H     | 17                  | 0.24     | 0.05                | 0.23       |
| (1,2622) | 1:71:A:LEU:HD11  | 1:57:A:VAL:H     | 17                  | 0.24     | 0.05                | 0.23       |
| (1,2622) | 1:71:A:LEU:HD13  | 1:57:A:VAL:H     | 17                  | 0.24     | 0.05                | 0.23       |
| (1,3028) | 1:71:A:LEU:HD13  | 1:72:A:ARG:HA    | 17                  | 0.24     | 0.02                | 0.24       |
| (1,3028) | 1:71:A:LEU:HD12  | 1:72:A:ARG:HA    | 17                  | 0.24     | 0.02                | 0.24       |
| (1,3028) | 1:71:A:LEU:HD11  | 1:72:A:ARG:HA    | 17                  | 0.24     | 0.02                | 0.24       |
| (1,3417) | 1:117:A:LEU:HG   | 1:117:A:LEU:HD11 | 17                  | 0.24     | 0.04                | 0.23       |
| (1,3417) | 1:117:A:LEU:HG   | 1:117:A:LEU:HD13 | 17                  | 0.24     | 0.04                | 0.23       |
| (1,3417) | 1:117:A:LEU:HG   | 1:117:A:LEU:HD12 | 17                  | 0.24     | 0.04                | 0.23       |
| (1,2307) | 1:117:A:LEU:HD13 | 1:86:A:TYR:HB2   | 17                  | 0.24     | 0.03                | 0.25       |
| (1,2307) | 1:117:A:LEU:HD11 | 1:86:A:TYR:HB2   | 17                  | 0.24     | 0.03                | 0.25       |
| (1,2307) | 1:117:A:LEU:HD12 | 1:86:A:TYR:HB2   | 17                  | 0.24     | 0.03                | 0.25       |
| (1,4153) | 1:18:A:GLN:HB3   | 1:18:A:GLN:H     | 17                  | 0.24     | 0.05                | 0.23       |
| (1,2618) | 1:34:A:ARG:HG3   | 1:34:A:ARG:H     | 17                  | 0.24     | 0.02                | 0.23       |
| (1,3341) | 1:41:A:ALA:HB2   | 1:28:A:ILE:HG22  | 17                  | 0.24     | 0.03                | 0.23       |
| (1,3341) | 1:41:A:ALA:HB3   | 1:28:A:ILE:HG21  | 17                  | 0.24     | 0.03                | 0.23       |
| (1,3341) | 1:41:A:ALA:HB3   | 1:28:A:ILE:HG23  | 17                  | 0.24     | 0.03                | 0.23       |
| (1,3341) | 1:41:A:ALA:HB1   | 1:28:A:ILE:HG23  | 17                  | 0.24     | 0.03                | 0.23       |
| (1,3341) | 1:41:A:ALA:HB2   | 1:28:A:ILE:HG23  | 17                  | 0.24     | 0.03                | 0.23       |
| (1,3341) | 1:41:A:ALA:HB1   | 1:28:A:ILE:HG21  | 17                  | 0.24     | 0.03                | 0.23       |
| (1,3341) | 1:41:A:ALA:HB3   | 1:28:A:ILE:HG22  | 17                  | 0.24     | 0.03                | 0.23       |
| (1,4299) | 1:65:A:ASN:HD22  | 1:65:A:ASN:HD21  | 17                  | 0.24     | 0.02                | 0.25       |
| (1,1736) | 1:77:A:LEU:HB3   | 1:77:A:LEU:HD13  | 17                  | 0.24     | 0.01                | 0.24       |
| (1,1736) | 1:77:A:LEU:HB3   | 1:77:A:LEU:HD11  | 17                  | 0.24     | 0.01                | 0.24       |
| (1,1736) | 1:77:A:LEU:HB3   | 1:77:A:LEU:HD12  | 17                  | 0.24     | 0.01                | 0.24       |
| (1,2713) | 1:53:A:PHE:HB3   | 1:75:A:LEU:HD13  | 17                  | 0.24     | 0.01                | 0.24       |
| (1,2713) | 1:53:A:PHE:HB3   | 1:75:A:LEU:HD11  | 17                  | 0.24     | 0.01                | 0.24       |
| (1,2713) | 1:53:A:PHE:HB3   | 1:75:A:LEU:HD12  | 17                  | 0.24     | 0.01                | 0.24       |
| (1,2605) | 1:31:A:LEU:HD23  | 1:30:A:PHE:HD1   | 17                  | 0.24     | 0.02                | 0.24       |
| (1,2605) | 1:31:A:LEU:HD22  | 1:30:A:PHE:HD2   | 17                  | 0.24     | 0.02                | 0.24       |
| (1,2605) | 1:31:A:LEU:HD21  | 1:30:A:PHE:HD2   | 17                  | 0.24     | 0.02                | 0.24       |
| (1,2605) | 1:31:A:LEU:HD21  | 1:30:A:PHE:HD1   | 17                  | 0.24     | 0.02                | 0.24       |
| (1,3209) | 1:124:A:VAL:HG12 | 1:124:A:VAL:HB   | 17                  | 0.24     | 0.01                | 0.24       |
| (1,3209) | 1:124:A:VAL:HG11 | 1:124:A:VAL:HB   | 17                  | 0.24     | 0.01                | 0.24       |
| (1,3209) | 1:124:A:VAL:HG13 | 1:124:A:VAL:HB   | 17                  | 0.24     | 0.01                | 0.24       |
| (1,4172) | 1:105:A:LEU:H    | 1:92:A:ALA:H     | 17                  | 0.24     | 0.02                | 0.24       |
| (1,2404) | 1:28:A:ILE:HD11  | 1:74:A:ALA:HA    | 17                  | 0.24     | 0.02                | 0.23       |
| (1,2404) | 1:28:A:ILE:HD12  | 1:74:A:ALA:HA    | 17                  | 0.24     | 0.02                | 0.23       |
| (1,2404) | 1:28:A:ILE:HD13  | 1:74:A:ALA:HA    | 17                  | 0.24     | 0.02                | 0.23       |
| (1,4017) | 1:32:A:ALA:HB1   | 1:35:A:PHE:H     | 17                  | 0.24     | 0.05                | 0.23       |
| (1,4017) | 1:32:A:ALA:HB2   | 1:35:A:PHE:H     | 17                  | 0.24     | 0.05                | 0.23       |
| (1,4017) | 1:32:A:ALA:HB3   | 1:35:A:PHE:H     | 17                  | 0.24     | 0.05                | 0.23       |

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| Key      | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,1395) | 1:31:A:LEU:HD21 | 1:39:A:PHE:HD2   | 17                  | 0.24     | 0.01                | 0.23       |
| (1,1395) | 1:31:A:LEU:HD23 | 1:39:A:PHE:HD2   | 17                  | 0.24     | 0.01                | 0.23       |
| (1,1395) | 1:31:A:LEU:HD22 | 1:39:A:PHE:HD2   | 17                  | 0.24     | 0.01                | 0.23       |
| (1,1395) | 1:31:A:LEU:HD22 | 1:39:A:PHE:HD1   | 17                  | 0.24     | 0.01                | 0.23       |
| (1,1395) | 1:31:A:LEU:HD23 | 1:39:A:PHE:HD1   | 17                  | 0.24     | 0.01                | 0.23       |
| (1,1395) | 1:31:A:LEU:HD21 | 1:39:A:PHE:HD1   | 17                  | 0.24     | 0.01                | 0.23       |
| (1,3874) | 1:85:A:LEU:HB3  | 1:86:A:TYR:H     | 17                  | 0.24     | 0.01                | 0.24       |
| (3,111)  | 1:111:A:GLU:HG2 | 1:112:A:HIS:HA   | 17                  | 0.24     | 0.08                | 0.2        |
| (1,1730) | 1:27:A:VAL:HA   | 1:66:A:LEU:HD21  | 17                  | 0.23     | 0.02                | 0.24       |
| (1,1730) | 1:27:A:VAL:HA   | 1:66:A:LEU:HD23  | 17                  | 0.23     | 0.02                | 0.24       |
| (1,1730) | 1:27:A:VAL:HA   | 1:66:A:LEU:HD22  | 17                  | 0.23     | 0.02                | 0.24       |
| (1,2210) | 1:105:A:LEU:HG  | 1:110:A:VAL:HG11 | 17                  | 0.23     | 0.01                | 0.23       |
| (1,2210) | 1:105:A:LEU:HG  | 1:110:A:VAL:HG12 | 17                  | 0.23     | 0.01                | 0.23       |
| (1,2210) | 1:105:A:LEU:HG  | 1:110:A:VAL:HG13 | 17                  | 0.23     | 0.01                | 0.23       |
| (1,1232) | 1:60:A:VAL:HG12 | 1:59:A:ARG:HD3   | 17                  | 0.23     | 0.03                | 0.23       |
| (1,1232) | 1:60:A:VAL:HG13 | 1:59:A:ARG:HD3   | 17                  | 0.23     | 0.03                | 0.23       |
| (1,1232) | 1:60:A:VAL:HG11 | 1:59:A:ARG:HD3   | 17                  | 0.23     | 0.03                | 0.23       |
| (1,3479) | 1:45:A:ALA:HB1  | 1:44:A:GLU:HB3   | 17                  | 0.23     | 0.07                | 0.22       |
| (1,3479) | 1:45:A:ALA:HB3  | 1:44:A:GLU:HB3   | 17                  | 0.23     | 0.07                | 0.22       |
| (1,3479) | 1:45:A:ALA:HB2  | 1:44:A:GLU:HB3   | 17                  | 0.23     | 0.07                | 0.22       |
| (1,3068) | 1:52:A:ILE:HG23 | 1:53:A:PHE:HB2   | 17                  | 0.23     | 0.13                | 0.18       |
| (1,3068) | 1:52:A:ILE:HG21 | 1:53:A:PHE:HB2   | 17                  | 0.23     | 0.13                | 0.18       |
| (1,3068) | 1:52:A:ILE:HG22 | 1:53:A:PHE:HB2   | 17                  | 0.23     | 0.13                | 0.18       |
| (1,3066) | 1:30:A:PHE:HB3  | 1:29:A:ALA:HB1   | 17                  | 0.23     | 0.03                | 0.23       |
| (1,3066) | 1:30:A:PHE:HB3  | 1:29:A:ALA:HB2   | 17                  | 0.23     | 0.03                | 0.23       |
| (1,3066) | 1:30:A:PHE:HB3  | 1:29:A:ALA:HB3   | 17                  | 0.23     | 0.03                | 0.23       |
| (1,3492) | 1:105:A:LEU:HB3 | 1:105:A:LEU:HD11 | 17                  | 0.23     | 0.02                | 0.23       |
| (1,3492) | 1:105:A:LEU:HB3 | 1:105:A:LEU:HD12 | 17                  | 0.23     | 0.02                | 0.23       |
| (1,3492) | 1:105:A:LEU:HB3 | 1:105:A:LEU:HD13 | 17                  | 0.23     | 0.02                | 0.23       |
| (1,3583) | 1:112:A:HIS:H   | 1:109:A:HIS:HA   | 17                  | 0.23     | 0.03                | 0.24       |
| (3,129)  | 1:71:A:LEU:HD12 | 1:60:A:VAL:HB    | 17                  | 0.23     | 0.02                | 0.23       |
| (3,129)  | 1:71:A:LEU:HD11 | 1:60:A:VAL:HB    | 17                  | 0.23     | 0.02                | 0.23       |
| (3,129)  | 1:71:A:LEU:HD13 | 1:60:A:VAL:HB    | 17                  | 0.23     | 0.02                | 0.23       |
| (1,1136) | 1:31:A:LEU:HD13 | 1:35:A:PHE:HD2   | 17                  | 0.23     | 0.06                | 0.22       |
| (1,1136) | 1:31:A:LEU:HD13 | 1:35:A:PHE:HD1   | 17                  | 0.23     | 0.06                | 0.22       |
| (1,1136) | 1:31:A:LEU:HD12 | 1:35:A:PHE:HD2   | 17                  | 0.23     | 0.06                | 0.22       |
| (1,1136) | 1:31:A:LEU:HD12 | 1:35:A:PHE:HD1   | 17                  | 0.23     | 0.06                | 0.22       |
| (1,1136) | 1:31:A:LEU:HD11 | 1:35:A:PHE:HD1   | 17                  | 0.23     | 0.06                | 0.22       |
| (1,1136) | 1:31:A:LEU:HD11 | 1:35:A:PHE:HD2   | 17                  | 0.23     | 0.06                | 0.22       |
| (1,2729) | 1:17:A:ASN:HB3  | 1:17:A:ASN:HB2   | 17                  | 0.23     | 0.02                | 0.23       |
| (1,3775) | 1:124:A:VAL:HA  | 1:125:A:GLN:H    | 17                  | 0.23     | 0.02                | 0.22       |
| (1,2527) | 1:123:A:ARG:H   | 1:123:A:ARG:HA   | 17                  | 0.23     | 0.01                | 0.23       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2560) | 1:86:A:TYR:HE2   | 1:86:A:TYR:HD2   | 17                  | 0.23     | 0.04                | 0.25       |
| (1,2560) | 1:86:A:TYR:HE1   | 1:86:A:TYR:HD1   | 17                  | 0.23     | 0.04                | 0.25       |
| (1,56)   | 1:84:A:TYR:H     | 1:84:A:TYR:HD1   | 17                  | 0.23     | 0.07                | 0.21       |
| (1,56)   | 1:84:A:TYR:H     | 1:84:A:TYR:HD2   | 17                  | 0.23     | 0.07                | 0.21       |
| (1,580)  | 1:98:A:ASP:HB2   | 1:100:A:ASN:HD21 | 17                  | 0.23     | 0.03                | 0.24       |
| (1,3396) | 1:71:A:LEU:HA    | 1:74:A:ALA:HB3   | 17                  | 0.23     | 0.05                | 0.22       |
| (1,3396) | 1:71:A:LEU:HA    | 1:74:A:ALA:HB1   | 17                  | 0.23     | 0.05                | 0.22       |
| (1,3396) | 1:71:A:LEU:HA    | 1:74:A:ALA:HB2   | 17                  | 0.23     | 0.05                | 0.22       |
| (1,3501) | 1:27:A:VAL:HG22  | 1:28:A:ILE:HA    | 17                  | 0.23     | 0.07                | 0.24       |
| (1,3501) | 1:27:A:VAL:HG23  | 1:28:A:ILE:HA    | 17                  | 0.23     | 0.07                | 0.24       |
| (1,3501) | 1:27:A:VAL:HG21  | 1:28:A:ILE:HA    | 17                  | 0.23     | 0.07                | 0.24       |
| (1,3580) | 1:111:A:GLU:HB2  | 1:109:A:HIS:HA   | 17                  | 0.23     | 0.01                | 0.23       |
| (1,1363) | 1:29:A:ALA:HA    | 1:32:A:ALA:HB2   | 17                  | 0.23     | 0.04                | 0.22       |
| (1,1363) | 1:29:A:ALA:HA    | 1:32:A:ALA:HB3   | 17                  | 0.23     | 0.04                | 0.22       |
| (1,1363) | 1:29:A:ALA:HA    | 1:32:A:ALA:HB1   | 17                  | 0.23     | 0.04                | 0.22       |
| (1,3311) | 1:68:A:LYS:HD3   | 1:57:A:VAL:HG13  | 17                  | 0.23     | 0.02                | 0.23       |
| (1,3311) | 1:68:A:LYS:HD3   | 1:57:A:VAL:HG11  | 17                  | 0.23     | 0.02                | 0.23       |
| (1,3311) | 1:68:A:LYS:HD3   | 1:57:A:VAL:HG12  | 17                  | 0.23     | 0.02                | 0.23       |
| (1,3336) | 1:71:A:LEU:HD23  | 1:74:A:ALA:H     | 17                  | 0.23     | 0.04                | 0.24       |
| (1,3336) | 1:71:A:LEU:HD22  | 1:74:A:ALA:H     | 17                  | 0.23     | 0.04                | 0.24       |
| (1,3336) | 1:71:A:LEU:HD21  | 1:74:A:ALA:H     | 17                  | 0.23     | 0.04                | 0.24       |
| (3,14)   | 1:82:A:TRP:HA    | 1:85:A:LEU:HB2   | 17                  | 0.23     | 0.03                | 0.24       |
| (1,3414) | 1:86:A:TYR:H     | 1:117:A:LEU:HD13 | 17                  | 0.22     | 0.09                | 0.18       |
| (1,3414) | 1:86:A:TYR:H     | 1:117:A:LEU:HD11 | 17                  | 0.22     | 0.09                | 0.18       |
| (1,3414) | 1:86:A:TYR:H     | 1:117:A:LEU:HD12 | 17                  | 0.22     | 0.09                | 0.18       |
| (1,1428) | 1:93:A:THR:HG21  | 1:101:A:PRO:HB3  | 17                  | 0.22     | 0.02                | 0.22       |
| (1,1428) | 1:93:A:THR:HG22  | 1:101:A:PRO:HB3  | 17                  | 0.22     | 0.02                | 0.22       |
| (1,1428) | 1:93:A:THR:HG23  | 1:101:A:PRO:HB3  | 17                  | 0.22     | 0.02                | 0.22       |
| (1,1552) | 1:124:A:VAL:HG12 | 1:124:A:VAL:HB   | 17                  | 0.22     | 0.02                | 0.23       |
| (1,1552) | 1:124:A:VAL:HG11 | 1:124:A:VAL:HB   | 17                  | 0.22     | 0.02                | 0.23       |
| (1,1552) | 1:124:A:VAL:HG13 | 1:124:A:VAL:HB   | 17                  | 0.22     | 0.02                | 0.23       |
| (1,1733) | 1:30:A:PHE:HD1   | 1:66:A:LEU:HD21  | 17                  | 0.22     | 0.02                | 0.23       |
| (1,1733) | 1:30:A:PHE:HD2   | 1:66:A:LEU:HD23  | 17                  | 0.22     | 0.02                | 0.23       |
| (1,1733) | 1:30:A:PHE:HD2   | 1:66:A:LEU:HD21  | 17                  | 0.22     | 0.02                | 0.23       |
| (1,1733) | 1:30:A:PHE:HD2   | 1:66:A:LEU:HD22  | 17                  | 0.22     | 0.02                | 0.23       |
| (1,1733) | 1:30:A:PHE:HD1   | 1:66:A:LEU:HD22  | 17                  | 0.22     | 0.02                | 0.23       |
| (1,1733) | 1:30:A:PHE:HD1   | 1:66:A:LEU:HD23  | 17                  | 0.22     | 0.02                | 0.23       |
| (1,1194) | 1:39:A:PHE:HB3   | 1:35:A:PHE:HB3   | 17                  | 0.22     | 0.01                | 0.22       |
| (1,2341) | 1:66:A:LEU:HD23  | 1:70:A:GLN:H     | 17                  | 0.22     | 0.03                | 0.22       |
| (1,2341) | 1:66:A:LEU:HD22  | 1:70:A:GLN:H     | 17                  | 0.22     | 0.03                | 0.22       |
| (1,2341) | 1:66:A:LEU:HD21  | 1:70:A:GLN:H     | 17                  | 0.22     | 0.03                | 0.22       |
| (1,1592) | 1:126:A:ALA:HB2  | 1:125:A:GLN:HG3  | 17                  | 0.22     | 0.02                | 0.22       |

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| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1592) | 1:126:A:ALA:HB1  | 1:125:A:GLN:HG3 | 17                  | 0.22     | 0.02                | 0.22       |
| (1,1592) | 1:126:A:ALA:HB3  | 1:125:A:GLN:HG3 | 17                  | 0.22     | 0.02                | 0.22       |
| (1,3166) | 1:75:A:LEU:HD23  | 1:53:A:PHE:HD1  | 17                  | 0.22     | 0.01                | 0.22       |
| (1,3166) | 1:75:A:LEU:HD22  | 1:53:A:PHE:HD1  | 17                  | 0.22     | 0.01                | 0.22       |
| (1,3166) | 1:75:A:LEU:HD23  | 1:53:A:PHE:HD2  | 17                  | 0.22     | 0.01                | 0.22       |
| (1,3166) | 1:75:A:LEU:HD22  | 1:53:A:PHE:HD2  | 17                  | 0.22     | 0.01                | 0.22       |
| (1,3166) | 1:75:A:LEU:HD21  | 1:53:A:PHE:HD1  | 17                  | 0.22     | 0.01                | 0.22       |
| (1,3166) | 1:75:A:LEU:HD21  | 1:53:A:PHE:HD2  | 17                  | 0.22     | 0.01                | 0.22       |
| (1,2434) | 1:86:A:TYR:HB2   | 1:117:A:LEU:HB3 | 17                  | 0.22     | 0.01                | 0.22       |
| (1,3662) | 1:83:A:ARG:H     | 1:82:A:TRP:HD1  | 17                  | 0.22     | 0.03                | 0.21       |
| (1,2444) | 1:53:A:PHE:HE1   | 1:53:A:PHE:HB2  | 17                  | 0.22     | 0.02                | 0.22       |
| (1,2444) | 1:53:A:PHE:HE2   | 1:53:A:PHE:HB2  | 17                  | 0.22     | 0.02                | 0.22       |
| (1,3080) | 1:125:A:GLN:HB2  | 1:125:A:GLN:HA  | 17                  | 0.22     | 0.03                | 0.23       |
| (1,3195) | 1:113:A:ALA:HA   | 1:113:A:ALA:H   | 17                  | 0.22     | 0.01                | 0.22       |
| (1,2515) | 1:122:A:ALA:HA   | 1:122:A:ALA:H   | 17                  | 0.22     | 0.01                | 0.21       |
| (1,3395) | 1:33:A:GLU:HB3   | 1:33:A:GLU:HA   | 17                  | 0.22     | 0.02                | 0.22       |
| (1,3535) | 1:74:A:ALA:HB2   | 1:28:A:ILE:HA   | 17                  | 0.21     | 0.01                | 0.22       |
| (1,3535) | 1:74:A:ALA:HB3   | 1:28:A:ILE:HA   | 17                  | 0.21     | 0.01                | 0.22       |
| (1,3535) | 1:74:A:ALA:HB1   | 1:28:A:ILE:HA   | 17                  | 0.21     | 0.01                | 0.22       |
| (1,3183) | 1:124:A:VAL:HG21 | 1:121:A:LYS:HA  | 17                  | 0.21     | 0.05                | 0.22       |
| (1,3183) | 1:124:A:VAL:HG22 | 1:121:A:LYS:HA  | 17                  | 0.21     | 0.05                | 0.22       |
| (1,3183) | 1:124:A:VAL:HG23 | 1:121:A:LYS:HA  | 17                  | 0.21     | 0.05                | 0.22       |
| (1,1419) | 1:77:A:LEU:HD13  | 1:25:A:LYS:HA   | 17                  | 0.21     | 0.03                | 0.2        |
| (1,1419) | 1:77:A:LEU:HD11  | 1:25:A:LYS:HA   | 17                  | 0.21     | 0.03                | 0.2        |
| (1,1419) | 1:77:A:LEU:HD12  | 1:25:A:LYS:HA   | 17                  | 0.21     | 0.03                | 0.2        |
| (1,1080) | 1:105:A:LEU:HD11 | 1:92:A:ALA:H    | 17                  | 0.21     | 0.01                | 0.21       |
| (1,1080) | 1:105:A:LEU:HD12 | 1:92:A:ALA:H    | 17                  | 0.21     | 0.01                | 0.21       |
| (1,1080) | 1:105:A:LEU:HD13 | 1:92:A:ALA:H    | 17                  | 0.21     | 0.01                | 0.21       |
| (3,34)   | 1:97:A:LEU:HD22  | 1:31:A:LEU:HD13 | 17                  | 0.21     | 0.07                | 0.24       |
| (3,34)   | 1:97:A:LEU:HD23  | 1:31:A:LEU:HD13 | 17                  | 0.21     | 0.07                | 0.24       |
| (3,34)   | 1:97:A:LEU:HD23  | 1:31:A:LEU:HD12 | 17                  | 0.21     | 0.07                | 0.24       |
| (3,34)   | 1:97:A:LEU:HD21  | 1:31:A:LEU:HD12 | 17                  | 0.21     | 0.07                | 0.24       |
| (3,34)   | 1:97:A:LEU:HD21  | 1:31:A:LEU:HD11 | 17                  | 0.21     | 0.07                | 0.24       |
| (3,34)   | 1:97:A:LEU:HD21  | 1:31:A:LEU:HD13 | 17                  | 0.21     | 0.07                | 0.24       |
| (3,34)   | 1:97:A:LEU:HD22  | 1:31:A:LEU:HD11 | 17                  | 0.21     | 0.07                | 0.24       |
| (3,34)   | 1:97:A:LEU:HD23  | 1:31:A:LEU:HD11 | 17                  | 0.21     | 0.07                | 0.24       |
| (1,1817) | 1:77:A:LEU:HG    | 1:77:A:LEU:HD21 | 17                  | 0.21     | 0.03                | 0.21       |
| (1,1817) | 1:77:A:LEU:HG    | 1:77:A:LEU:HD22 | 17                  | 0.21     | 0.03                | 0.21       |
| (1,1817) | 1:77:A:LEU:HG    | 1:77:A:LEU:HD23 | 17                  | 0.21     | 0.03                | 0.21       |
| (1,3260) | 1:121:A:LYS:HG2  | 1:121:A:LYS:HB2 | 17                  | 0.21     | 0.02                | 0.21       |
| (1,3562) | 1:104:A:GLU:HB3  | 1:91:A:GLY:HA3  | 17                  | 0.21     | 0.01                | 0.21       |
| (1,3139) | 1:69:A:THR:HB    | 1:69:A:THR:H    | 17                  | 0.21     | 0.0                 | 0.21       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,3181) | 1:108:A:GLN:HG3 | 1:108:A:GLN:HA  | 17                  | 0.21     | 0.02                | 0.22       |
| (1,1951) | 1:108:A:GLN:HA  | 1:111:A:GLU:HB3 | 17                  | 0.21     | 0.01                | 0.21       |
| (1,3476) | 1:107:A:GLU:HG2 | 1:108:A:GLN:H   | 17                  | 0.21     | 0.03                | 0.21       |
| (3,92)   | 1:88:A:VAL:HG22 | 1:49:A:LYS:HA   | 17                  | 0.21     | 0.11                | 0.17       |
| (3,92)   | 1:88:A:VAL:HG23 | 1:87:A:GLY:HA2  | 17                  | 0.21     | 0.11                | 0.17       |
| (3,92)   | 1:88:A:VAL:HG22 | 1:87:A:GLY:HA2  | 17                  | 0.21     | 0.11                | 0.17       |
| (3,92)   | 1:88:A:VAL:HG21 | 1:87:A:GLY:HA2  | 17                  | 0.21     | 0.11                | 0.17       |
| (1,1628) | 1:87:A:GLY:HA3  | 1:113:A:ALA:HB1 | 17                  | 0.21     | 0.04                | 0.2        |
| (1,1628) | 1:87:A:GLY:HA3  | 1:113:A:ALA:HB3 | 17                  | 0.21     | 0.04                | 0.2        |
| (1,1628) | 1:87:A:GLY:HA3  | 1:113:A:ALA:HB2 | 17                  | 0.21     | 0.04                | 0.2        |
| (1,3325) | 1:77:A:LEU:HB3  | 1:77:A:LEU:HD13 | 17                  | 0.21     | 0.01                | 0.21       |
| (1,3325) | 1:77:A:LEU:HB3  | 1:77:A:LEU:HD11 | 17                  | 0.21     | 0.01                | 0.21       |
| (1,3325) | 1:77:A:LEU:HB3  | 1:77:A:LEU:HD12 | 17                  | 0.21     | 0.01                | 0.21       |
| (1,1508) | 1:29:A:ALA:H    | 1:28:A:ILE:HG22 | 17                  | 0.21     | 0.01                | 0.21       |
| (1,1508) | 1:29:A:ALA:H    | 1:28:A:ILE:HG21 | 17                  | 0.21     | 0.01                | 0.21       |
| (1,1508) | 1:29:A:ALA:H    | 1:28:A:ILE:HG23 | 17                  | 0.21     | 0.01                | 0.21       |
| (1,3591) | 1:93:A:THR:HB   | 1:88:A:VAL:HG13 | 17                  | 0.21     | 0.03                | 0.2        |
| (1,3591) | 1:93:A:THR:HB   | 1:88:A:VAL:HG12 | 17                  | 0.21     | 0.03                | 0.2        |
| (1,3591) | 1:93:A:THR:HB   | 1:88:A:VAL:HG11 | 17                  | 0.21     | 0.03                | 0.2        |
| (1,2727) | 1:86:A:TYR:HB3  | 1:86:A:TYR:H    | 17                  | 0.2      | 0.01                | 0.2        |
| (1,100)  | 1:35:A:PHE:HE2  | 1:35:A:PHE:H    | 17                  | 0.2      | 0.02                | 0.2        |
| (1,100)  | 1:35:A:PHE:HE1  | 1:35:A:PHE:H    | 17                  | 0.2      | 0.02                | 0.2        |
| (1,3179) | 1:111:A:GLU:HA  | 1:111:A:GLU:H   | 17                  | 0.2      | 0.01                | 0.2        |
| (1,1616) | 1:109:A:HIS:HB2 | 1:108:A:GLN:H   | 17                  | 0.2      | 0.02                | 0.21       |
| (1,3749) | 1:123:A:ARG:H   | 1:121:A:LYS:H   | 17                  | 0.2      | 0.01                | 0.2        |
| (1,1337) | 1:78:A:TYR:HD2  | 1:28:A:ILE:HD11 | 17                  | 0.2      | 0.02                | 0.2        |
| (1,1337) | 1:78:A:TYR:HD1  | 1:28:A:ILE:HD11 | 17                  | 0.2      | 0.02                | 0.2        |
| (1,1337) | 1:78:A:TYR:HD1  | 1:28:A:ILE:HD12 | 17                  | 0.2      | 0.02                | 0.2        |
| (1,1337) | 1:78:A:TYR:HD2  | 1:28:A:ILE:HD12 | 17                  | 0.2      | 0.02                | 0.2        |
| (1,1337) | 1:78:A:TYR:HD2  | 1:28:A:ILE:HD13 | 17                  | 0.2      | 0.02                | 0.2        |
| (1,1337) | 1:78:A:TYR:HD1  | 1:28:A:ILE:HD13 | 17                  | 0.2      | 0.02                | 0.2        |
| (1,2164) | 1:120:A:ALA:HA  | 1:121:A:LYS:H   | 17                  | 0.2      | 0.01                | 0.2        |
| (1,1456) | 1:57:A:VAL:HA   | 1:60:A:VAL:HB   | 17                  | 0.2      | 0.01                | 0.19       |
| (1,2888) | 1:29:A:ALA:HA   | 1:32:A:ALA:HB2  | 17                  | 0.2      | 0.04                | 0.19       |
| (1,2888) | 1:29:A:ALA:HA   | 1:32:A:ALA:HB3  | 17                  | 0.2      | 0.04                | 0.19       |
| (1,2888) | 1:29:A:ALA:HA   | 1:32:A:ALA:HB1  | 17                  | 0.2      | 0.04                | 0.19       |
| (1,3783) | 1:117:A:LEU:HB3 | 1:117:A:LEU:H   | 17                  | 0.2      | 0.08                | 0.15       |
| (1,2035) | 1:52:A:ILE:HG13 | 1:97:A:LEU:HD22 | 17                  | 0.2      | 0.03                | 0.21       |
| (1,2035) | 1:52:A:ILE:HG13 | 1:97:A:LEU:HD23 | 17                  | 0.2      | 0.03                | 0.21       |
| (1,2035) | 1:52:A:ILE:HG13 | 1:97:A:LEU:HD21 | 17                  | 0.2      | 0.03                | 0.21       |
| (1,2221) | 1:31:A:LEU:HA   | 1:60:A:VAL:HB   | 17                  | 0.2      | 0.04                | 0.19       |
| (1,2992) | 1:20:A:LYS:HB3  | 1:20:A:LYS:H    | 17                  | 0.2      | 0.04                | 0.18       |

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| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,3506) | 1:60:A:VAL:HG12  | 1:35:A:PHE:HZ   | 17                  | 0.2      | 0.02                | 0.19       |
| (1,3506) | 1:60:A:VAL:HG13  | 1:35:A:PHE:HZ   | 17                  | 0.2      | 0.02                | 0.19       |
| (1,3506) | 1:60:A:VAL:HG11  | 1:35:A:PHE:HZ   | 17                  | 0.2      | 0.02                | 0.19       |
| (1,3901) | 1:79:A:THR:H     | 1:77:A:LEU:HB2  | 17                  | 0.2      | 0.01                | 0.19       |
| (1,3961) | 1:57:A:VAL:H     | 1:56:A:LEU:HB3  | 17                  | 0.2      | 0.03                | 0.21       |
| (1,3221) | 1:37:A:HIS:HB2   | 1:99:A:GLY:HA2  | 17                  | 0.2      | 0.06                | 0.23       |
| (1,3032) | 1:121:A:LYS:HG3  | 1:121:A:LYS:HE3 | 17                  | 0.19     | 0.04                | 0.17       |
| (1,3698) | 1:30:A:PHE:HD1   | 1:30:A:PHE:H    | 17                  | 0.19     | 0.02                | 0.19       |
| (1,3698) | 1:30:A:PHE:HD2   | 1:30:A:PHE:H    | 17                  | 0.19     | 0.02                | 0.19       |
| (1,3717) | 1:35:A:PHE:H     | 1:39:A:PHE:HE2  | 17                  | 0.19     | 0.01                | 0.19       |
| (1,3717) | 1:35:A:PHE:H     | 1:39:A:PHE:HE1  | 17                  | 0.19     | 0.01                | 0.19       |
| (1,2927) | 1:31:A:LEU:HD21  | 1:39:A:PHE:HD2  | 17                  | 0.19     | 0.01                | 0.19       |
| (1,2927) | 1:31:A:LEU:HD23  | 1:39:A:PHE:HD2  | 17                  | 0.19     | 0.01                | 0.19       |
| (1,2927) | 1:31:A:LEU:HD22  | 1:39:A:PHE:HD2  | 17                  | 0.19     | 0.01                | 0.19       |
| (1,2927) | 1:31:A:LEU:HD22  | 1:39:A:PHE:HD1  | 17                  | 0.19     | 0.01                | 0.19       |
| (1,2927) | 1:31:A:LEU:HD23  | 1:39:A:PHE:HD1  | 17                  | 0.19     | 0.01                | 0.19       |
| (1,2927) | 1:31:A:LEU:HD21  | 1:39:A:PHE:HD1  | 17                  | 0.19     | 0.01                | 0.19       |
| (1,1321) | 1:124:A:VAL:HG12 | 1:125:A:GLN:H   | 17                  | 0.19     | 0.01                | 0.19       |
| (1,1321) | 1:124:A:VAL:HG11 | 1:125:A:GLN:H   | 17                  | 0.19     | 0.01                | 0.19       |
| (1,1321) | 1:124:A:VAL:HG13 | 1:125:A:GLN:H   | 17                  | 0.19     | 0.01                | 0.19       |
| (1,3250) | 1:41:A:ALA:HA    | 1:41:A:ALA:HB2  | 17                  | 0.19     | 0.03                | 0.19       |
| (1,3250) | 1:41:A:ALA:HA    | 1:41:A:ALA:HB3  | 17                  | 0.19     | 0.03                | 0.19       |
| (1,3250) | 1:41:A:ALA:HA    | 1:41:A:ALA:HB1  | 17                  | 0.19     | 0.03                | 0.19       |
| (1,4036) | 1:31:A:LEU:H     | 1:31:A:LEU:HD11 | 17                  | 0.19     | 0.04                | 0.2        |
| (1,4036) | 1:31:A:LEU:H     | 1:31:A:LEU:HD13 | 17                  | 0.19     | 0.04                | 0.2        |
| (1,4036) | 1:31:A:LEU:H     | 1:31:A:LEU:HD12 | 17                  | 0.19     | 0.04                | 0.2        |
| (1,3165) | 1:126:A:ALA:HB2  | 1:125:A:GLN:HG3 | 17                  | 0.19     | 0.02                | 0.19       |
| (1,3165) | 1:126:A:ALA:HB1  | 1:125:A:GLN:HG3 | 17                  | 0.19     | 0.02                | 0.19       |
| (1,3165) | 1:126:A:ALA:HB3  | 1:125:A:GLN:HG3 | 17                  | 0.19     | 0.02                | 0.19       |
| (1,2969) | 1:93:A:THR:HG21  | 1:101:A:PRO:HB3 | 17                  | 0.19     | 0.02                | 0.18       |
| (1,2969) | 1:93:A:THR:HG22  | 1:101:A:PRO:HB3 | 17                  | 0.19     | 0.02                | 0.18       |
| (1,2969) | 1:93:A:THR:HG23  | 1:101:A:PRO:HB3 | 17                  | 0.19     | 0.02                | 0.18       |
| (1,2754) | 1:60:A:VAL:HG12  | 1:59:A:ARG:HD3  | 17                  | 0.19     | 0.03                | 0.18       |
| (1,2754) | 1:60:A:VAL:HG13  | 1:59:A:ARG:HD3  | 17                  | 0.19     | 0.03                | 0.18       |
| (1,2754) | 1:60:A:VAL:HG11  | 1:59:A:ARG:HD3  | 17                  | 0.19     | 0.03                | 0.18       |
| (1,2037) | 1:57:A:VAL:HG22  | 1:57:A:VAL:HG11 | 17                  | 0.19     | 0.03                | 0.19       |
| (1,2037) | 1:57:A:VAL:HG21  | 1:57:A:VAL:HG11 | 17                  | 0.19     | 0.03                | 0.19       |
| (1,2037) | 1:57:A:VAL:HG23  | 1:57:A:VAL:HG11 | 17                  | 0.19     | 0.03                | 0.19       |
| (1,2037) | 1:57:A:VAL:HG21  | 1:57:A:VAL:HG12 | 17                  | 0.19     | 0.03                | 0.19       |
| (1,2037) | 1:57:A:VAL:HG23  | 1:57:A:VAL:HG13 | 17                  | 0.19     | 0.03                | 0.19       |
| (1,2037) | 1:57:A:VAL:HG22  | 1:57:A:VAL:HG12 | 17                  | 0.19     | 0.03                | 0.19       |
| (1,2037) | 1:57:A:VAL:HG23  | 1:57:A:VAL:HG12 | 17                  | 0.19     | 0.03                | 0.19       |

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| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,2037) | 1:57:A:VAL:HG22  | 1:57:A:VAL:HG13 | 17                  | 0.19     | 0.03                | 0.19       |
| (1,1206) | 1:117:A:LEU:HD13 | 1:86:A:TYR:HB2  | 17                  | 0.19     | 0.03                | 0.2        |
| (1,1206) | 1:117:A:LEU:HD11 | 1:86:A:TYR:HB2  | 17                  | 0.19     | 0.03                | 0.2        |
| (1,1206) | 1:117:A:LEU:HD12 | 1:86:A:TYR:HB2  | 17                  | 0.19     | 0.03                | 0.2        |
| (1,2711) | 1:35:A:PHE:HB2   | 1:35:A:PHE:HE2  | 17                  | 0.19     | 0.02                | 0.19       |
| (1,2711) | 1:35:A:PHE:HB2   | 1:35:A:PHE:HE1  | 17                  | 0.19     | 0.02                | 0.19       |
| (1,1556) | 1:59:A:ARG:HB2   | 1:58:A:ASP:HB2  | 17                  | 0.19     | 0.01                | 0.19       |
| (1,3422) | 1:77:A:LEU:HG    | 1:77:A:LEU:HD21 | 17                  | 0.19     | 0.03                | 0.19       |
| (1,3422) | 1:77:A:LEU:HG    | 1:77:A:LEU:HD22 | 17                  | 0.19     | 0.03                | 0.19       |
| (1,3422) | 1:77:A:LEU:HG    | 1:77:A:LEU:HD23 | 17                  | 0.19     | 0.03                | 0.19       |
| (1,1671) | 1:78:A:TYR:HA    | 1:28:A:ILE:HG12 | 17                  | 0.19     | 0.01                | 0.18       |
| (1,1588) | 1:74:A:ALA:HB1   | 1:74:A:ALA:HA   | 17                  | 0.18     | 0.03                | 0.19       |
| (1,1588) | 1:74:A:ALA:HB2   | 1:74:A:ALA:HA   | 17                  | 0.18     | 0.03                | 0.19       |
| (1,1588) | 1:74:A:ALA:HB3   | 1:74:A:ALA:HA   | 17                  | 0.18     | 0.03                | 0.19       |
| (1,3320) | 1:27:A:VAL:HA    | 1:66:A:LEU:HD21 | 17                  | 0.18     | 0.02                | 0.19       |
| (1,3320) | 1:27:A:VAL:HA    | 1:66:A:LEU:HD23 | 17                  | 0.18     | 0.02                | 0.19       |
| (1,3320) | 1:27:A:VAL:HA    | 1:66:A:LEU:HD22 | 17                  | 0.18     | 0.02                | 0.19       |
| (1,3595) | 1:108:A:GLN:HA   | 1:111:A:GLU:HB3 | 17                  | 0.18     | 0.01                | 0.18       |
| (1,2960) | 1:77:A:LEU:HD13  | 1:25:A:LYS:HA   | 17                  | 0.18     | 0.03                | 0.17       |
| (1,2960) | 1:77:A:LEU:HD11  | 1:25:A:LYS:HA   | 17                  | 0.18     | 0.03                | 0.17       |
| (1,2960) | 1:77:A:LEU:HD12  | 1:25:A:LYS:HA   | 17                  | 0.18     | 0.03                | 0.17       |
| (1,3232) | 1:92:A:ALA:H     | 1:105:A:LEU:HB2 | 17                  | 0.18     | 0.02                | 0.18       |
| (1,3781) | 1:119:A:GLU:HA   | 1:119:A:GLU:H   | 17                  | 0.18     | 0.02                | 0.18       |
| (1,1409) | 1:57:A:VAL:HG22  | 1:57:A:VAL:HG11 | 17                  | 0.18     | 0.03                | 0.19       |
| (1,1409) | 1:57:A:VAL:HG21  | 1:57:A:VAL:HG11 | 17                  | 0.18     | 0.03                | 0.19       |
| (1,1409) | 1:57:A:VAL:HG23  | 1:57:A:VAL:HG11 | 17                  | 0.18     | 0.03                | 0.19       |
| (1,1409) | 1:57:A:VAL:HG21  | 1:57:A:VAL:HG12 | 17                  | 0.18     | 0.03                | 0.19       |
| (1,1409) | 1:57:A:VAL:HG23  | 1:57:A:VAL:HG13 | 17                  | 0.18     | 0.03                | 0.19       |
| (1,1409) | 1:57:A:VAL:HG22  | 1:57:A:VAL:HG12 | 17                  | 0.18     | 0.03                | 0.19       |
| (1,1409) | 1:57:A:VAL:HG23  | 1:57:A:VAL:HG12 | 17                  | 0.18     | 0.03                | 0.19       |
| (1,1409) | 1:57:A:VAL:HG22  | 1:57:A:VAL:HG13 | 17                  | 0.18     | 0.03                | 0.19       |
| (1,3322) | 1:30:A:PHE:HD1   | 1:66:A:LEU:HD21 | 17                  | 0.18     | 0.02                | 0.19       |
| (1,3322) | 1:30:A:PHE:HD2   | 1:66:A:LEU:HD23 | 17                  | 0.18     | 0.02                | 0.19       |
| (1,3322) | 1:30:A:PHE:HD2   | 1:66:A:LEU:HD21 | 17                  | 0.18     | 0.02                | 0.19       |
| (1,3322) | 1:30:A:PHE:HD2   | 1:66:A:LEU:HD22 | 17                  | 0.18     | 0.02                | 0.19       |
| (1,3322) | 1:30:A:PHE:HD1   | 1:66:A:LEU:HD22 | 17                  | 0.18     | 0.02                | 0.19       |
| (1,3322) | 1:30:A:PHE:HD1   | 1:66:A:LEU:HD23 | 17                  | 0.18     | 0.02                | 0.19       |
| (1,451)  | 1:32:A:ALA:HB1   | 1:35:A:PHE:H    | 17                  | 0.18     | 0.05                | 0.17       |
| (1,451)  | 1:32:A:ALA:HB2   | 1:35:A:PHE:H    | 17                  | 0.18     | 0.05                | 0.17       |
| (1,451)  | 1:32:A:ALA:HB3   | 1:35:A:PHE:H    | 17                  | 0.18     | 0.05                | 0.17       |
| (1,2639) | 1:71:A:LEU:HD11  | 1:71:A:LEU:HB2  | 17                  | 0.18     | 0.02                | 0.17       |
| (1,2639) | 1:71:A:LEU:HD13  | 1:71:A:LEU:HB2  | 17                  | 0.18     | 0.02                | 0.17       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2639) | 1:71:A:LEU:HD12  | 1:71:A:LEU:HB2   | 17                  | 0.18     | 0.02                | 0.17       |
| (1,2629) | 1:53:A:PHE:HZ    | 1:71:A:LEU:HB2   | 17                  | 0.18     | 0.02                | 0.18       |
| (1,1877) | 1:27:A:VAL:HG23  | 1:27:A:VAL:H     | 17                  | 0.18     | 0.02                | 0.18       |
| (1,1877) | 1:27:A:VAL:HG21  | 1:27:A:VAL:H     | 17                  | 0.18     | 0.02                | 0.18       |
| (1,1877) | 1:27:A:VAL:HG22  | 1:27:A:VAL:H     | 17                  | 0.18     | 0.02                | 0.18       |
| (1,3378) | 1:67:A:SER:HB3   | 1:66:A:LEU:HA    | 17                  | 0.17     | 0.01                | 0.17       |
| (1,1382) | 1:57:A:VAL:HG23  | 1:53:A:PHE:HE2   | 17                  | 0.17     | 0.03                | 0.17       |
| (1,1382) | 1:57:A:VAL:HG22  | 1:53:A:PHE:HE2   | 17                  | 0.17     | 0.03                | 0.17       |
| (1,1382) | 1:57:A:VAL:HG23  | 1:53:A:PHE:HE1   | 17                  | 0.17     | 0.03                | 0.17       |
| (1,1382) | 1:57:A:VAL:HG21  | 1:53:A:PHE:HE1   | 17                  | 0.17     | 0.03                | 0.17       |
| (1,1382) | 1:57:A:VAL:HG21  | 1:53:A:PHE:HE2   | 17                  | 0.17     | 0.03                | 0.17       |
| (1,1382) | 1:57:A:VAL:HG22  | 1:53:A:PHE:HE1   | 17                  | 0.17     | 0.03                | 0.17       |
| (1,1511) | 1:28:A:ILE:HA    | 1:28:A:ILE:HG21  | 17                  | 0.17     | 0.02                | 0.17       |
| (1,1511) | 1:28:A:ILE:HA    | 1:28:A:ILE:HG23  | 17                  | 0.17     | 0.02                | 0.17       |
| (1,1511) | 1:28:A:ILE:HA    | 1:28:A:ILE:HG22  | 17                  | 0.17     | 0.02                | 0.17       |
| (1,1812) | 1:117:A:LEU:HA   | 1:117:A:LEU:HD11 | 17                  | 0.17     | 0.05                | 0.14       |
| (1,1812) | 1:117:A:LEU:HA   | 1:117:A:LEU:HD12 | 17                  | 0.17     | 0.05                | 0.14       |
| (1,1812) | 1:117:A:LEU:HA   | 1:117:A:LEU:HD13 | 17                  | 0.17     | 0.05                | 0.14       |
| (1,1928) | 1:105:A:LEU:HB3  | 1:109:A:HIS:HB2  | 17                  | 0.17     | 0.01                | 0.17       |
| (1,397)  | 1:57:A:VAL:H     | 1:56:A:LEU:HB3   | 17                  | 0.17     | 0.03                | 0.18       |
| (1,2489) | 1:28:A:ILE:HA    | 1:28:A:ILE:HG21  | 17                  | 0.17     | 0.02                | 0.17       |
| (1,2489) | 1:28:A:ILE:HA    | 1:28:A:ILE:HG23  | 17                  | 0.17     | 0.02                | 0.17       |
| (1,2489) | 1:28:A:ILE:HA    | 1:28:A:ILE:HG22  | 17                  | 0.17     | 0.02                | 0.17       |
| (1,4133) | 1:82:A:TRP:HE1   | 1:82:A:TRP:HD1   | 17                  | 0.17     | 0.01                | 0.17       |
| (1,2712) | 1:39:A:PHE:HB3   | 1:35:A:PHE:HB3   | 17                  | 0.17     | 0.01                | 0.17       |
| (1,2288) | 1:70:A:GLN:HA    | 1:70:A:GLN:HG3   | 17                  | 0.17     | 0.03                | 0.17       |
| (1,1726) | 1:66:A:LEU:HD11  | 1:66:A:LEU:HA    | 17                  | 0.17     | 0.03                | 0.18       |
| (1,1726) | 1:66:A:LEU:HD12  | 1:66:A:LEU:HA    | 17                  | 0.17     | 0.03                | 0.18       |
| (1,1726) | 1:66:A:LEU:HD13  | 1:66:A:LEU:HA    | 17                  | 0.17     | 0.03                | 0.18       |
| (1,3053) | 1:29:A:ALA:H     | 1:28:A:ILE:HG22  | 17                  | 0.17     | 0.02                | 0.17       |
| (1,3053) | 1:29:A:ALA:H     | 1:28:A:ILE:HG21  | 17                  | 0.17     | 0.02                | 0.17       |
| (1,3053) | 1:29:A:ALA:H     | 1:28:A:ILE:HG23  | 17                  | 0.17     | 0.02                | 0.17       |
| (1,3197) | 1:87:A:GLY:HA3   | 1:113:A:ALA:HB1  | 17                  | 0.17     | 0.04                | 0.16       |
| (1,3197) | 1:87:A:GLY:HA3   | 1:113:A:ALA:HB3  | 17                  | 0.17     | 0.04                | 0.16       |
| (1,3197) | 1:87:A:GLY:HA3   | 1:113:A:ALA:HB2  | 17                  | 0.17     | 0.04                | 0.16       |
| (1,2621) | 1:105:A:LEU:HD11 | 1:92:A:ALA:H     | 17                  | 0.17     | 0.02                | 0.17       |
| (1,2621) | 1:105:A:LEU:HD12 | 1:92:A:ALA:H     | 17                  | 0.17     | 0.02                | 0.17       |
| (1,2621) | 1:105:A:LEU:HD13 | 1:92:A:ALA:H     | 17                  | 0.17     | 0.02                | 0.17       |
| (1,2855) | 1:78:A:TYR:HD2   | 1:28:A:ILE:HD11  | 17                  | 0.17     | 0.02                | 0.16       |
| (1,2855) | 1:78:A:TYR:HD1   | 1:28:A:ILE:HD11  | 17                  | 0.17     | 0.02                | 0.16       |
| (1,2855) | 1:78:A:TYR:HD1   | 1:28:A:ILE:HD12  | 17                  | 0.17     | 0.02                | 0.16       |
| (1,2855) | 1:78:A:TYR:HD2   | 1:28:A:ILE:HD12  | 17                  | 0.17     | 0.02                | 0.16       |

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| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,2855) | 1:78:A:TYR:HD2   | 1:28:A:ILE:HD13 | 17                  | 0.17     | 0.02                | 0.16       |
| (1,2855) | 1:78:A:TYR:HD1   | 1:28:A:ILE:HD13 | 17                  | 0.17     | 0.02                | 0.16       |
| (1,3917) | 1:74:A:ALA:HA    | 1:75:A:LEU:H    | 17                  | 0.17     | 0.01                | 0.16       |
| (1,1440) | 1:105:A:LEU:H    | 1:101:A:PRO:HD3 | 17                  | 0.16     | 0.01                | 0.17       |
| (1,1108) | 1:56:A:LEU:HD13  | 1:52:A:ILE:HG12 | 17                  | 0.16     | 0.02                | 0.17       |
| (1,1108) | 1:56:A:LEU:HD11  | 1:52:A:ILE:HG12 | 17                  | 0.16     | 0.02                | 0.17       |
| (1,1108) | 1:56:A:LEU:HD12  | 1:52:A:ILE:HG12 | 17                  | 0.16     | 0.02                | 0.17       |
| (1,1325) | 1:53:A:PHE:HE1   | 1:75:A:LEU:HB3  | 17                  | 0.16     | 0.02                | 0.16       |
| (1,1325) | 1:53:A:PHE:HE2   | 1:75:A:LEU:HB3  | 17                  | 0.16     | 0.02                | 0.16       |
| (1,2530) | 1:33:A:GLU:HA    | 1:34:A:ARG:H    | 17                  | 0.16     | 0.01                | 0.16       |
| (1,3230) | 1:68:A:LYS:HB2   | 1:68:A:LYS:HA   | 17                  | 0.16     | 0.05                | 0.14       |
| (1,134)  | 1:123:A:ARG:H    | 1:121:A:LYS:H   | 17                  | 0.16     | 0.01                | 0.16       |
| (1,2514) | 1:120:A:ALA:H    | 1:120:A:ALA:HA  | 17                  | 0.16     | 0.01                | 0.16       |
| (1,2840) | 1:124:A:VAL:HG12 | 1:125:A:GLN:H   | 17                  | 0.16     | 0.01                | 0.16       |
| (1,2840) | 1:124:A:VAL:HG11 | 1:125:A:GLN:H   | 17                  | 0.16     | 0.01                | 0.16       |
| (1,2840) | 1:124:A:VAL:HG13 | 1:125:A:GLN:H   | 17                  | 0.16     | 0.01                | 0.16       |
| (1,1638) | 1:124:A:VAL:HG11 | 1:124:A:VAL:HA  | 17                  | 0.16     | 0.01                | 0.16       |
| (1,1638) | 1:124:A:VAL:HG13 | 1:124:A:VAL:HA  | 17                  | 0.16     | 0.01                | 0.16       |
| (1,1638) | 1:124:A:VAL:HG12 | 1:124:A:VAL:HA  | 17                  | 0.16     | 0.01                | 0.16       |
| (1,4317) | 1:93:A:THR:HB    | 1:102:A:CYS:H   | 17                  | 0.16     | 0.02                | 0.15       |
| (1,2995) | 1:60:A:VAL:H     | 1:60:A:VAL:HB   | 17                  | 0.16     | 0.01                | 0.16       |
| (1,3582) | 1:110:A:VAL:H    | 1:109:A:HIS:HA  | 17                  | 0.16     | 0.01                | 0.16       |
| (1,4193) | 1:69:A:THR:HB    | 1:72:A:ARG:H    | 17                  | 0.16     | 0.01                | 0.16       |
| (1,80)   | 1:30:A:PHE:HD1   | 1:30:A:PHE:H    | 17                  | 0.16     | 0.02                | 0.15       |
| (1,80)   | 1:30:A:PHE:HD2   | 1:30:A:PHE:H    | 17                  | 0.16     | 0.02                | 0.15       |
| (1,2045) | 1:77:A:LEU:H     | 1:78:A:TYR:H    | 17                  | 0.16     | 0.03                | 0.16       |
| (1,4212) | 1:115:A:LYS:HE3  | 1:115:A:LYS:H   | 17                  | 0.16     | 0.02                | 0.16       |
| (1,3241) | 1:52:A:ILE:HG13  | 1:97:A:LEU:HD22 | 17                  | 0.16     | 0.03                | 0.17       |
| (1,3241) | 1:52:A:ILE:HG13  | 1:97:A:LEU:HD23 | 17                  | 0.16     | 0.03                | 0.17       |
| (1,3241) | 1:52:A:ILE:HG13  | 1:97:A:LEU:HD21 | 17                  | 0.16     | 0.03                | 0.17       |
| (1,2351) | 1:110:A:VAL:HG21 | 1:109:A:HIS:HA  | 17                  | 0.15     | 0.02                | 0.15       |
| (1,2351) | 1:110:A:VAL:HG22 | 1:109:A:HIS:HA  | 17                  | 0.15     | 0.02                | 0.15       |
| (1,2351) | 1:110:A:VAL:HG23 | 1:109:A:HIS:HA  | 17                  | 0.15     | 0.02                | 0.15       |
| (1,3185) | 1:109:A:HIS:HB2  | 1:108:A:GLN:H   | 17                  | 0.15     | 0.01                | 0.16       |
| (1,2637) | 1:71:A:LEU:HB3   | 1:71:A:LEU:HG   | 17                  | 0.15     | 0.01                | 0.15       |
| (1,3916) | 1:71:A:LEU:HA    | 1:74:A:ALA:H    | 17                  | 0.15     | 0.01                | 0.15       |
| (1,3830) | 1:101:A:PRO:HD3  | 1:100:A:ASN:H   | 17                  | 0.15     | 0.02                | 0.15       |
| (1,1775) | 1:88:A:VAL:HA    | 1:47:A:PRO:HB3  | 17                  | 0.15     | 0.02                | 0.15       |
| (1,3940) | 1:62:A:GLY:HA3   | 1:63:A:GLU:H    | 17                  | 0.15     | 0.02                | 0.15       |
| (1,3000) | 1:57:A:VAL:HA    | 1:60:A:VAL:HB   | 17                  | 0.15     | 0.01                | 0.14       |
| (1,311)  | 1:79:A:THR:H     | 1:77:A:LEU:HB2  | 17                  | 0.15     | 0.01                | 0.14       |
| (1,1439) | 1:103:A:GLY:HA3  | 1:101:A:PRO:HD3 | 17                  | 0.15     | 0.01                | 0.15       |

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| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,3130) | 1:123:A:ARG:HG2  | 1:123:A:ARG:H   | 17                  | 0.15     | 0.02                | 0.14       |
| (1,1352) | 1:122:A:ALA:HB3  | 1:122:A:ALA:H   | 17                  | 0.14     | 0.02                | 0.14       |
| (1,1352) | 1:122:A:ALA:HB1  | 1:122:A:ALA:H   | 17                  | 0.14     | 0.02                | 0.14       |
| (1,1352) | 1:122:A:ALA:HB2  | 1:122:A:ALA:H   | 17                  | 0.14     | 0.02                | 0.14       |
| (1,101)  | 1:35:A:PHE:H     | 1:39:A:PHE:HE2  | 17                  | 0.14     | 0.01                | 0.14       |
| (1,101)  | 1:35:A:PHE:H     | 1:39:A:PHE:HE1  | 17                  | 0.14     | 0.01                | 0.14       |
| (1,4270) | 1:75:A:LEU:HB3   | 1:74:A:ALA:H    | 17                  | 0.14     | 0.02                | 0.14       |
| (1,1239) | 1:79:A:THR:H     | 1:78:A:TYR:HE2  | 17                  | 0.14     | 0.01                | 0.14       |
| (1,1239) | 1:79:A:THR:H     | 1:78:A:TYR:HE1  | 17                  | 0.14     | 0.01                | 0.14       |
| (1,2118) | 1:69:A:THR:HB    | 1:69:A:THR:HG23 | 17                  | 0.14     | 0.01                | 0.14       |
| (1,2118) | 1:69:A:THR:HB    | 1:69:A:THR:HG22 | 17                  | 0.14     | 0.01                | 0.14       |
| (1,2118) | 1:69:A:THR:HB    | 1:69:A:THR:HG21 | 17                  | 0.14     | 0.01                | 0.14       |
| (1,3120) | 1:59:A:ARG:HB2   | 1:58:A:ASP:HB2  | 17                  | 0.14     | 0.01                | 0.14       |
| (1,3502) | 1:27:A:VAL:HG23  | 1:27:A:VAL:H    | 17                  | 0.14     | 0.02                | 0.14       |
| (1,3502) | 1:27:A:VAL:HG21  | 1:27:A:VAL:H    | 17                  | 0.14     | 0.02                | 0.14       |
| (1,3502) | 1:27:A:VAL:HG22  | 1:27:A:VAL:H    | 17                  | 0.14     | 0.02                | 0.14       |
| (1,3059) | 1:28:A:ILE:HB    | 1:28:A:ILE:HG22 | 17                  | 0.14     | 0.03                | 0.15       |
| (1,3059) | 1:28:A:ILE:HB    | 1:28:A:ILE:HG21 | 17                  | 0.14     | 0.03                | 0.15       |
| (1,3059) | 1:28:A:ILE:HB    | 1:28:A:ILE:HG23 | 17                  | 0.14     | 0.03                | 0.15       |
| (1,3087) | 1:56:A:LEU:HG    | 1:56:A:LEU:HA   | 17                  | 0.14     | 0.01                | 0.14       |
| (3,137)  | 1:123:A:ARG:H    | 1:123:A:ARG:HA  | 17                  | 0.14     | 0.01                | 0.14       |
| (1,2612) | 1:30:A:PHE:HD2   | 1:34:A:ARG:HG2  | 17                  | 0.14     | 0.01                | 0.14       |
| (1,2612) | 1:30:A:PHE:HD1   | 1:34:A:ARG:HG2  | 17                  | 0.14     | 0.01                | 0.14       |
| (1,4148) | 1:25:A:LYS:HB2   | 1:26:A:GLU:H    | 17                  | 0.14     | 0.01                | 0.14       |
| (1,1240) | 1:78:A:TYR:HE2   | 1:79:A:THR:HB   | 17                  | 0.14     | 0.01                | 0.14       |
| (1,1240) | 1:78:A:TYR:HE1   | 1:79:A:THR:HB   | 17                  | 0.14     | 0.01                | 0.14       |
| (1,2648) | 1:56:A:LEU:HD13  | 1:52:A:ILE:HG12 | 17                  | 0.14     | 0.02                | 0.14       |
| (1,2648) | 1:56:A:LEU:HD11  | 1:52:A:ILE:HG12 | 17                  | 0.14     | 0.02                | 0.14       |
| (1,2648) | 1:56:A:LEU:HD12  | 1:52:A:ILE:HG12 | 17                  | 0.14     | 0.02                | 0.14       |
| (1,1275) | 1:84:A:TYR:HE1   | 1:84:A:TYR:HB3  | 17                  | 0.14     | 0.03                | 0.14       |
| (1,1275) | 1:84:A:TYR:HE2   | 1:84:A:TYR:HB3  | 17                  | 0.14     | 0.03                | 0.14       |
| (1,1906) | 1:105:A:LEU:HB3  | 1:101:A:PRO:HB3 | 17                  | 0.13     | 0.01                | 0.13       |
| (1,3205) | 1:124:A:VAL:HA   | 1:124:A:VAL:HB  | 17                  | 0.13     | 0.01                | 0.14       |
| (1,3208) | 1:124:A:VAL:HG11 | 1:124:A:VAL:HA  | 17                  | 0.13     | 0.01                | 0.13       |
| (1,3208) | 1:124:A:VAL:HG13 | 1:124:A:VAL:HA  | 17                  | 0.13     | 0.01                | 0.13       |
| (1,3208) | 1:124:A:VAL:HG12 | 1:124:A:VAL:HA  | 17                  | 0.13     | 0.01                | 0.13       |
| (1,4228) | 1:123:A:ARG:HB3  | 1:124:A:VAL:H   | 17                  | 0.13     | 0.01                | 0.13       |
| (1,1796) | 1:53:A:PHE:HE1   | 1:68:A:LYS:HA   | 17                  | 0.13     | 0.01                | 0.13       |
| (1,1796) | 1:53:A:PHE:HE2   | 1:68:A:LYS:HA   | 17                  | 0.13     | 0.01                | 0.13       |
| (1,872)  | 1:56:A:LEU:HB3   | 1:56:A:LEU:HA   | 17                  | 0.13     | 0.01                | 0.13       |
| (1,4194) | 1:107:A:GLU:H    | 1:106:A:ASP:HA  | 17                  | 0.13     | 0.02                | 0.12       |
| (1,3244) | 1:78:A:TYR:HA    | 1:28:A:ILE:HG12 | 17                  | 0.12     | 0.01                | 0.12       |

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| Key      | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,1526) | 1:54:A:GLN:HB3  | 1:54:A:GLN:HA    | 17                  | 0.12     | 0.01                | 0.12       |
| (1,3568) | 1:105:A:LEU:HB3 | 1:109:A:HIS:HB2  | 17                  | 0.12     | 0.01                | 0.12       |
| (3,48)   | 1:72:A:ARG:HD3  | 1:72:A:ARG:HB3   | 17                  | 0.12     | 0.01                | 0.11       |
| (1,1158) | 1:120:A:ALA:HB2 | 1:82:A:TRP:HD1   | 16                  | 0.75     | 0.17                | 0.78       |
| (1,1158) | 1:120:A:ALA:HB3 | 1:82:A:TRP:HD1   | 16                  | 0.75     | 0.17                | 0.78       |
| (1,1158) | 1:120:A:ALA:HB1 | 1:82:A:TRP:HD1   | 16                  | 0.75     | 0.17                | 0.78       |
| (1,720)  | 1:120:A:ALA:H   | 1:85:A:LEU:HD21  | 16                  | 0.7      | 0.18                | 0.7        |
| (1,720)  | 1:120:A:ALA:H   | 1:85:A:LEU:HD22  | 16                  | 0.7      | 0.18                | 0.7        |
| (1,720)  | 1:120:A:ALA:H   | 1:85:A:LEU:HD23  | 16                  | 0.7      | 0.18                | 0.7        |
| (1,2681) | 1:120:A:ALA:HB2 | 1:82:A:TRP:HD1   | 16                  | 0.7      | 0.16                | 0.72       |
| (1,2681) | 1:120:A:ALA:HB3 | 1:82:A:TRP:HD1   | 16                  | 0.7      | 0.16                | 0.72       |
| (1,2681) | 1:120:A:ALA:HB1 | 1:82:A:TRP:HD1   | 16                  | 0.7      | 0.16                | 0.72       |
| (1,4084) | 1:20:A:LYS:HB3  | 1:22:A:ASN:HD22  | 16                  | 0.64     | 0.34                | 0.66       |
| (1,1334) | 1:81:A:SER:HB3  | 1:84:A:TYR:HD2   | 16                  | 0.53     | 0.08                | 0.55       |
| (1,1334) | 1:81:A:SER:HB3  | 1:84:A:TYR:HD1   | 16                  | 0.53     | 0.08                | 0.55       |
| (3,59)   | 1:117:A:LEU:HA  | 1:85:A:LEU:HD21  | 16                  | 0.48     | 0.22                | 0.5        |
| (3,59)   | 1:117:A:LEU:HA  | 1:85:A:LEU:HD22  | 16                  | 0.48     | 0.22                | 0.5        |
| (3,59)   | 1:117:A:LEU:HA  | 1:85:A:LEU:HD23  | 16                  | 0.48     | 0.22                | 0.5        |
| (1,2852) | 1:81:A:SER:HB3  | 1:84:A:TYR:HD2   | 16                  | 0.48     | 0.09                | 0.5        |
| (1,2852) | 1:81:A:SER:HB3  | 1:84:A:TYR:HD1   | 16                  | 0.48     | 0.09                | 0.5        |
| (1,4007) | 1:41:A:ALA:HB2  | 1:41:A:ALA:H     | 16                  | 0.46     | 0.05                | 0.48       |
| (1,4007) | 1:41:A:ALA:HB3  | 1:41:A:ALA:H     | 16                  | 0.46     | 0.05                | 0.48       |
| (1,4007) | 1:41:A:ALA:HB1  | 1:41:A:ALA:H     | 16                  | 0.46     | 0.05                | 0.48       |
| (1,2172) | 1:34:A:ARG:HD3  | 1:60:A:VAL:HG13  | 16                  | 0.44     | 0.08                | 0.41       |
| (1,2172) | 1:34:A:ARG:HD3  | 1:60:A:VAL:HG11  | 16                  | 0.44     | 0.08                | 0.41       |
| (1,2172) | 1:34:A:ARG:HD3  | 1:60:A:VAL:HG12  | 16                  | 0.44     | 0.08                | 0.41       |
| (3,126)  | 1:21:A:LEU:HD22 | 1:22:A:ASN:H     | 16                  | 0.44     | 0.12                | 0.47       |
| (3,126)  | 1:21:A:LEU:HD23 | 1:22:A:ASN:H     | 16                  | 0.44     | 0.12                | 0.47       |
| (3,126)  | 1:21:A:LEU:HD21 | 1:22:A:ASN:H     | 16                  | 0.44     | 0.12                | 0.47       |
| (1,442)  | 1:41:A:ALA:HB2  | 1:41:A:ALA:H     | 16                  | 0.43     | 0.05                | 0.44       |
| (1,442)  | 1:41:A:ALA:HB3  | 1:41:A:ALA:H     | 16                  | 0.43     | 0.05                | 0.44       |
| (1,442)  | 1:41:A:ALA:HB1  | 1:41:A:ALA:H     | 16                  | 0.43     | 0.05                | 0.44       |
| (3,124)  | 1:88:A:VAL:HG23 | 1:88:A:VAL:H     | 16                  | 0.42     | 0.05                | 0.42       |
| (3,124)  | 1:88:A:VAL:HG22 | 1:88:A:VAL:H     | 16                  | 0.42     | 0.05                | 0.42       |
| (3,124)  | 1:88:A:VAL:HG23 | 1:84:A:TYR:HE2   | 16                  | 0.42     | 0.05                | 0.42       |
| (3,124)  | 1:88:A:VAL:HG21 | 1:88:A:VAL:H     | 16                  | 0.42     | 0.05                | 0.42       |
| (1,3446) | 1:65:A:ASN:HD22 | 1:20:A:LYS:HG2   | 16                  | 0.41     | 0.1                 | 0.38       |
| (1,3627) | 1:100:A:ASN:H   | 1:100:A:ASN:HD21 | 16                  | 0.37     | 0.1                 | 0.36       |
| (1,1480) | 1:64:A:MET:HE1  | 1:63:A:GLU:H     | 16                  | 0.36     | 0.15                | 0.32       |
| (1,1480) | 1:64:A:MET:HE2  | 1:63:A:GLU:H     | 16                  | 0.36     | 0.15                | 0.32       |
| (1,1480) | 1:64:A:MET:HE3  | 1:63:A:GLU:H     | 16                  | 0.36     | 0.15                | 0.32       |
| (1,12)   | 1:100:A:ASN:H   | 1:100:A:ASN:HD21 | 16                  | 0.32     | 0.1                 | 0.32       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,3135) | 1:68:A:LYS:HD3  | 1:68:A:LYS:HB2  | 16                  | 0.32     | 0.06                | 0.34       |
| (1,3021) | 1:64:A:MET:HE1  | 1:63:A:GLU:H    | 16                  | 0.31     | 0.15                | 0.26       |
| (1,3021) | 1:64:A:MET:HE2  | 1:63:A:GLU:H    | 16                  | 0.31     | 0.15                | 0.26       |
| (1,3021) | 1:64:A:MET:HE3  | 1:63:A:GLU:H    | 16                  | 0.31     | 0.15                | 0.26       |
| (1,2933) | 1:95:A:VAL:HG23 | 1:99:A:GLY:H    | 16                  | 0.3      | 0.04                | 0.3        |
| (1,2933) | 1:95:A:VAL:HG22 | 1:99:A:GLY:H    | 16                  | 0.3      | 0.04                | 0.3        |
| (1,2933) | 1:95:A:VAL:HG21 | 1:99:A:GLY:H    | 16                  | 0.3      | 0.04                | 0.3        |
| (1,1881) | 1:113:A:ALA:HB3 | 1:88:A:VAL:HA   | 16                  | 0.3      | 0.1                 | 0.29       |
| (1,1881) | 1:113:A:ALA:HB2 | 1:88:A:VAL:HA   | 16                  | 0.3      | 0.1                 | 0.29       |
| (1,1881) | 1:113:A:ALA:HB1 | 1:88:A:VAL:HA   | 16                  | 0.3      | 0.1                 | 0.29       |
| (1,3599) | 1:92:A:ALA:HB3  | 1:113:A:ALA:HB3 | 16                  | 0.28     | 0.09                | 0.3        |
| (1,3599) | 1:92:A:ALA:HB3  | 1:113:A:ALA:HB1 | 16                  | 0.28     | 0.09                | 0.3        |
| (1,3599) | 1:92:A:ALA:HB2  | 1:113:A:ALA:HB1 | 16                  | 0.28     | 0.09                | 0.3        |
| (1,3599) | 1:92:A:ALA:HB2  | 1:113:A:ALA:HB2 | 16                  | 0.28     | 0.09                | 0.3        |
| (1,3599) | 1:92:A:ALA:HB1  | 1:113:A:ALA:HB1 | 16                  | 0.28     | 0.09                | 0.3        |
| (1,3599) | 1:92:A:ALA:HB1  | 1:113:A:ALA:HB2 | 16                  | 0.28     | 0.09                | 0.3        |
| (1,3599) | 1:92:A:ALA:HB1  | 1:113:A:ALA:HB3 | 16                  | 0.28     | 0.09                | 0.3        |
| (1,4006) | 1:42:A:GLU:HB3  | 1:41:A:ALA:H    | 16                  | 0.28     | 0.02                | 0.28       |
| (1,117)  | 1:27:A:VAL:HG13 | 1:26:A:GLU:H    | 16                  | 0.28     | 0.05                | 0.26       |
| (1,117)  | 1:27:A:VAL:HG11 | 1:26:A:GLU:H    | 16                  | 0.28     | 0.05                | 0.26       |
| (1,117)  | 1:27:A:VAL:HG12 | 1:26:A:GLU:H    | 16                  | 0.28     | 0.05                | 0.26       |
| (1,1365) | 1:32:A:ALA:HB3  | 1:28:A:ILE:HG22 | 16                  | 0.27     | 0.06                | 0.29       |
| (1,1365) | 1:32:A:ALA:HB1  | 1:28:A:ILE:HG21 | 16                  | 0.27     | 0.06                | 0.29       |
| (1,1365) | 1:32:A:ALA:HB1  | 1:28:A:ILE:HG23 | 16                  | 0.27     | 0.06                | 0.29       |
| (1,1365) | 1:32:A:ALA:HB2  | 1:28:A:ILE:HG23 | 16                  | 0.27     | 0.06                | 0.29       |
| (1,1365) | 1:32:A:ALA:HB2  | 1:28:A:ILE:HG22 | 16                  | 0.27     | 0.06                | 0.29       |
| (1,1365) | 1:32:A:ALA:HB3  | 1:28:A:ILE:HG23 | 16                  | 0.27     | 0.06                | 0.29       |
| (1,1365) | 1:32:A:ALA:HB3  | 1:28:A:ILE:HG21 | 16                  | 0.27     | 0.06                | 0.29       |
| (3,83)   | 1:114:A:ARG:HB2 | 1:113:A:ALA:HB1 | 16                  | 0.26     | 0.07                | 0.26       |
| (3,83)   | 1:114:A:ARG:HB2 | 1:113:A:ALA:HB3 | 16                  | 0.26     | 0.07                | 0.26       |
| (3,83)   | 1:114:A:ARG:HB2 | 1:113:A:ALA:HB2 | 16                  | 0.26     | 0.07                | 0.26       |
| (1,4109) | 1:97:A:LEU:HD11 | 1:98:A:ASP:H    | 16                  | 0.26     | 0.11                | 0.22       |
| (1,4109) | 1:97:A:LEU:HD13 | 1:98:A:ASP:H    | 16                  | 0.26     | 0.11                | 0.22       |
| (1,4109) | 1:97:A:LEU:HD12 | 1:98:A:ASP:H    | 16                  | 0.26     | 0.11                | 0.22       |
| (1,3508) | 1:113:A:ALA:HB3 | 1:88:A:VAL:HA   | 16                  | 0.25     | 0.1                 | 0.24       |
| (1,3508) | 1:113:A:ALA:HB2 | 1:88:A:VAL:HA   | 16                  | 0.25     | 0.1                 | 0.24       |
| (1,3508) | 1:113:A:ALA:HB1 | 1:88:A:VAL:HA   | 16                  | 0.25     | 0.1                 | 0.24       |
| (1,2336) | 1:64:A:MET:HE1  | 1:31:A:LEU:HA   | 16                  | 0.24     | 0.1                 | 0.2        |
| (1,2336) | 1:64:A:MET:HE2  | 1:31:A:LEU:HA   | 16                  | 0.24     | 0.1                 | 0.2        |
| (1,2336) | 1:64:A:MET:HE3  | 1:31:A:LEU:HA   | 16                  | 0.24     | 0.1                 | 0.2        |
| (1,441)  | 1:42:A:GLU:HB3  | 1:41:A:ALA:H    | 16                  | 0.24     | 0.02                | 0.24       |
| (1,2891) | 1:32:A:ALA:HB3  | 1:28:A:ILE:HG22 | 16                  | 0.24     | 0.06                | 0.25       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,2891) | 1:32:A:ALA:HB1  | 1:28:A:ILE:HG21 | 16                  | 0.24     | 0.06                | 0.25       |
| (1,2891) | 1:32:A:ALA:HB1  | 1:28:A:ILE:HG23 | 16                  | 0.24     | 0.06                | 0.25       |
| (1,2891) | 1:32:A:ALA:HB2  | 1:28:A:ILE:HG23 | 16                  | 0.24     | 0.06                | 0.25       |
| (1,2891) | 1:32:A:ALA:HB2  | 1:28:A:ILE:HG22 | 16                  | 0.24     | 0.06                | 0.25       |
| (1,2891) | 1:32:A:ALA:HB3  | 1:28:A:ILE:HG23 | 16                  | 0.24     | 0.06                | 0.25       |
| (1,2891) | 1:32:A:ALA:HB3  | 1:28:A:ILE:HG21 | 16                  | 0.24     | 0.06                | 0.25       |
| (1,3465) | 1:88:A:VAL:HG23 | 1:85:A:LEU:HB3  | 16                  | 0.24     | 0.05                | 0.24       |
| (1,3465) | 1:88:A:VAL:HG21 | 1:85:A:LEU:HB3  | 16                  | 0.24     | 0.05                | 0.24       |
| (1,3465) | 1:88:A:VAL:HG22 | 1:85:A:LEU:HB3  | 16                  | 0.24     | 0.05                | 0.24       |
| (1,2745) | 1:34:A:ARG:HD3  | 1:34:A:ARG:HG3  | 16                  | 0.23     | 0.01                | 0.23       |
| (1,3437) | 1:21:A:LEU:HB2  | 1:21:A:LEU:HD13 | 16                  | 0.23     | 0.07                | 0.23       |
| (1,3437) | 1:21:A:LEU:HB2  | 1:21:A:LEU:HD11 | 16                  | 0.23     | 0.07                | 0.23       |
| (1,3437) | 1:21:A:LEU:HB2  | 1:21:A:LEU:HD12 | 16                  | 0.23     | 0.07                | 0.23       |
| (1,3430) | 1:45:A:ALA:HB3  | 1:84:A:TYR:HA   | 16                  | 0.22     | 0.05                | 0.22       |
| (1,3430) | 1:45:A:ALA:HB2  | 1:84:A:TYR:HA   | 16                  | 0.22     | 0.05                | 0.22       |
| (1,3430) | 1:45:A:ALA:HB1  | 1:84:A:TYR:HA   | 16                  | 0.22     | 0.05                | 0.22       |
| (1,1629) | 1:116:A:GLN:HG3 | 1:113:A:ALA:HB3 | 16                  | 0.21     | 0.05                | 0.22       |
| (1,1629) | 1:116:A:GLN:HG3 | 1:113:A:ALA:HB2 | 16                  | 0.21     | 0.05                | 0.22       |
| (1,1629) | 1:116:A:GLN:HG3 | 1:113:A:ALA:HB1 | 16                  | 0.21     | 0.05                | 0.22       |
| (1,4069) | 1:13:A:ASP:HB2  | 1:13:A:ASP:H    | 16                  | 0.21     | 0.02                | 0.2        |
| (1,234)  | 1:95:A:VAL:HG23 | 1:99:A:GLY:H    | 16                  | 0.2      | 0.04                | 0.2        |
| (1,234)  | 1:95:A:VAL:HG22 | 1:99:A:GLY:H    | 16                  | 0.2      | 0.04                | 0.2        |
| (1,234)  | 1:95:A:VAL:HG21 | 1:99:A:GLY:H    | 16                  | 0.2      | 0.04                | 0.2        |
| (1,3744) | 1:35:A:PHE:HD2  | 1:39:A:PHE:H    | 16                  | 0.2      | 0.06                | 0.18       |
| (1,3744) | 1:35:A:PHE:HD1  | 1:39:A:PHE:H    | 16                  | 0.2      | 0.06                | 0.18       |
| (1,1773) | 1:24:A:SER:HA   | 1:27:A:VAL:HG23 | 16                  | 0.2      | 0.04                | 0.2        |
| (1,1773) | 1:24:A:SER:HA   | 1:27:A:VAL:HG21 | 16                  | 0.2      | 0.04                | 0.2        |
| (1,1773) | 1:24:A:SER:HA   | 1:27:A:VAL:HG22 | 16                  | 0.2      | 0.04                | 0.2        |
| (1,2116) | 1:45:A:ALA:HB3  | 1:84:A:TYR:HA   | 16                  | 0.2      | 0.05                | 0.19       |
| (1,2116) | 1:45:A:ALA:HB2  | 1:84:A:TYR:HA   | 16                  | 0.2      | 0.05                | 0.19       |
| (1,2116) | 1:45:A:ALA:HB1  | 1:84:A:TYR:HA   | 16                  | 0.2      | 0.05                | 0.19       |
| (1,4202) | 1:127:A:GLN:H   | 1:127:A:GLN:HB3 | 16                  | 0.18     | 0.06                | 0.19       |
| (1,1253) | 1:47:A:PRO:HB3  | 1:87:A:GLY:HA2  | 16                  | 0.18     | 0.01                | 0.18       |
| (1,2169) | 1:22:A:ASN:HB3  | 1:22:A:ASN:H    | 16                  | 0.18     | 0.02                | 0.18       |
| (1,4323) | 1:62:A:GLY:H    | 1:68:A:LYS:HD2  | 16                  | 0.18     | 0.07                | 0.16       |
| (1,512)  | 1:13:A:ASP:HB2  | 1:13:A:ASP:H    | 16                  | 0.18     | 0.02                | 0.18       |
| (1,2672) | 1:31:A:LEU:HD13 | 1:35:A:PHE:HD2  | 16                  | 0.18     | 0.05                | 0.16       |
| (1,2672) | 1:31:A:LEU:HD13 | 1:35:A:PHE:HD1  | 16                  | 0.18     | 0.05                | 0.16       |
| (1,2672) | 1:31:A:LEU:HD12 | 1:35:A:PHE:HD2  | 16                  | 0.18     | 0.05                | 0.16       |
| (1,2672) | 1:31:A:LEU:HD12 | 1:35:A:PHE:HD1  | 16                  | 0.18     | 0.05                | 0.16       |
| (1,2672) | 1:31:A:LEU:HD11 | 1:35:A:PHE:HD1  | 16                  | 0.18     | 0.05                | 0.16       |
| (1,2672) | 1:31:A:LEU:HD11 | 1:35:A:PHE:HD2  | 16                  | 0.18     | 0.05                | 0.16       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,4225) | 1:122:A:ALA:HB2 | 1:123:A:ARG:H   | 16                  | 0.17     | 0.02                | 0.18       |
| (1,4225) | 1:122:A:ALA:HB3 | 1:123:A:ARG:H   | 16                  | 0.17     | 0.02                | 0.18       |
| (1,4225) | 1:122:A:ALA:HB1 | 1:123:A:ARG:H   | 16                  | 0.17     | 0.02                | 0.18       |
| (1,1049) | 1:59:A:ARG:HB2  | 1:60:A:VAL:HG12 | 16                  | 0.17     | 0.02                | 0.18       |
| (1,1049) | 1:59:A:ARG:HB2  | 1:60:A:VAL:HG13 | 16                  | 0.17     | 0.02                | 0.18       |
| (1,1049) | 1:59:A:ARG:HB2  | 1:60:A:VAL:HG11 | 16                  | 0.17     | 0.02                | 0.18       |
| (1,4019) | 1:33:A:GLU:HB3  | 1:34:A:ARG:H    | 16                  | 0.17     | 0.03                | 0.16       |
| (1,1713) | 1:20:A:LYS:H    | 1:20:A:LYS:HD3  | 16                  | 0.16     | 0.04                | 0.17       |
| (1,3935) | 1:63:A:GLU:HB3  | 1:65:A:ASN:H    | 16                  | 0.15     | 0.02                | 0.15       |
| (1,3537) | 1:51:A:GLY:HA2  | 1:54:A:GLN:HB2  | 16                  | 0.15     | 0.02                | 0.15       |
| (1,2197) | 1:39:A:PHE:HD2  | 1:56:A:LEU:HA   | 16                  | 0.15     | 0.02                | 0.14       |
| (1,2197) | 1:39:A:PHE:HD1  | 1:56:A:LEU:HA   | 16                  | 0.15     | 0.02                | 0.14       |
| (1,665)  | 1:122:A:ALA:HB2 | 1:123:A:ARG:H   | 16                  | 0.15     | 0.02                | 0.15       |
| (1,665)  | 1:122:A:ALA:HB3 | 1:123:A:ARG:H   | 16                  | 0.15     | 0.02                | 0.15       |
| (1,665)  | 1:122:A:ALA:HB1 | 1:123:A:ARG:H   | 16                  | 0.15     | 0.02                | 0.15       |
| (1,3306) | 1:128:A:ARG:HG2 | 1:128:A:ARG:HD2 | 16                  | 0.14     | 0.02                | 0.14       |
| (1,3118) | 1:58:A:ASP:HA   | 1:58:A:ASP:HB2  | 16                  | 0.14     | 0.01                | 0.14       |
| (1,3040) | 1:52:A:ILE:HA   | 1:52:A:ILE:HG12 | 16                  | 0.14     | 0.02                | 0.14       |
| (1,3907) | 1:76:A:ARG:HD2  | 1:77:A:LEU:H    | 16                  | 0.13     | 0.02                | 0.12       |
| (1,2775) | 1:47:A:PRO:HB3  | 1:87:A:GLY:HA2  | 16                  | 0.13     | 0.01                | 0.13       |
| (1,3753) | 1:107:A:GLU:H   | 1:106:A:ASP:H   | 16                  | 0.13     | 0.01                | 0.13       |
| (1,3523) | 1:56:A:LEU:HG   | 1:56:A:LEU:HB3  | 16                  | 0.13     | 0.02                | 0.13       |
| (1,1707) | 1:70:A:GLN:HG3  | 1:70:A:GLN:HB3  | 16                  | 0.13     | 0.0                 | 0.13       |
| (1,2786) | 1:82:A:TRP:HH2  | 1:82:A:TRP:HE1  | 16                  | 0.12     | 0.01                | 0.12       |
| (1,4339) | 1:116:A:GLN:HG3 | 1:115:A:LYS:H   | 16                  | 0.12     | 0.01                | 0.12       |
| (1,359)  | 1:62:A:GLY:HA3  | 1:63:A:GLU:H    | 16                  | 0.12     | 0.01                | 0.12       |
| (1,4203) | 1:106:A:ASP:HB2 | 1:109:A:HIS:H   | 16                  | 0.12     | 0.0                 | 0.12       |
| (1,3263) | 1:121:A:LYS:HG2 | 1:122:A:ALA:H   | 16                  | 0.12     | 0.01                | 0.11       |
| (1,4331) | 1:104:A:GLU:HG2 | 1:104:A:GLU:H   | 16                  | 0.12     | 0.01                | 0.11       |
| (1,3108) | 1:102:A:CYS:H   | 1:101:A:PRO:HB3 | 16                  | 0.12     | 0.01                | 0.12       |
| (1,1356) | 1:61:A:ALA:HB1  | 1:57:A:VAL:HG12 | 15                  | 0.53     | 0.12                | 0.58       |
| (1,1356) | 1:61:A:ALA:HB2  | 1:57:A:VAL:HG12 | 15                  | 0.53     | 0.12                | 0.58       |
| (1,1356) | 1:61:A:ALA:HB3  | 1:57:A:VAL:HG12 | 15                  | 0.53     | 0.12                | 0.58       |
| (1,1356) | 1:61:A:ALA:HB2  | 1:57:A:VAL:HG13 | 15                  | 0.53     | 0.12                | 0.58       |
| (1,1356) | 1:61:A:ALA:HB1  | 1:57:A:VAL:HG13 | 15                  | 0.53     | 0.12                | 0.58       |
| (1,1356) | 1:61:A:ALA:HB1  | 1:57:A:VAL:HG11 | 15                  | 0.53     | 0.12                | 0.58       |
| (1,1356) | 1:61:A:ALA:HB3  | 1:57:A:VAL:HG13 | 15                  | 0.53     | 0.12                | 0.58       |
| (1,2880) | 1:61:A:ALA:HB1  | 1:57:A:VAL:HG12 | 15                  | 0.49     | 0.12                | 0.54       |
| (1,2880) | 1:61:A:ALA:HB2  | 1:57:A:VAL:HG12 | 15                  | 0.49     | 0.12                | 0.54       |
| (1,2880) | 1:61:A:ALA:HB3  | 1:57:A:VAL:HG12 | 15                  | 0.49     | 0.12                | 0.54       |
| (1,2880) | 1:61:A:ALA:HB2  | 1:57:A:VAL:HG13 | 15                  | 0.49     | 0.12                | 0.54       |
| (1,2880) | 1:61:A:ALA:HB1  | 1:57:A:VAL:HG13 | 15                  | 0.49     | 0.12                | 0.54       |

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| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,2880) | 1:61:A:ALA:HB1   | 1:57:A:VAL:HG11 | 15                  | 0.49     | 0.12                | 0.54       |
| (1,2880) | 1:61:A:ALA:HB3   | 1:57:A:VAL:HG13 | 15                  | 0.49     | 0.12                | 0.54       |
| (1,3943) | 1:66:A:LEU:HD12  | 1:62:A:GLY:H    | 15                  | 0.48     | 0.09                | 0.51       |
| (1,3943) | 1:66:A:LEU:HD13  | 1:62:A:GLY:H    | 15                  | 0.48     | 0.09                | 0.51       |
| (1,3943) | 1:66:A:LEU:HD11  | 1:62:A:GLY:H    | 15                  | 0.48     | 0.09                | 0.51       |
| (1,363)  | 1:66:A:LEU:HD12  | 1:62:A:GLY:H    | 15                  | 0.44     | 0.09                | 0.46       |
| (1,363)  | 1:66:A:LEU:HD13  | 1:62:A:GLY:H    | 15                  | 0.44     | 0.09                | 0.46       |
| (1,363)  | 1:66:A:LEU:HD11  | 1:62:A:GLY:H    | 15                  | 0.44     | 0.09                | 0.46       |
| (3,84)   | 1:84:A:TYR:HE2   | 1:84:A:TYR:HA   | 15                  | 0.41     | 0.05                | 0.41       |
| (3,84)   | 1:84:A:TYR:HE1   | 1:84:A:TYR:HA   | 15                  | 0.41     | 0.05                | 0.41       |
| (3,123)  | 1:50:A:ILE:HD12  | 1:79:A:THR:HA   | 15                  | 0.41     | 0.15                | 0.4        |
| (3,123)  | 1:50:A:ILE:HD13  | 1:79:A:THR:HA   | 15                  | 0.41     | 0.15                | 0.4        |
| (3,123)  | 1:50:A:ILE:HD11  | 1:79:A:THR:HA   | 15                  | 0.41     | 0.15                | 0.4        |
| (1,1874) | 1:70:A:GLN:HE21  | 1:27:A:VAL:HG12 | 15                  | 0.41     | 0.07                | 0.42       |
| (1,1874) | 1:70:A:GLN:HE21  | 1:27:A:VAL:HG13 | 15                  | 0.41     | 0.07                | 0.42       |
| (1,1874) | 1:70:A:GLN:HE21  | 1:27:A:VAL:HG11 | 15                  | 0.41     | 0.07                | 0.42       |
| (1,2268) | 1:110:A:VAL:HG12 | 1:89:A:LYS:H    | 15                  | 0.37     | 0.11                | 0.39       |
| (1,2268) | 1:110:A:VAL:HG13 | 1:89:A:LYS:H    | 15                  | 0.37     | 0.11                | 0.39       |
| (1,2268) | 1:110:A:VAL:HG11 | 1:89:A:LYS:H    | 15                  | 0.37     | 0.11                | 0.39       |
| (1,2861) | 1:84:A:TYR:HE2   | 1:84:A:TYR:HA   | 15                  | 0.36     | 0.05                | 0.36       |
| (1,2861) | 1:84:A:TYR:HE1   | 1:84:A:TYR:HA   | 15                  | 0.36     | 0.05                | 0.36       |
| (1,3498) | 1:70:A:GLN:HE21  | 1:27:A:VAL:HG12 | 15                  | 0.36     | 0.07                | 0.38       |
| (1,3498) | 1:70:A:GLN:HE21  | 1:27:A:VAL:HG13 | 15                  | 0.36     | 0.07                | 0.38       |
| (1,3498) | 1:70:A:GLN:HE21  | 1:27:A:VAL:HG11 | 15                  | 0.36     | 0.07                | 0.38       |
| (1,2094) | 1:95:A:VAL:HG22  | 1:97:A:LEU:HD23 | 15                  | 0.36     | 0.19                | 0.32       |
| (1,2094) | 1:95:A:VAL:HG22  | 1:97:A:LEU:HD21 | 15                  | 0.36     | 0.19                | 0.32       |
| (1,2094) | 1:95:A:VAL:HG21  | 1:97:A:LEU:HD21 | 15                  | 0.36     | 0.19                | 0.32       |
| (1,2094) | 1:95:A:VAL:HG22  | 1:97:A:LEU:HD22 | 15                  | 0.36     | 0.19                | 0.32       |
| (1,2094) | 1:95:A:VAL:HG23  | 1:97:A:LEU:HD21 | 15                  | 0.36     | 0.19                | 0.32       |
| (1,2094) | 1:95:A:VAL:HG23  | 1:97:A:LEU:HD22 | 15                  | 0.36     | 0.19                | 0.32       |
| (1,2094) | 1:95:A:VAL:HG21  | 1:97:A:LEU:HD22 | 15                  | 0.36     | 0.19                | 0.32       |
| (1,2094) | 1:95:A:VAL:HG21  | 1:97:A:LEU:HD23 | 15                  | 0.36     | 0.19                | 0.32       |
| (1,3845) | 1:95:A:VAL:HG13  | 1:96:A:ASP:H    | 15                  | 0.36     | 0.19                | 0.29       |
| (1,3845) | 1:95:A:VAL:HG11  | 1:96:A:ASP:H    | 15                  | 0.36     | 0.19                | 0.29       |
| (1,3845) | 1:95:A:VAL:HG12  | 1:96:A:ASP:H    | 15                  | 0.36     | 0.19                | 0.29       |
| (1,3941) | 1:63:A:GLU:H     | 1:61:A:ALA:HB1  | 15                  | 0.28     | 0.14                | 0.23       |
| (1,3941) | 1:63:A:GLU:H     | 1:61:A:ALA:HB2  | 15                  | 0.28     | 0.14                | 0.23       |
| (1,3941) | 1:63:A:GLU:H     | 1:61:A:ALA:HB3  | 15                  | 0.28     | 0.14                | 0.23       |
| (1,829)  | 1:41:A:ALA:HB2   | 1:41:A:ALA:H    | 15                  | 0.26     | 0.03                | 0.27       |
| (1,829)  | 1:41:A:ALA:HB3   | 1:41:A:ALA:H    | 15                  | 0.26     | 0.03                | 0.27       |
| (1,829)  | 1:41:A:ALA:HB1   | 1:41:A:ALA:H    | 15                  | 0.26     | 0.03                | 0.27       |
| (1,2480) | 1:71:A:LEU:HB2   | 1:27:A:VAL:HG12 | 15                  | 0.25     | 0.08                | 0.29       |

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| Key      | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,2480) | 1:71:A:LEU:HB2  | 1:27:A:VAL:HG13  | 15                  | 0.25     | 0.08                | 0.29       |
| (1,2480) | 1:71:A:LEU:HB2  | 1:27:A:VAL:HG11  | 15                  | 0.25     | 0.08                | 0.29       |
| (1,2583) | 1:60:A:VAL:HG13 | 1:34:A:ARG:HG2   | 15                  | 0.25     | 0.07                | 0.27       |
| (1,2583) | 1:60:A:VAL:HG11 | 1:34:A:ARG:HG2   | 15                  | 0.25     | 0.07                | 0.27       |
| (1,2583) | 1:60:A:VAL:HG12 | 1:34:A:ARG:HG2   | 15                  | 0.25     | 0.07                | 0.27       |
| (1,549)  | 1:97:A:LEU:HD11 | 1:98:A:ASP:H     | 15                  | 0.22     | 0.11                | 0.18       |
| (1,549)  | 1:97:A:LEU:HD13 | 1:98:A:ASP:H     | 15                  | 0.22     | 0.11                | 0.18       |
| (1,549)  | 1:97:A:LEU:HD12 | 1:98:A:ASP:H     | 15                  | 0.22     | 0.11                | 0.18       |
| (1,4016) | 1:15:A:MET:HA   | 1:15:A:MET:H     | 15                  | 0.21     | 0.05                | 0.2        |
| (1,1553) | 1:57:A:VAL:HG12 | 1:61:A:ALA:H     | 15                  | 0.21     | 0.08                | 0.18       |
| (1,1553) | 1:57:A:VAL:HG13 | 1:61:A:ALA:H     | 15                  | 0.21     | 0.08                | 0.18       |
| (1,1553) | 1:57:A:VAL:HG11 | 1:61:A:ALA:H     | 15                  | 0.21     | 0.08                | 0.18       |
| (1,4150) | 1:17:A:ASN:HB3  | 1:18:A:GLN:H     | 15                  | 0.19     | 0.05                | 0.2        |
| (1,1397) | 1:31:A:LEU:HD22 | 1:60:A:VAL:HG11  | 15                  | 0.19     | 0.06                | 0.19       |
| (1,1397) | 1:31:A:LEU:HD22 | 1:60:A:VAL:HG13  | 15                  | 0.19     | 0.06                | 0.19       |
| (1,1397) | 1:31:A:LEU:HD21 | 1:60:A:VAL:HG12  | 15                  | 0.19     | 0.06                | 0.19       |
| (1,1397) | 1:31:A:LEU:HD21 | 1:60:A:VAL:HG11  | 15                  | 0.19     | 0.06                | 0.19       |
| (1,1397) | 1:31:A:LEU:HD23 | 1:60:A:VAL:HG13  | 15                  | 0.19     | 0.06                | 0.19       |
| (1,1397) | 1:31:A:LEU:HD22 | 1:60:A:VAL:HG12  | 15                  | 0.19     | 0.06                | 0.19       |
| (1,1397) | 1:31:A:LEU:HD21 | 1:60:A:VAL:HG13  | 15                  | 0.19     | 0.06                | 0.19       |
| (1,1397) | 1:31:A:LEU:HD23 | 1:60:A:VAL:HG12  | 15                  | 0.19     | 0.06                | 0.19       |
| (3,94)   | 1:56:A:LEU:HB2  | 1:75:A:LEU:HD13  | 15                  | 0.18     | 0.03                | 0.18       |
| (3,94)   | 1:56:A:LEU:HB2  | 1:75:A:LEU:HD11  | 15                  | 0.18     | 0.03                | 0.18       |
| (3,94)   | 1:56:A:LEU:HB2  | 1:75:A:LEU:HD12  | 15                  | 0.18     | 0.03                | 0.18       |
| (1,3200) | 1:116:A:GLN:HG3 | 1:113:A:ALA:HB3  | 15                  | 0.18     | 0.05                | 0.17       |
| (1,3200) | 1:116:A:GLN:HG3 | 1:113:A:ALA:HB1  | 15                  | 0.18     | 0.05                | 0.17       |
| (1,3200) | 1:116:A:GLN:HG3 | 1:113:A:ALA:HB2  | 15                  | 0.18     | 0.05                | 0.17       |
| (1,2950) | 1:75:A:LEU:HD11 | 1:75:A:LEU:H     | 15                  | 0.17     | 0.04                | 0.16       |
| (1,2950) | 1:75:A:LEU:HD12 | 1:75:A:LEU:H     | 15                  | 0.17     | 0.04                | 0.16       |
| (1,2950) | 1:75:A:LEU:HD13 | 1:75:A:LEU:H     | 15                  | 0.17     | 0.04                | 0.16       |
| (1,3768) | 1:130:A:GLU:H   | 1:130:A:GLU:HA   | 15                  | 0.17     | 0.03                | 0.16       |
| (1,3160) | 1:74:A:ALA:HB1  | 1:74:A:ALA:HA    | 15                  | 0.16     | 0.02                | 0.17       |
| (1,3160) | 1:74:A:ALA:HB2  | 1:74:A:ALA:HA    | 15                  | 0.16     | 0.02                | 0.17       |
| (1,3160) | 1:74:A:ALA:HB3  | 1:74:A:ALA:HA    | 15                  | 0.16     | 0.02                | 0.17       |
| (1,477)  | 1:31:A:LEU:H    | 1:31:A:LEU:HD11  | 15                  | 0.16     | 0.03                | 0.16       |
| (1,477)  | 1:31:A:LEU:H    | 1:31:A:LEU:HD13  | 15                  | 0.16     | 0.03                | 0.16       |
| (1,477)  | 1:31:A:LEU:H    | 1:31:A:LEU:HD12  | 15                  | 0.16     | 0.03                | 0.16       |
| (1,3477) | 1:15:A:MET:HG3  | 1:15:A:MET:HB2   | 15                  | 0.16     | 0.02                | 0.16       |
| (1,3415) | 1:117:A:LEU:HA  | 1:117:A:LEU:HD12 | 15                  | 0.15     | 0.05                | 0.15       |
| (1,3415) | 1:117:A:LEU:HA  | 1:117:A:LEU:HD13 | 15                  | 0.15     | 0.05                | 0.15       |
| (1,3415) | 1:117:A:LEU:HA  | 1:117:A:LEU:HD11 | 15                  | 0.15     | 0.05                | 0.15       |
| (1,4316) | 1:95:A:VAL:H    | 1:94:A:ARG:HB3   | 15                  | 0.15     | 0.03                | 0.14       |

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| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,2283) | 1:33:A:GLU:HG2   | 1:33:A:GLU:HA   | 15                  | 0.15     | 0.04                | 0.14       |
| (1,4343) | 1:118:A:GLU:H    | 1:119:A:GLU:H   | 15                  | 0.15     | 0.02                | 0.14       |
| (1,1410) | 1:110:A:VAL:HG22 | 1:108:A:GLN:H   | 15                  | 0.15     | 0.03                | 0.14       |
| (1,1410) | 1:110:A:VAL:HG21 | 1:108:A:GLN:H   | 15                  | 0.15     | 0.03                | 0.14       |
| (1,1410) | 1:110:A:VAL:HG23 | 1:108:A:GLN:H   | 15                  | 0.15     | 0.03                | 0.14       |
| (1,3552) | 1:123:A:ARG:HG2  | 1:124:A:VAL:HA  | 15                  | 0.14     | 0.02                | 0.16       |
| (1,4198) | 1:127:A:GLN:HA   | 1:127:A:GLN:H   | 15                  | 0.14     | 0.02                | 0.15       |
| (1,2140) | 1:84:A:TYR:HB2   | 1:82:A:TRP:HA   | 15                  | 0.14     | 0.01                | 0.14       |
| (1,1412) | 1:39:A:PHE:HZ    | 1:75:A:LEU:HD12 | 15                  | 0.14     | 0.02                | 0.14       |
| (1,1412) | 1:39:A:PHE:HZ    | 1:75:A:LEU:HD13 | 15                  | 0.14     | 0.02                | 0.14       |
| (1,1412) | 1:39:A:PHE:HZ    | 1:75:A:LEU:HD11 | 15                  | 0.14     | 0.02                | 0.14       |
| (1,3134) | 1:15:A:MET:HB2   | 1:15:A:MET:HG2  | 15                  | 0.14     | 0.02                | 0.14       |
| (1,3797) | 1:44:A:GLU:HA    | 1:44:A:GLU:H    | 15                  | 0.14     | 0.02                | 0.14       |
| (1,2579) | 1:59:A:ARG:HB2   | 1:60:A:VAL:HG12 | 15                  | 0.14     | 0.02                | 0.15       |
| (1,2579) | 1:59:A:ARG:HB2   | 1:60:A:VAL:HG13 | 15                  | 0.14     | 0.02                | 0.15       |
| (1,2579) | 1:59:A:ARG:HB2   | 1:60:A:VAL:HG11 | 15                  | 0.14     | 0.02                | 0.15       |
| (1,1599) | 1:53:A:PHE:HB3   | 1:75:A:LEU:HD23 | 15                  | 0.14     | 0.02                | 0.13       |
| (1,1599) | 1:53:A:PHE:HB3   | 1:75:A:LEU:HD22 | 15                  | 0.14     | 0.02                | 0.13       |
| (1,1599) | 1:53:A:PHE:HB3   | 1:75:A:LEU:HD21 | 15                  | 0.14     | 0.02                | 0.13       |
| (1,2875) | 1:122:A:ALA:HB3  | 1:122:A:ALA:H   | 15                  | 0.13     | 0.01                | 0.13       |
| (1,2875) | 1:122:A:ALA:HB1  | 1:122:A:ALA:H   | 15                  | 0.13     | 0.01                | 0.13       |
| (1,2875) | 1:122:A:ALA:HB2  | 1:122:A:ALA:H   | 15                  | 0.13     | 0.01                | 0.13       |
| (1,3275) | 1:119:A:GLU:HA   | 1:119:A:GLU:HG2 | 15                  | 0.12     | 0.01                | 0.12       |
| (1,645)  | 1:115:A:LYS:HE3  | 1:115:A:LYS:H   | 15                  | 0.12     | 0.02                | 0.12       |
| (1,1819) | 1:112:A:HIS:HA   | 1:112:A:HIS:H   | 15                  | 0.12     | 0.01                | 0.12       |
| (1,3801) | 1:108:A:GLN:HA   | 1:108:A:GLN:H   | 15                  | 0.11     | 0.01                | 0.11       |
| (1,1920) | 1:101:A:PRO:HG3  | 1:101:A:PRO:HD2 | 15                  | 0.11     | 0.0                 | 0.11       |
| (1,2617) | 1:21:A:LEU:HD23  | 1:30:A:PHE:HD1  | 14                  | 0.96     | 0.1                 | 0.96       |
| (1,2617) | 1:21:A:LEU:HD21  | 1:30:A:PHE:HD2  | 14                  | 0.96     | 0.1                 | 0.96       |
| (1,2617) | 1:21:A:LEU:HD22  | 1:30:A:PHE:HD1  | 14                  | 0.96     | 0.1                 | 0.96       |
| (1,2617) | 1:21:A:LEU:HD21  | 1:30:A:PHE:HD1  | 14                  | 0.96     | 0.1                 | 0.96       |
| (1,2617) | 1:21:A:LEU:HD23  | 1:30:A:PHE:HD2  | 14                  | 0.96     | 0.1                 | 0.96       |
| (1,1065) | 1:21:A:LEU:HD12  | 1:21:A:LEU:H    | 14                  | 0.85     | 0.07                | 0.86       |
| (1,1065) | 1:21:A:LEU:HD11  | 1:21:A:LEU:H    | 14                  | 0.85     | 0.07                | 0.86       |
| (1,1065) | 1:21:A:LEU:HD13  | 1:21:A:LEU:H    | 14                  | 0.85     | 0.07                | 0.86       |
| (1,2602) | 1:21:A:LEU:HD12  | 1:21:A:LEU:H    | 14                  | 0.81     | 0.07                | 0.83       |
| (1,2602) | 1:21:A:LEU:HD11  | 1:21:A:LEU:H    | 14                  | 0.81     | 0.07                | 0.83       |
| (1,2602) | 1:21:A:LEU:HD13  | 1:21:A:LEU:H    | 14                  | 0.81     | 0.07                | 0.83       |
| (1,524)  | 1:20:A:LYS:HB3   | 1:22:A:ASN:HD22 | 14                  | 0.67     | 0.3                 | 0.62       |
| (1,2142) | 1:21:A:LEU:HD12  | 1:30:A:PHE:HA   | 14                  | 0.63     | 0.06                | 0.63       |
| (1,2142) | 1:21:A:LEU:HD13  | 1:30:A:PHE:HA   | 14                  | 0.63     | 0.06                | 0.63       |
| (1,2142) | 1:21:A:LEU:HD11  | 1:30:A:PHE:HA   | 14                  | 0.63     | 0.06                | 0.63       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,2926) | 1:21:A:LEU:HB2  | 1:21:A:LEU:HD22 | 14                  | 0.61     | 0.05                | 0.6        |
| (1,2926) | 1:21:A:LEU:HB2  | 1:21:A:LEU:HD23 | 14                  | 0.61     | 0.05                | 0.6        |
| (1,2926) | 1:21:A:LEU:HB2  | 1:21:A:LEU:HD21 | 14                  | 0.61     | 0.05                | 0.6        |
| (1,3541) | 1:64:A:MET:HB2  | 1:21:A:LEU:HD21 | 14                  | 0.55     | 0.06                | 0.56       |
| (1,3541) | 1:64:A:MET:HB2  | 1:21:A:LEU:HD22 | 14                  | 0.55     | 0.06                | 0.56       |
| (1,3541) | 1:64:A:MET:HB2  | 1:21:A:LEU:HD23 | 14                  | 0.55     | 0.06                | 0.56       |
| (1,4132) | 1:60:A:VAL:HG13 | 1:34:A:ARG:HE   | 14                  | 0.51     | 0.1                 | 0.55       |
| (1,4132) | 1:60:A:VAL:HG11 | 1:34:A:ARG:HE   | 14                  | 0.51     | 0.1                 | 0.55       |
| (1,4132) | 1:60:A:VAL:HG12 | 1:34:A:ARG:HE   | 14                  | 0.51     | 0.1                 | 0.55       |
| (1,2458) | 1:21:A:LEU:HA   | 1:21:A:LEU:HD12 | 14                  | 0.47     | 0.08                | 0.44       |
| (1,2458) | 1:21:A:LEU:HA   | 1:21:A:LEU:HD13 | 14                  | 0.47     | 0.08                | 0.44       |
| (1,2458) | 1:21:A:LEU:HA   | 1:21:A:LEU:HD11 | 14                  | 0.47     | 0.08                | 0.44       |
| (3,36)   | 1:49:A:LYS:HB2  | 1:52:A:ILE:HD11 | 14                  | 0.47     | 0.11                | 0.5        |
| (3,36)   | 1:49:A:LYS:HB2  | 1:52:A:ILE:HD13 | 14                  | 0.47     | 0.11                | 0.5        |
| (3,36)   | 1:48:A:LEU:HD21 | 1:49:A:LYS:HB2  | 14                  | 0.47     | 0.11                | 0.5        |
| (3,36)   | 1:50:A:ILE:HG21 | 1:49:A:LYS:HB2  | 14                  | 0.47     | 0.11                | 0.5        |
| (3,36)   | 1:50:A:ILE:HG23 | 1:49:A:LYS:HB2  | 14                  | 0.47     | 0.11                | 0.5        |
| (3,36)   | 1:49:A:LYS:HB2  | 1:52:A:ILE:HD12 | 14                  | 0.47     | 0.11                | 0.5        |
| (1,570)  | 1:60:A:VAL:HG13 | 1:34:A:ARG:HE   | 14                  | 0.45     | 0.1                 | 0.49       |
| (1,570)  | 1:60:A:VAL:HG11 | 1:34:A:ARG:HE   | 14                  | 0.45     | 0.1                 | 0.49       |
| (1,570)  | 1:60:A:VAL:HG12 | 1:34:A:ARG:HE   | 14                  | 0.45     | 0.1                 | 0.49       |
| (1,2003) | 1:48:A:LEU:HB3  | 1:48:A:LEU:HD11 | 14                  | 0.44     | 0.01                | 0.44       |
| (1,2003) | 1:48:A:LEU:HB3  | 1:48:A:LEU:HD13 | 14                  | 0.44     | 0.01                | 0.44       |
| (1,2179) | 1:52:A:ILE:HG22 | 1:48:A:LEU:HB3  | 14                  | 0.42     | 0.11                | 0.39       |
| (1,2179) | 1:52:A:ILE:HG23 | 1:48:A:LEU:HB3  | 14                  | 0.42     | 0.11                | 0.39       |
| (1,2179) | 1:52:A:ILE:HG21 | 1:48:A:LEU:HB3  | 14                  | 0.42     | 0.11                | 0.39       |
| (1,3024) | 1:64:A:MET:HE3  | 1:65:A:ASN:HB3  | 14                  | 0.4      | 0.06                | 0.4        |
| (1,3024) | 1:64:A:MET:HE2  | 1:65:A:ASN:HB3  | 14                  | 0.4      | 0.06                | 0.4        |
| (1,3024) | 1:64:A:MET:HE1  | 1:65:A:ASN:HB3  | 14                  | 0.4      | 0.06                | 0.4        |
| (1,2178) | 1:48:A:LEU:HB2  | 1:52:A:ILE:HG22 | 14                  | 0.39     | 0.14                | 0.34       |
| (1,2178) | 1:48:A:LEU:HB2  | 1:52:A:ILE:HG23 | 14                  | 0.39     | 0.14                | 0.34       |
| (1,2178) | 1:48:A:LEU:HB2  | 1:52:A:ILE:HG21 | 14                  | 0.39     | 0.14                | 0.34       |
| (1,2201) | 1:64:A:MET:HB2  | 1:21:A:LEU:HD21 | 14                  | 0.38     | 0.06                | 0.38       |
| (1,2201) | 1:64:A:MET:HB2  | 1:21:A:LEU:HD22 | 14                  | 0.38     | 0.06                | 0.38       |
| (1,2201) | 1:64:A:MET:HB2  | 1:21:A:LEU:HD23 | 14                  | 0.38     | 0.06                | 0.38       |
| (1,4197) | 1:66:A:LEU:HD23 | 1:67:A:SER:H    | 14                  | 0.38     | 0.06                | 0.37       |
| (1,4197) | 1:66:A:LEU:HD22 | 1:67:A:SER:H    | 14                  | 0.38     | 0.06                | 0.37       |
| (1,2099) | 1:21:A:LEU:HB2  | 1:21:A:LEU:HD22 | 14                  | 0.37     | 0.05                | 0.36       |
| (1,2099) | 1:21:A:LEU:HB2  | 1:21:A:LEU:HD23 | 14                  | 0.37     | 0.05                | 0.36       |
| (1,2099) | 1:21:A:LEU:HB2  | 1:21:A:LEU:HD21 | 14                  | 0.37     | 0.05                | 0.36       |
| (1,1735) | 1:66:A:LEU:HD23 | 1:67:A:SER:H    | 14                  | 0.37     | 0.06                | 0.36       |
| (1,1735) | 1:66:A:LEU:HD22 | 1:67:A:SER:H    | 14                  | 0.37     | 0.06                | 0.36       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,2542) | 1:21:A:LEU:HD12 | 1:30:A:PHE:HA   | 14                  | 0.36     | 0.06                | 0.36       |
| (1,2542) | 1:21:A:LEU:HD13 | 1:30:A:PHE:HA   | 14                  | 0.36     | 0.06                | 0.36       |
| (1,2542) | 1:21:A:LEU:HD11 | 1:30:A:PHE:HA   | 14                  | 0.36     | 0.06                | 0.36       |
| (1,4180) | 1:95:A:VAL:H    | 1:48:A:LEU:HD12 | 14                  | 0.34     | 0.11                | 0.35       |
| (1,4180) | 1:95:A:VAL:H    | 1:48:A:LEU:HD13 | 14                  | 0.34     | 0.11                | 0.35       |
| (1,4180) | 1:95:A:VAL:H    | 1:48:A:LEU:HD11 | 14                  | 0.34     | 0.11                | 0.35       |
| (1,3216) | 1:48:A:LEU:HG   | 1:84:A:TYR:HD2  | 14                  | 0.31     | 0.04                | 0.33       |
| (1,3216) | 1:48:A:LEU:HG   | 1:84:A:TYR:HD1  | 14                  | 0.31     | 0.04                | 0.33       |
| (1,3769) | 1:130:A:GLU:H   | 1:129:A:ALA:HB3 | 14                  | 0.29     | 0.04                | 0.28       |
| (1,3769) | 1:130:A:GLU:H   | 1:129:A:ALA:HB1 | 14                  | 0.29     | 0.04                | 0.28       |
| (1,3769) | 1:130:A:GLU:H   | 1:129:A:ALA:HB2 | 14                  | 0.29     | 0.04                | 0.28       |
| (1,618)  | 1:95:A:VAL:H    | 1:48:A:LEU:HD12 | 14                  | 0.28     | 0.11                | 0.29       |
| (1,618)  | 1:95:A:VAL:H    | 1:48:A:LEU:HD13 | 14                  | 0.28     | 0.11                | 0.29       |
| (1,618)  | 1:95:A:VAL:H    | 1:48:A:LEU:HD11 | 14                  | 0.28     | 0.11                | 0.29       |
| (1,2005) | 1:95:A:VAL:HG21 | 1:48:A:LEU:HD12 | 14                  | 0.28     | 0.08                | 0.3        |
| (1,2005) | 1:95:A:VAL:HG23 | 1:48:A:LEU:HD12 | 14                  | 0.28     | 0.08                | 0.3        |
| (1,2005) | 1:95:A:VAL:HG21 | 1:48:A:LEU:HD13 | 14                  | 0.28     | 0.08                | 0.3        |
| (1,2005) | 1:95:A:VAL:HG22 | 1:48:A:LEU:HD12 | 14                  | 0.28     | 0.08                | 0.3        |
| (1,2005) | 1:95:A:VAL:HG23 | 1:48:A:LEU:HD11 | 14                  | 0.28     | 0.08                | 0.3        |
| (1,2005) | 1:95:A:VAL:HG22 | 1:48:A:LEU:HD11 | 14                  | 0.28     | 0.08                | 0.3        |
| (1,2005) | 1:95:A:VAL:HG21 | 1:48:A:LEU:HD11 | 14                  | 0.28     | 0.08                | 0.3        |
| (3,22)   | 1:48:A:LEU:H    | 1:48:A:LEU:HD11 | 14                  | 0.27     | 0.11                | 0.26       |
| (3,22)   | 1:48:A:LEU:H    | 1:48:A:LEU:HD12 | 14                  | 0.27     | 0.11                | 0.26       |
| (3,22)   | 1:48:A:LEU:HD13 | 1:97:A:LEU:H    | 14                  | 0.27     | 0.11                | 0.26       |
| (3,22)   | 1:48:A:LEU:HD11 | 1:97:A:LEU:H    | 14                  | 0.27     | 0.11                | 0.26       |
| (3,22)   | 1:48:A:LEU:HD12 | 1:97:A:LEU:H    | 14                  | 0.27     | 0.11                | 0.26       |
| (3,22)   | 1:48:A:LEU:H    | 1:48:A:LEU:HD13 | 14                  | 0.27     | 0.11                | 0.26       |
| (1,154)  | 1:130:A:GLU:H   | 1:129:A:ALA:HB3 | 14                  | 0.26     | 0.04                | 0.25       |
| (1,154)  | 1:130:A:GLU:H   | 1:129:A:ALA:HB1 | 14                  | 0.26     | 0.04                | 0.25       |
| (1,154)  | 1:130:A:GLU:H   | 1:129:A:ALA:HB2 | 14                  | 0.26     | 0.04                | 0.25       |
| (1,2025) | 1:97:A:LEU:HD21 | 1:35:A:PHE:HD2  | 14                  | 0.25     | 0.1                 | 0.26       |
| (1,2025) | 1:97:A:LEU:HD22 | 1:35:A:PHE:HD2  | 14                  | 0.25     | 0.1                 | 0.26       |
| (1,2025) | 1:97:A:LEU:HD23 | 1:35:A:PHE:HD2  | 14                  | 0.25     | 0.1                 | 0.26       |
| (1,2025) | 1:97:A:LEU:HD22 | 1:35:A:PHE:HD1  | 14                  | 0.25     | 0.1                 | 0.26       |
| (1,2025) | 1:97:A:LEU:HD23 | 1:35:A:PHE:HD1  | 14                  | 0.25     | 0.1                 | 0.26       |
| (1,2769) | 1:43:A:GLY:HA2  | 1:42:A:GLU:HB2  | 14                  | 0.25     | 0.05                | 0.26       |
| (1,3536) | 1:66:A:LEU:HB3  | 1:62:A:GLY:HA3  | 14                  | 0.23     | 0.03                | 0.23       |
| (1,1831) | 1:21:A:LEU:HG   | 1:21:A:LEU:HB3  | 14                  | 0.22     | 0.02                | 0.22       |
| (1,1513) | 1:52:A:ILE:HG23 | 1:53:A:PHE:HB3  | 14                  | 0.2      | 0.06                | 0.18       |
| (1,1513) | 1:52:A:ILE:HG21 | 1:53:A:PHE:HB3  | 14                  | 0.2      | 0.06                | 0.18       |
| (1,1513) | 1:52:A:ILE:HG22 | 1:53:A:PHE:HB3  | 14                  | 0.2      | 0.06                | 0.18       |
| (1,1886) | 1:102:A:CYS:HB3 | 1:49:A:LYS:HA   | 14                  | 0.2      | 0.06                | 0.21       |

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| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,3441) | 1:21:A:LEU:HG    | 1:21:A:LEU:HB3  | 14                  | 0.19     | 0.02                | 0.19       |
| (1,1371) | 1:28:A:ILE:HD11  | 1:75:A:LEU:H    | 14                  | 0.19     | 0.04                | 0.18       |
| (1,1371) | 1:28:A:ILE:HD12  | 1:75:A:LEU:H    | 14                  | 0.19     | 0.04                | 0.18       |
| (1,1371) | 1:28:A:ILE:HD13  | 1:75:A:LEU:H    | 14                  | 0.19     | 0.04                | 0.18       |
| (1,2299) | 1:55:A:ASP:HB3   | 1:96:A:ASP:HA   | 14                  | 0.17     | 0.03                | 0.17       |
| (1,2804) | 1:66:A:LEU:HB3   | 1:60:A:VAL:HB   | 14                  | 0.16     | 0.01                | 0.17       |
| (1,3369) | 1:24:A:SER:HA    | 1:27:A:VAL:HG23 | 14                  | 0.16     | 0.03                | 0.18       |
| (1,3369) | 1:24:A:SER:HA    | 1:27:A:VAL:HG21 | 14                  | 0.16     | 0.03                | 0.18       |
| (1,3369) | 1:24:A:SER:HA    | 1:27:A:VAL:HG22 | 14                  | 0.16     | 0.03                | 0.18       |
| (1,4040) | 1:25:A:LYS:HG3   | 1:25:A:LYS:H    | 14                  | 0.16     | 0.01                | 0.16       |
| (1,4345) | 1:117:A:LEU:HA   | 1:121:A:LYS:H   | 14                  | 0.15     | 0.03                | 0.16       |
| (1,2719) | 1:117:A:LEU:HD13 | 1:86:A:TYR:HB2  | 14                  | 0.15     | 0.02                | 0.15       |
| (1,2719) | 1:117:A:LEU:HD11 | 1:86:A:TYR:HB2  | 14                  | 0.15     | 0.02                | 0.15       |
| (1,2719) | 1:117:A:LEU:HD12 | 1:86:A:TYR:HB2  | 14                  | 0.15     | 0.02                | 0.15       |
| (1,2469) | 1:53:A:PHE:HZ    | 1:72:A:ARG:HG3  | 14                  | 0.15     | 0.02                | 0.15       |
| (1,2079) | 1:66:A:LEU:HD12  | 1:62:A:GLY:H    | 14                  | 0.14     | 0.02                | 0.14       |
| (1,2079) | 1:66:A:LEU:HD13  | 1:62:A:GLY:H    | 14                  | 0.14     | 0.02                | 0.14       |
| (1,2079) | 1:66:A:LEU:HD11  | 1:62:A:GLY:H    | 14                  | 0.14     | 0.02                | 0.14       |
| (1,2774) | 1:91:A:GLY:HA3   | 1:90:A:PRO:HB2  | 14                  | 0.14     | 0.02                | 0.14       |
| (1,3035) | 1:25:A:LYS:H     | 1:25:A:LYS:HG2  | 14                  | 0.13     | 0.05                | 0.11       |
| (1,1486) | 1:25:A:LYS:HG3   | 1:26:A:GLU:HA   | 14                  | 0.13     | 0.02                | 0.12       |
| (1,1636) | 1:124:A:VAL:HA   | 1:125:A:GLN:HG3 | 14                  | 0.12     | 0.01                | 0.12       |
| (1,483)  | 1:25:A:LYS:HG3   | 1:25:A:LYS:H    | 14                  | 0.12     | 0.01                | 0.12       |
| (1,2978) | 1:105:A:LEU:H    | 1:101:A:PRO:HD3 | 14                  | 0.11     | 0.01                | 0.11       |
| (1,587)  | 1:25:A:LYS:HB2   | 1:26:A:GLU:H    | 14                  | 0.11     | 0.01                | 0.11       |
| (1,2318) | 1:108:A:GLN:HA   | 1:108:A:GLN:HB3 | 14                  | 0.11     | 0.01                | 0.11       |
| (3,116)  | 1:95:A:VAL:H     | 1:48:A:LEU:HD12 | 13                  | 0.88     | 0.15                | 0.94       |
| (3,116)  | 1:95:A:VAL:H     | 1:48:A:LEU:HD11 | 13                  | 0.88     | 0.15                | 0.94       |
| (1,1866) | 1:83:A:ARG:HD3   | 1:45:A:ALA:HB1  | 13                  | 0.39     | 0.04                | 0.4        |
| (1,1866) | 1:83:A:ARG:HD3   | 1:45:A:ALA:HB3  | 13                  | 0.39     | 0.04                | 0.4        |
| (1,1866) | 1:83:A:ARG:HD3   | 1:45:A:ALA:HB2  | 13                  | 0.39     | 0.04                | 0.4        |
| (1,1684) | 1:48:A:LEU:HD13  | 1:50:A:ILE:HA   | 13                  | 0.38     | 0.08                | 0.39       |
| (1,1684) | 1:48:A:LEU:HD12  | 1:50:A:ILE:HA   | 13                  | 0.38     | 0.08                | 0.39       |
| (1,241)  | 1:95:A:VAL:HG13  | 1:96:A:ASP:H    | 13                  | 0.35     | 0.18                | 0.29       |
| (1,241)  | 1:95:A:VAL:HG11  | 1:96:A:ASP:H    | 13                  | 0.35     | 0.18                | 0.29       |
| (1,241)  | 1:95:A:VAL:HG12  | 1:96:A:ASP:H    | 13                  | 0.35     | 0.18                | 0.29       |
| (1,3987) | 1:50:A:ILE:HG22  | 1:50:A:ILE:H    | 13                  | 0.33     | 0.25                | 0.19       |
| (1,3987) | 1:50:A:ILE:HG21  | 1:50:A:ILE:H    | 13                  | 0.33     | 0.25                | 0.19       |
| (1,3987) | 1:50:A:ILE:HG23  | 1:50:A:ILE:H    | 13                  | 0.33     | 0.25                | 0.19       |
| (1,3481) | 1:83:A:ARG:HD3   | 1:45:A:ALA:HB1  | 13                  | 0.33     | 0.04                | 0.34       |
| (1,3481) | 1:83:A:ARG:HD3   | 1:45:A:ALA:HB3  | 13                  | 0.33     | 0.04                | 0.34       |
| (1,3481) | 1:83:A:ARG:HD3   | 1:45:A:ALA:HB2  | 13                  | 0.33     | 0.04                | 0.34       |

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| Key      | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,3258) | 1:48:A:LEU:HD13 | 1:50:A:ILE:HA    | 13                  | 0.32     | 0.08                | 0.33       |
| (1,3258) | 1:48:A:LEU:HD12 | 1:50:A:ILE:HA    | 13                  | 0.32     | 0.08                | 0.33       |
| (1,2569) | 1:82:A:TRP:HZ2  | 1:124:A:VAL:HG21 | 13                  | 0.32     | 0.09                | 0.34       |
| (1,2569) | 1:82:A:TRP:HZ2  | 1:124:A:VAL:HG22 | 13                  | 0.32     | 0.09                | 0.34       |
| (1,2569) | 1:82:A:TRP:HZ2  | 1:124:A:VAL:HG23 | 13                  | 0.32     | 0.09                | 0.34       |
| (1,822)  | 1:49:A:LYS:H    | 1:52:A:ILE:HD11  | 13                  | 0.3      | 0.08                | 0.29       |
| (1,822)  | 1:49:A:LYS:H    | 1:52:A:ILE:HD13  | 13                  | 0.3      | 0.08                | 0.29       |
| (1,822)  | 1:49:A:LYS:H    | 1:52:A:ILE:HD12  | 13                  | 0.3      | 0.08                | 0.29       |
| (1,2149) | 1:21:A:LEU:HD23 | 1:30:A:PHE:HD1   | 13                  | 0.27     | 0.09                | 0.26       |
| (1,2149) | 1:21:A:LEU:HD21 | 1:30:A:PHE:HD2   | 13                  | 0.27     | 0.09                | 0.26       |
| (1,2149) | 1:21:A:LEU:HD22 | 1:30:A:PHE:HD1   | 13                  | 0.27     | 0.09                | 0.26       |
| (1,2149) | 1:21:A:LEU:HD21 | 1:30:A:PHE:HD1   | 13                  | 0.27     | 0.09                | 0.26       |
| (1,2149) | 1:21:A:LEU:HD23 | 1:30:A:PHE:HD2   | 13                  | 0.27     | 0.09                | 0.26       |
| (1,1403) | 1:95:A:VAL:HG21 | 1:95:A:VAL:HG11  | 13                  | 0.25     | 0.09                | 0.25       |
| (1,1403) | 1:95:A:VAL:HG23 | 1:95:A:VAL:HG11  | 13                  | 0.25     | 0.09                | 0.25       |
| (1,1403) | 1:95:A:VAL:HG23 | 1:95:A:VAL:HG12  | 13                  | 0.25     | 0.09                | 0.25       |
| (1,1403) | 1:95:A:VAL:HG23 | 1:95:A:VAL:HG13  | 13                  | 0.25     | 0.09                | 0.25       |
| (1,1403) | 1:95:A:VAL:HG21 | 1:95:A:VAL:HG12  | 13                  | 0.25     | 0.09                | 0.25       |
| (1,1403) | 1:95:A:VAL:HG21 | 1:95:A:VAL:HG13  | 13                  | 0.25     | 0.09                | 0.25       |
| (1,1403) | 1:95:A:VAL:HG22 | 1:95:A:VAL:HG12  | 13                  | 0.25     | 0.09                | 0.25       |
| (1,993)  | 1:79:A:THR:HG22 | 1:75:A:LEU:HA    | 13                  | 0.21     | 0.05                | 0.2        |
| (1,993)  | 1:79:A:THR:HG23 | 1:75:A:LEU:HA    | 13                  | 0.21     | 0.05                | 0.2        |
| (1,993)  | 1:79:A:THR:HG21 | 1:75:A:LEU:HA    | 13                  | 0.21     | 0.05                | 0.2        |
| (1,2529) | 1:79:A:THR:HG22 | 1:75:A:LEU:HA    | 13                  | 0.18     | 0.04                | 0.17       |
| (1,2529) | 1:79:A:THR:HG23 | 1:75:A:LEU:HA    | 13                  | 0.18     | 0.04                | 0.17       |
| (1,2529) | 1:79:A:THR:HG21 | 1:75:A:LEU:HA    | 13                  | 0.18     | 0.04                | 0.17       |
| (1,635)  | 1:127:A:GLN:H   | 1:127:A:GLN:HB3  | 13                  | 0.18     | 0.05                | 0.17       |
| (1,2930) | 1:31:A:LEU:HD22 | 1:60:A:VAL:HG11  | 13                  | 0.18     | 0.05                | 0.16       |
| (1,2930) | 1:31:A:LEU:HD22 | 1:60:A:VAL:HG13  | 13                  | 0.18     | 0.05                | 0.16       |
| (1,2930) | 1:31:A:LEU:HD21 | 1:60:A:VAL:HG12  | 13                  | 0.18     | 0.05                | 0.16       |
| (1,2930) | 1:31:A:LEU:HD21 | 1:60:A:VAL:HG11  | 13                  | 0.18     | 0.05                | 0.16       |
| (1,2930) | 1:31:A:LEU:HD22 | 1:60:A:VAL:HG12  | 13                  | 0.18     | 0.05                | 0.16       |
| (1,2930) | 1:31:A:LEU:HD21 | 1:60:A:VAL:HG13  | 13                  | 0.18     | 0.05                | 0.16       |
| (1,2930) | 1:31:A:LEU:HD23 | 1:60:A:VAL:HG12  | 13                  | 0.18     | 0.05                | 0.16       |
| (1,3370) | 1:24:A:SER:HA   | 1:27:A:VAL:HG13  | 13                  | 0.18     | 0.03                | 0.19       |
| (1,3370) | 1:24:A:SER:HA   | 1:27:A:VAL:HG11  | 13                  | 0.18     | 0.03                | 0.19       |
| (1,3370) | 1:24:A:SER:HA   | 1:27:A:VAL:HG12  | 13                  | 0.18     | 0.03                | 0.19       |
| (1,3673) | 1:49:A:LYS:H    | 1:50:A:ILE:H     | 13                  | 0.18     | 0.01                | 0.18       |
| (1,2893) | 1:50:A:ILE:HB   | 1:50:A:ILE:HG22  | 13                  | 0.15     | 0.02                | 0.15       |
| (1,2893) | 1:50:A:ILE:HB   | 1:50:A:ILE:HG21  | 13                  | 0.15     | 0.02                | 0.15       |
| (1,2893) | 1:50:A:ILE:HB   | 1:50:A:ILE:HG23  | 13                  | 0.15     | 0.02                | 0.15       |
| (1,2899) | 1:28:A:ILE:HD11 | 1:75:A:LEU:H     | 13                  | 0.14     | 0.04                | 0.13       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,2899) | 1:28:A:ILE:HD12 | 1:75:A:LEU:H    | 13                  | 0.14     | 0.04                | 0.13       |
| (1,2899) | 1:28:A:ILE:HD13 | 1:75:A:LEU:H    | 13                  | 0.14     | 0.04                | 0.13       |
| (1,1032) | 1:85:A:LEU:H    | 1:84:A:TYR:HE1  | 13                  | 0.14     | 0.02                | 0.14       |
| (1,1032) | 1:85:A:LEU:H    | 1:84:A:TYR:HE2  | 13                  | 0.14     | 0.02                | 0.14       |
| (1,2295) | 1:121:A:LYS:HG2 | 1:121:A:LYS:HD3 | 13                  | 0.14     | 0.03                | 0.13       |
| (1,1756) | 1:79:A:THR:HG22 | 1:84:A:TYR:HE2  | 13                  | 0.13     | 0.03                | 0.12       |
| (1,1756) | 1:79:A:THR:HG21 | 1:84:A:TYR:HE2  | 13                  | 0.13     | 0.03                | 0.12       |
| (1,1756) | 1:79:A:THR:HG22 | 1:84:A:TYR:HE1  | 13                  | 0.13     | 0.03                | 0.12       |
| (1,1756) | 1:79:A:THR:HG23 | 1:84:A:TYR:HE1  | 13                  | 0.13     | 0.03                | 0.12       |
| (1,1756) | 1:79:A:THR:HG21 | 1:84:A:TYR:HE1  | 13                  | 0.13     | 0.03                | 0.12       |
| (1,1756) | 1:79:A:THR:HG23 | 1:84:A:TYR:HE2  | 13                  | 0.13     | 0.03                | 0.12       |
| (1,756)  | 1:93:A:THR:HB   | 1:102:A:CYS:H   | 13                  | 0.12     | 0.02                | 0.12       |
| (1,1727) | 1:66:A:LEU:HD13 | 1:30:A:PHE:HD1  | 13                  | 0.12     | 0.02                | 0.11       |
| (1,1727) | 1:66:A:LEU:HD11 | 1:30:A:PHE:HD2  | 13                  | 0.12     | 0.02                | 0.11       |
| (1,1727) | 1:66:A:LEU:HD13 | 1:30:A:PHE:HD2  | 13                  | 0.12     | 0.02                | 0.11       |
| (1,1727) | 1:66:A:LEU:HD12 | 1:30:A:PHE:HD2  | 13                  | 0.12     | 0.02                | 0.11       |
| (1,1727) | 1:66:A:LEU:HD11 | 1:30:A:PHE:HD1  | 13                  | 0.12     | 0.02                | 0.11       |
| (1,1727) | 1:66:A:LEU:HD12 | 1:30:A:PHE:HD1  | 13                  | 0.12     | 0.02                | 0.11       |
| (1,3820) | 1:101:A:PRO:HB3 | 1:103:A:GLY:H   | 13                  | 0.12     | 0.0                 | 0.12       |
| (1,3859) | 1:90:A:PRO:HB2  | 1:91:A:GLY:H    | 13                  | 0.12     | 0.02                | 0.11       |
| (1,3824) | 1:102:A:CYS:H   | 1:100:A:ASN:HB3 | 13                  | 0.12     | 0.01                | 0.12       |
| (1,2846) | 1:53:A:PHE:HE1  | 1:75:A:LEU:HB3  | 13                  | 0.12     | 0.01                | 0.12       |
| (1,2846) | 1:53:A:PHE:HE2  | 1:75:A:LEU:HB3  | 13                  | 0.12     | 0.01                | 0.12       |
| (1,3839) | 1:65:A:ASN:HB3  | 1:65:A:ASN:HD21 | 12                  | 0.34     | 0.05                | 0.34       |
| (1,2409) | 1:49:A:LYS:H    | 1:52:A:ILE:HD11 | 12                  | 0.27     | 0.07                | 0.24       |
| (1,2409) | 1:49:A:LYS:H    | 1:52:A:ILE:HD13 | 12                  | 0.27     | 0.07                | 0.24       |
| (1,2409) | 1:49:A:LYS:H    | 1:52:A:ILE:HD12 | 12                  | 0.27     | 0.07                | 0.24       |
| (3,106)  | 1:68:A:LYS:HD2  | 1:68:A:LYS:HA   | 12                  | 0.25     | 0.12                | 0.19       |
| (1,852)  | 1:65:A:ASN:HB3  | 1:65:A:ASN:HD21 | 12                  | 0.24     | 0.05                | 0.24       |
| (1,527)  | 1:65:A:ASN:HB3  | 1:65:A:ASN:HD21 | 12                  | 0.22     | 0.05                | 0.22       |
| (1,4037) | 1:27:A:VAL:HG22 | 1:29:A:ALA:H    | 12                  | 0.21     | 0.06                | 0.2        |
| (1,4037) | 1:27:A:VAL:HG21 | 1:29:A:ALA:H    | 12                  | 0.21     | 0.06                | 0.2        |
| (1,4037) | 1:27:A:VAL:HG23 | 1:29:A:ALA:H    | 12                  | 0.21     | 0.06                | 0.2        |
| (1,2505) | 1:126:A:ALA:HA  | 1:126:A:ALA:H   | 12                  | 0.2      | 0.04                | 0.22       |
| (1,827)  | 1:45:A:ALA:HB1  | 1:45:A:ALA:H    | 12                  | 0.2      | 0.03                | 0.2        |
| (1,827)  | 1:45:A:ALA:HB3  | 1:45:A:ALA:H    | 12                  | 0.2      | 0.03                | 0.2        |
| (1,827)  | 1:45:A:ALA:HB2  | 1:45:A:ALA:H    | 12                  | 0.2      | 0.03                | 0.2        |
| (1,2416) | 1:45:A:ALA:HB1  | 1:45:A:ALA:H    | 12                  | 0.16     | 0.03                | 0.16       |
| (1,2416) | 1:45:A:ALA:HB3  | 1:45:A:ALA:H    | 12                  | 0.16     | 0.03                | 0.16       |
| (1,2416) | 1:45:A:ALA:HB2  | 1:45:A:ALA:H    | 12                  | 0.16     | 0.03                | 0.16       |
| (1,3457) | 1:20:A:LYS:HE3  | 1:19:A:PRO:HA   | 12                  | 0.16     | 0.05                | 0.15       |
| (1,830)  | 1:129:A:ALA:HB1 | 1:127:A:GLN:HB3 | 12                  | 0.15     | 0.07                | 0.14       |

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| Key      | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,830)  | 1:129:A:ALA:HB2 | 1:127:A:GLN:HB3  | 12                  | 0.15     | 0.07                | 0.14       |
| (1,830)  | 1:129:A:ALA:HB3 | 1:127:A:GLN:HB3  | 12                  | 0.15     | 0.07                | 0.14       |
| (1,1725) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HG    | 12                  | 0.15     | 0.03                | 0.15       |
| (1,1725) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HG    | 12                  | 0.15     | 0.03                | 0.15       |
| (1,1725) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HG    | 12                  | 0.15     | 0.03                | 0.15       |
| (1,4320) | 1:62:A:GLY:H    | 1:66:A:LEU:H     | 12                  | 0.14     | 0.02                | 0.14       |
| (1,3879) | 1:127:A:GLN:H   | 1:127:A:GLN:HG2  | 12                  | 0.14     | 0.02                | 0.14       |
| (1,3757) | 1:116:A:GLN:H   | 1:117:A:LEU:H    | 12                  | 0.13     | 0.02                | 0.12       |
| (3,90)   | 1:115:A:LYS:HG3 | 1:116:A:GLN:HG3  | 12                  | 0.12     | 0.01                | 0.12       |
| (1,3372) | 1:88:A:VAL:HA   | 1:47:A:PRO:HB3   | 12                  | 0.12     | 0.01                | 0.12       |
| (1,983)  | 1:55:A:ASP:HB3  | 1:55:A:ASP:HA    | 12                  | 0.12     | 0.02                | 0.11       |
| (1,2160) | 1:82:A:TRP:HZ3  | 1:82:A:TRP:HB2   | 12                  | 0.12     | 0.01                | 0.12       |
| (3,149)  | 1:82:A:TRP:HE1  | 1:82:A:TRP:HE3   | 12                  | 0.12     | 0.01                | 0.11       |
| (3,149)  | 1:82:A:TRP:HE1  | 1:86:A:TYR:HD1   | 12                  | 0.12     | 0.01                | 0.11       |
| (3,149)  | 1:82:A:TRP:HE1  | 1:86:A:TYR:HD2   | 12                  | 0.12     | 0.01                | 0.11       |
| (1,2047) | 1:60:A:VAL:H    | 1:61:A:ALA:H     | 12                  | 0.12     | 0.01                | 0.12       |
| (1,4176) | 1:97:A:LEU:HD11 | 1:97:A:LEU:H     | 11                  | 0.33     | 0.13                | 0.4        |
| (1,4176) | 1:97:A:LEU:HD12 | 1:97:A:LEU:H     | 11                  | 0.33     | 0.13                | 0.4        |
| (1,4176) | 1:97:A:LEU:HD13 | 1:97:A:LEU:H     | 11                  | 0.33     | 0.13                | 0.4        |
| (1,423)  | 1:50:A:ILE:HG22 | 1:50:A:ILE:H     | 11                  | 0.33     | 0.25                | 0.15       |
| (1,423)  | 1:50:A:ILE:HG21 | 1:50:A:ILE:H     | 11                  | 0.33     | 0.25                | 0.15       |
| (1,423)  | 1:50:A:ILE:HG23 | 1:50:A:ILE:H     | 11                  | 0.33     | 0.25                | 0.15       |
| (1,2088) | 1:82:A:TRP:HZ2  | 1:124:A:VAL:HG21 | 11                  | 0.31     | 0.02                | 0.32       |
| (1,2088) | 1:82:A:TRP:HZ2  | 1:124:A:VAL:HG22 | 11                  | 0.31     | 0.02                | 0.32       |
| (1,2088) | 1:82:A:TRP:HZ2  | 1:124:A:VAL:HG23 | 11                  | 0.31     | 0.02                | 0.32       |
| (1,614)  | 1:97:A:LEU:HD11 | 1:97:A:LEU:H     | 11                  | 0.3      | 0.13                | 0.36       |
| (1,614)  | 1:97:A:LEU:HD12 | 1:97:A:LEU:H     | 11                  | 0.3      | 0.13                | 0.36       |
| (1,614)  | 1:97:A:LEU:HD13 | 1:97:A:LEU:H     | 11                  | 0.3      | 0.13                | 0.36       |
| (1,1073) | 1:97:A:LEU:HD11 | 1:97:A:LEU:H     | 11                  | 0.29     | 0.13                | 0.36       |
| (1,1073) | 1:97:A:LEU:HD12 | 1:97:A:LEU:H     | 11                  | 0.29     | 0.13                | 0.36       |
| (1,1073) | 1:97:A:LEU:HD13 | 1:97:A:LEU:H     | 11                  | 0.29     | 0.13                | 0.36       |
| (1,2546) | 1:73:A:SER:HA   | 1:73:A:SER:HB3   | 11                  | 0.26     | 0.01                | 0.26       |
| (1,2937) | 1:95:A:VAL:HG21 | 1:95:A:VAL:HG11  | 11                  | 0.25     | 0.07                | 0.24       |
| (1,2937) | 1:95:A:VAL:HG23 | 1:95:A:VAL:HG11  | 11                  | 0.25     | 0.07                | 0.24       |
| (1,2937) | 1:95:A:VAL:HG23 | 1:95:A:VAL:HG13  | 11                  | 0.25     | 0.07                | 0.24       |
| (1,2937) | 1:95:A:VAL:HG21 | 1:95:A:VAL:HG12  | 11                  | 0.25     | 0.07                | 0.24       |
| (1,2937) | 1:95:A:VAL:HG23 | 1:95:A:VAL:HG12  | 11                  | 0.25     | 0.07                | 0.24       |
| (1,2937) | 1:95:A:VAL:HG21 | 1:95:A:VAL:HG13  | 11                  | 0.25     | 0.07                | 0.24       |
| (1,2937) | 1:95:A:VAL:HG22 | 1:95:A:VAL:HG12  | 11                  | 0.25     | 0.07                | 0.24       |
| (1,1414) | 1:74:A:ALA:HB2  | 1:75:A:LEU:HD12  | 11                  | 0.18     | 0.07                | 0.15       |
| (1,1414) | 1:74:A:ALA:HB3  | 1:75:A:LEU:HD13  | 11                  | 0.18     | 0.07                | 0.15       |
| (1,1414) | 1:74:A:ALA:HB2  | 1:75:A:LEU:HD11  | 11                  | 0.18     | 0.07                | 0.15       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1414) | 1:74:A:ALA:HB2  | 1:75:A:LEU:HD13 | 11                  | 0.18     | 0.07                | 0.15       |
| (1,1414) | 1:74:A:ALA:HB3  | 1:75:A:LEU:HD12 | 11                  | 0.18     | 0.07                | 0.15       |
| (1,1414) | 1:74:A:ALA:HB3  | 1:75:A:LEU:HD11 | 11                  | 0.18     | 0.07                | 0.15       |
| (3,122)  | 1:27:A:VAL:HG23 | 1:28:A:ILE:HD12 | 11                  | 0.18     | 0.07                | 0.16       |
| (3,122)  | 1:27:A:VAL:HG23 | 1:28:A:ILE:HD13 | 11                  | 0.18     | 0.07                | 0.16       |
| (3,122)  | 1:27:A:VAL:HG21 | 1:28:A:ILE:HD11 | 11                  | 0.18     | 0.07                | 0.16       |
| (3,122)  | 1:27:A:VAL:HG21 | 1:28:A:ILE:HD13 | 11                  | 0.18     | 0.07                | 0.16       |
| (3,122)  | 1:27:A:VAL:HG23 | 1:28:A:ILE:HD11 | 11                  | 0.18     | 0.07                | 0.16       |
| (3,122)  | 1:27:A:VAL:HG21 | 1:28:A:ILE:HD12 | 11                  | 0.18     | 0.07                | 0.16       |
| (3,122)  | 1:27:A:VAL:HG22 | 1:28:A:ILE:HD12 | 11                  | 0.18     | 0.07                | 0.16       |
| (1,128)  | 1:35:A:PHE:HD2  | 1:39:A:PHE:H    | 11                  | 0.18     | 0.06                | 0.15       |
| (1,128)  | 1:35:A:PHE:HD1  | 1:39:A:PHE:H    | 11                  | 0.18     | 0.06                | 0.15       |
| (1,1350) | 1:129:A:ALA:HB2 | 1:129:A:ALA:H   | 11                  | 0.16     | 0.03                | 0.16       |
| (1,1350) | 1:129:A:ALA:HB1 | 1:129:A:ALA:H   | 11                  | 0.16     | 0.03                | 0.16       |
| (1,1350) | 1:129:A:ALA:HB3 | 1:129:A:ALA:H   | 11                  | 0.16     | 0.03                | 0.16       |
| (1,4301) | 1:97:A:LEU:HB2  | 1:97:A:LEU:H    | 11                  | 0.16     | 0.02                | 0.15       |
| (1,4344) | 1:120:A:ALA:H   | 1:119:A:GLU:HG2 | 11                  | 0.16     | 0.04                | 0.14       |
| (1,3172) | 1:25:A:LYS:HE3  | 1:25:A:LYS:HA   | 11                  | 0.14     | 0.05                | 0.12       |
| (1,2185) | 1:53:A:PHE:H    | 1:97:A:LEU:HD23 | 11                  | 0.14     | 0.02                | 0.13       |
| (1,2185) | 1:53:A:PHE:H    | 1:97:A:LEU:HD21 | 11                  | 0.14     | 0.02                | 0.13       |
| (1,3315) | 1:66:A:LEU:HD12 | 1:66:A:LEU:HA   | 11                  | 0.14     | 0.02                | 0.13       |
| (1,3315) | 1:66:A:LEU:HD11 | 1:66:A:LEU:HA   | 11                  | 0.14     | 0.02                | 0.13       |
| (1,3315) | 1:66:A:LEU:HD13 | 1:66:A:LEU:HA   | 11                  | 0.14     | 0.02                | 0.13       |
| (1,2052) | 1:65:A:ASN:H    | 1:66:A:LEU:H    | 11                  | 0.14     | 0.02                | 0.14       |
| (1,1718) | 1:18:A:GLN:HB3  | 1:19:A:PRO:HD2  | 11                  | 0.13     | 0.02                | 0.13       |
| (1,1546) | 1:56:A:LEU:HD13 | 1:52:A:ILE:HG13 | 11                  | 0.13     | 0.02                | 0.13       |
| (1,1546) | 1:56:A:LEU:HD11 | 1:52:A:ILE:HG13 | 11                  | 0.13     | 0.02                | 0.13       |
| (1,1546) | 1:56:A:LEU:HD12 | 1:52:A:ILE:HG13 | 11                  | 0.13     | 0.02                | 0.13       |
| (1,1709) | 1:72:A:ARG:HB3  | 1:53:A:PHE:HE1  | 11                  | 0.13     | 0.02                | 0.13       |
| (1,1709) | 1:72:A:ARG:HB3  | 1:53:A:PHE:HE2  | 11                  | 0.13     | 0.02                | 0.13       |
| (1,4060) | 1:97:A:LEU:HD21 | 1:39:A:PHE:H    | 11                  | 0.12     | 0.01                | 0.11       |
| (1,4060) | 1:97:A:LEU:HD22 | 1:39:A:PHE:H    | 11                  | 0.12     | 0.01                | 0.11       |
| (1,4060) | 1:97:A:LEU:HD23 | 1:39:A:PHE:H    | 11                  | 0.12     | 0.01                | 0.11       |
| (1,4258) | 1:52:A:ILE:HG12 | 1:56:A:LEU:H    | 11                  | 0.11     | 0.01                | 0.12       |
| (1,2312) | 1:77:A:LEU:HG   | 1:77:A:LEU:H    | 11                  | 0.1      | 0.0                 | 0.1        |
| (1,1769) | 1:72:A:ARG:HD3  | 1:72:A:ARG:HA   | 11                  | 0.1      | 0.0                 | 0.1        |
| (1,4087) | 1:65:A:ASN:HB2  | 1:65:A:ASN:HD21 | 10                  | 0.38     | 0.05                | 0.41       |
| (1,528)  | 1:65:A:ASN:HB2  | 1:65:A:ASN:HD21 | 10                  | 0.34     | 0.06                | 0.37       |
| (1,1315) | 1:95:A:VAL:HG22 | 1:97:A:LEU:HD21 | 10                  | 0.32     | 0.16                | 0.32       |
| (1,1315) | 1:95:A:VAL:HG23 | 1:97:A:LEU:HD21 | 10                  | 0.32     | 0.16                | 0.32       |
| (1,1315) | 1:95:A:VAL:HG21 | 1:97:A:LEU:HD21 | 10                  | 0.32     | 0.16                | 0.32       |
| (1,1315) | 1:95:A:VAL:HG22 | 1:97:A:LEU:HD22 | 10                  | 0.32     | 0.16                | 0.32       |

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| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1315) | 1:95:A:VAL:HG23  | 1:97:A:LEU:HD22 | 10                  | 0.32     | 0.16                | 0.32       |
| (1,1315) | 1:95:A:VAL:HG21  | 1:97:A:LEU:HD22 | 10                  | 0.32     | 0.16                | 0.32       |
| (1,1315) | 1:95:A:VAL:HG21  | 1:97:A:LEU:HD23 | 10                  | 0.32     | 0.16                | 0.32       |
| (3,148)  | 1:22:A:ASN:H     | 1:22:A:ASN:HB2  | 10                  | 0.32     | 0.1                 | 0.28       |
| (3,148)  | 1:22:A:ASN:H     | 1:65:A:ASN:HB3  | 10                  | 0.32     | 0.1                 | 0.28       |
| (1,1698) | 1:44:A:GLU:HG2   | 1:45:A:ALA:HB3  | 10                  | 0.29     | 0.08                | 0.29       |
| (1,1698) | 1:44:A:GLU:HG2   | 1:45:A:ALA:HB1  | 10                  | 0.29     | 0.08                | 0.29       |
| (1,1698) | 1:44:A:GLU:HG2   | 1:45:A:ALA:HB2  | 10                  | 0.29     | 0.08                | 0.29       |
| (3,64)   | 1:55:A:ASP:HB2   | 1:52:A:ILE:HG21 | 10                  | 0.27     | 0.09                | 0.26       |
| (3,64)   | 1:102:A:CYS:HB2  | 1:52:A:ILE:HG22 | 10                  | 0.27     | 0.09                | 0.26       |
| (3,64)   | 1:55:A:ASP:HB2   | 1:52:A:ILE:HG23 | 10                  | 0.27     | 0.09                | 0.26       |
| (3,64)   | 1:55:A:ASP:HB2   | 1:52:A:ILE:HG22 | 10                  | 0.27     | 0.09                | 0.26       |
| (3,64)   | 1:102:A:CYS:HB2  | 1:52:A:ILE:HG21 | 10                  | 0.27     | 0.09                | 0.26       |
| (1,3282) | 1:44:A:GLU:HG2   | 1:45:A:ALA:HB3  | 10                  | 0.25     | 0.08                | 0.24       |
| (1,3282) | 1:44:A:GLU:HG2   | 1:45:A:ALA:HB1  | 10                  | 0.25     | 0.08                | 0.24       |
| (1,3282) | 1:44:A:GLU:HG2   | 1:45:A:ALA:HB2  | 10                  | 0.25     | 0.08                | 0.24       |
| (1,1030) | 1:86:A:TYR:HE2   | 1:86:A:TYR:HB2  | 10                  | 0.23     | 0.07                | 0.25       |
| (1,1030) | 1:86:A:TYR:HE1   | 1:86:A:TYR:HB2  | 10                  | 0.23     | 0.07                | 0.25       |
| (1,1890) | 1:100:A:ASN:HD22 | 1:98:A:ASP:HB3  | 10                  | 0.2      | 0.02                | 0.2        |
| (1,1889) | 1:65:A:ASN:H     | 1:65:A:ASN:HB3  | 10                  | 0.2      | 0.05                | 0.2        |
| (1,753)  | 1:92:A:ALA:HB2   | 1:91:A:GLY:H    | 10                  | 0.2      | 0.04                | 0.2        |
| (1,753)  | 1:92:A:ALA:HB3   | 1:91:A:GLY:H    | 10                  | 0.2      | 0.04                | 0.2        |
| (1,753)  | 1:92:A:ALA:HB1   | 1:91:A:GLY:H    | 10                  | 0.2      | 0.04                | 0.2        |
| (1,1399) | 1:95:A:VAL:HG21  | 1:95:A:VAL:H    | 10                  | 0.19     | 0.05                | 0.2        |
| (1,1399) | 1:95:A:VAL:HG23  | 1:95:A:VAL:H    | 10                  | 0.19     | 0.05                | 0.2        |
| (1,1399) | 1:95:A:VAL:HG22  | 1:95:A:VAL:H    | 10                  | 0.19     | 0.05                | 0.2        |
| (1,3113) | 1:57:A:VAL:HG12  | 1:61:A:ALA:H    | 10                  | 0.19     | 0.06                | 0.2        |
| (1,3113) | 1:57:A:VAL:HG11  | 1:61:A:ALA:H    | 10                  | 0.19     | 0.06                | 0.2        |
| (1,3113) | 1:57:A:VAL:HG13  | 1:61:A:ALA:H    | 10                  | 0.19     | 0.06                | 0.2        |
| (1,853)  | 1:65:A:ASN:HB2   | 1:65:A:ASN:HD21 | 10                  | 0.19     | 0.06                | 0.22       |
| (1,1690) | 1:42:A:GLU:HG2   | 1:41:A:ALA:HB2  | 10                  | 0.16     | 0.04                | 0.15       |
| (1,1690) | 1:42:A:GLU:HG2   | 1:41:A:ALA:HB3  | 10                  | 0.16     | 0.04                | 0.15       |
| (1,1690) | 1:42:A:GLU:HG2   | 1:41:A:ALA:HB1  | 10                  | 0.16     | 0.04                | 0.15       |
| (1,3520) | 1:100:A:ASN:HD22 | 1:98:A:ASP:HB3  | 10                  | 0.15     | 0.02                | 0.15       |
| (1,3210) | 1:128:A:ARG:HA   | 1:128:A:ARG:HB3 | 10                  | 0.15     | 0.02                | 0.15       |
| (1,3299) | 1:20:A:LYS:H     | 1:20:A:LYS:HD3  | 10                  | 0.15     | 0.02                | 0.15       |
| (1,2871) | 1:129:A:ALA:HB2  | 1:129:A:ALA:H   | 10                  | 0.14     | 0.03                | 0.14       |
| (1,2871) | 1:129:A:ALA:HB3  | 1:129:A:ALA:H   | 10                  | 0.14     | 0.03                | 0.14       |
| (1,4295) | 1:116:A:GLN:HA   | 1:117:A:LEU:H   | 10                  | 0.12     | 0.01                | 0.12       |
| (1,4223) | 1:123:A:ARG:H    | 1:125:A:GLN:HG3 | 10                  | 0.12     | 0.01                | 0.12       |
| (1,4106) | 1:99:A:GLY:HA3   | 1:98:A:ASP:H    | 10                  | 0.12     | 0.01                | 0.12       |
| (1,2949) | 1:39:A:PHE:HZ    | 1:75:A:LEU:HD12 | 10                  | 0.12     | 0.01                | 0.11       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2949) | 1:39:A:PHE:HZ    | 1:75:A:LEU:HD13  | 10                  | 0.12     | 0.01                | 0.11       |
| (1,2949) | 1:39:A:PHE:HZ    | 1:75:A:LEU:HD11  | 10                  | 0.12     | 0.01                | 0.11       |
| (1,1954) | 1:116:A:GLN:H    | 1:113:A:ALA:HA   | 10                  | 0.11     | 0.01                | 0.11       |
| (1,1578) | 1:70:A:GLN:HB3   | 1:66:A:LEU:HA    | 10                  | 0.11     | 0.01                | 0.11       |
| (1,1635) | 1:121:A:LYS:HB2  | 1:117:A:LEU:HD11 | 9                   | 0.6      | 0.04                | 0.61       |
| (1,1635) | 1:121:A:LYS:HB2  | 1:117:A:LEU:HD12 | 9                   | 0.6      | 0.04                | 0.61       |
| (1,1635) | 1:121:A:LYS:HB2  | 1:117:A:LEU:HD13 | 9                   | 0.6      | 0.04                | 0.61       |
| (1,1157) | 1:117:A:LEU:HD11 | 1:82:A:TRP:HD1   | 9                   | 0.6      | 0.07                | 0.62       |
| (1,1157) | 1:117:A:LEU:HD12 | 1:82:A:TRP:HD1   | 9                   | 0.6      | 0.07                | 0.62       |
| (1,1157) | 1:117:A:LEU:HD13 | 1:82:A:TRP:HD1   | 9                   | 0.6      | 0.07                | 0.62       |
| (1,2680) | 1:117:A:LEU:HD11 | 1:82:A:TRP:HD1   | 9                   | 0.55     | 0.07                | 0.57       |
| (1,2680) | 1:117:A:LEU:HD12 | 1:82:A:TRP:HD1   | 9                   | 0.55     | 0.07                | 0.57       |
| (1,2680) | 1:117:A:LEU:HD13 | 1:82:A:TRP:HD1   | 9                   | 0.55     | 0.07                | 0.57       |
| (1,3204) | 1:121:A:LYS:HB2  | 1:117:A:LEU:HD11 | 9                   | 0.55     | 0.04                | 0.56       |
| (1,3204) | 1:121:A:LYS:HB2  | 1:117:A:LEU:HD12 | 9                   | 0.55     | 0.04                | 0.56       |
| (1,3204) | 1:121:A:LYS:HB2  | 1:117:A:LEU:HD13 | 9                   | 0.55     | 0.04                | 0.56       |
| (3,87)   | 1:117:A:LEU:HD11 | 1:121:A:LYS:H    | 9                   | 0.33     | 0.08                | 0.34       |
| (3,87)   | 1:117:A:LEU:HD12 | 1:121:A:LYS:H    | 9                   | 0.33     | 0.08                | 0.34       |
| (3,87)   | 1:117:A:LEU:HD13 | 1:121:A:LYS:H    | 9                   | 0.33     | 0.08                | 0.34       |
| (1,1813) | 1:117:A:LEU:HD13 | 1:117:A:LEU:HB3  | 9                   | 0.33     | 0.02                | 0.32       |
| (1,1813) | 1:117:A:LEU:HD11 | 1:117:A:LEU:HB3  | 9                   | 0.33     | 0.02                | 0.32       |
| (1,1813) | 1:117:A:LEU:HD12 | 1:117:A:LEU:HB3  | 9                   | 0.33     | 0.02                | 0.32       |
| (1,4126) | 1:59:A:ARG:HE    | 1:97:A:LEU:HD11  | 9                   | 0.32     | 0.08                | 0.31       |
| (1,4126) | 1:59:A:ARG:HE    | 1:97:A:LEU:HD13  | 9                   | 0.32     | 0.08                | 0.31       |
| (1,1960) | 1:121:A:LYS:HG3  | 1:117:A:LEU:HD12 | 9                   | 0.31     | 0.08                | 0.33       |
| (1,1960) | 1:121:A:LYS:HG3  | 1:117:A:LEU:HD13 | 9                   | 0.31     | 0.08                | 0.33       |
| (1,1960) | 1:121:A:LYS:HG3  | 1:117:A:LEU:HD11 | 9                   | 0.31     | 0.08                | 0.33       |
| (1,2836) | 1:95:A:VAL:HG22  | 1:97:A:LEU:HD21  | 9                   | 0.31     | 0.15                | 0.35       |
| (1,2836) | 1:95:A:VAL:HG23  | 1:97:A:LEU:HD21  | 9                   | 0.31     | 0.15                | 0.35       |
| (1,2836) | 1:95:A:VAL:HG21  | 1:97:A:LEU:HD21  | 9                   | 0.31     | 0.15                | 0.35       |
| (1,2836) | 1:95:A:VAL:HG22  | 1:97:A:LEU:HD22  | 9                   | 0.31     | 0.15                | 0.35       |
| (1,2836) | 1:95:A:VAL:HG23  | 1:97:A:LEU:HD22  | 9                   | 0.31     | 0.15                | 0.35       |
| (1,2836) | 1:95:A:VAL:HG21  | 1:97:A:LEU:HD22  | 9                   | 0.31     | 0.15                | 0.35       |
| (1,2836) | 1:95:A:VAL:HG21  | 1:97:A:LEU:HD23  | 9                   | 0.31     | 0.15                | 0.35       |
| (1,3416) | 1:117:A:LEU:HD13 | 1:117:A:LEU:HB3  | 9                   | 0.3      | 0.01                | 0.3        |
| (1,3416) | 1:117:A:LEU:HD11 | 1:117:A:LEU:HB3  | 9                   | 0.3      | 0.01                | 0.3        |
| (1,3416) | 1:117:A:LEU:HD12 | 1:117:A:LEU:HB3  | 9                   | 0.3      | 0.01                | 0.3        |
| (1,564)  | 1:59:A:ARG:HE    | 1:97:A:LEU:HD11  | 9                   | 0.27     | 0.08                | 0.26       |
| (1,564)  | 1:59:A:ARG:HE    | 1:97:A:LEU:HD13  | 9                   | 0.27     | 0.08                | 0.26       |
| (1,4119) | 1:66:A:LEU:HB2   | 1:70:A:GLN:HE22  | 9                   | 0.26     | 0.12                | 0.23       |
| (1,2415) | 1:45:A:ALA:HB3   | 1:84:A:TYR:HD2   | 9                   | 0.25     | 0.08                | 0.27       |
| (1,2415) | 1:45:A:ALA:HB2   | 1:84:A:TYR:HD2   | 9                   | 0.25     | 0.08                | 0.27       |

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| Key      | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,2415) | 1:45:A:ALA:HB1  | 1:84:A:TYR:HD1   | 9                   | 0.25     | 0.08                | 0.27       |
| (1,2415) | 1:45:A:ALA:HB3  | 1:84:A:TYR:HD1   | 9                   | 0.25     | 0.08                | 0.27       |
| (1,2415) | 1:45:A:ALA:HB1  | 1:84:A:TYR:HD2   | 9                   | 0.25     | 0.08                | 0.27       |
| (1,3786) | 1:27:A:VAL:HG11 | 1:21:A:LEU:H     | 9                   | 0.24     | 0.08                | 0.27       |
| (1,3786) | 1:27:A:VAL:HG12 | 1:21:A:LEU:H     | 9                   | 0.24     | 0.08                | 0.27       |
| (1,3786) | 1:27:A:VAL:HG13 | 1:21:A:LEU:H     | 9                   | 0.24     | 0.08                | 0.27       |
| (1,1357) | 1:74:A:ALA:HB2  | 1:31:A:LEU:HD11  | 9                   | 0.21     | 0.06                | 0.22       |
| (1,1357) | 1:74:A:ALA:HB3  | 1:31:A:LEU:HD12  | 9                   | 0.21     | 0.06                | 0.22       |
| (1,1357) | 1:74:A:ALA:HB3  | 1:31:A:LEU:HD11  | 9                   | 0.21     | 0.06                | 0.22       |
| (1,1357) | 1:74:A:ALA:HB2  | 1:31:A:LEU:HD12  | 9                   | 0.21     | 0.06                | 0.22       |
| (1,1357) | 1:74:A:ALA:HB2  | 1:31:A:LEU:HD13  | 9                   | 0.21     | 0.06                | 0.22       |
| (1,3497) | 1:27:A:VAL:HA   | 1:27:A:VAL:HG11  | 9                   | 0.2      | 0.08                | 0.16       |
| (1,3497) | 1:27:A:VAL:HA   | 1:27:A:VAL:HG12  | 9                   | 0.2      | 0.08                | 0.16       |
| (1,3497) | 1:27:A:VAL:HA   | 1:27:A:VAL:HG13  | 9                   | 0.2      | 0.08                | 0.16       |
| (1,3515) | 1:102:A:CYS:HB3 | 1:49:A:LYS:HA    | 9                   | 0.19     | 0.03                | 0.2        |
| (1,1681) | 1:40:A:SER:HA   | 1:41:A:ALA:HB1   | 9                   | 0.18     | 0.05                | 0.19       |
| (1,1681) | 1:40:A:SER:HA   | 1:41:A:ALA:HB3   | 9                   | 0.18     | 0.05                | 0.19       |
| (1,478)  | 1:27:A:VAL:HG22 | 1:29:A:ALA:H     | 9                   | 0.18     | 0.04                | 0.19       |
| (1,478)  | 1:27:A:VAL:HG21 | 1:29:A:ALA:H     | 9                   | 0.18     | 0.04                | 0.19       |
| (1,478)  | 1:27:A:VAL:HG23 | 1:29:A:ALA:H     | 9                   | 0.18     | 0.04                | 0.19       |
| (1,1126) | 1:86:A:TYR:HE1  | 1:86:A:TYR:HB3   | 9                   | 0.17     | 0.03                | 0.17       |
| (1,1126) | 1:86:A:TYR:HE2  | 1:86:A:TYR:HB3   | 9                   | 0.17     | 0.03                | 0.17       |
| (1,3519) | 1:65:A:ASN:H    | 1:65:A:ASN:HB3   | 9                   | 0.17     | 0.04                | 0.17       |
| (3,54)   | 1:71:A:LEU:HB3  | 1:75:A:LEU:HD12  | 9                   | 0.16     | 0.03                | 0.16       |
| (3,54)   | 1:71:A:LEU:HB3  | 1:75:A:LEU:HD11  | 9                   | 0.16     | 0.03                | 0.16       |
| (3,54)   | 1:71:A:LEU:HB3  | 1:75:A:LEU:HD13  | 9                   | 0.16     | 0.03                | 0.16       |
| (1,3979) | 1:50:A:ILE:HA   | 1:51:A:GLY:H     | 9                   | 0.14     | 0.03                | 0.14       |
| (1,3887) | 1:81:A:SER:HB2  | 1:82:A:TRP:H     | 9                   | 0.13     | 0.02                | 0.13       |
| (1,3314) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HG    | 9                   | 0.13     | 0.02                | 0.12       |
| (1,3314) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HG    | 9                   | 0.13     | 0.02                | 0.12       |
| (1,1464) | 1:102:A:CYS:HB3 | 1:103:A:GLY:H    | 9                   | 0.12     | 0.01                | 0.12       |
| (1,1004) | 1:82:A:TRP:HA   | 1:86:A:TYR:HD1   | 9                   | 0.12     | 0.01                | 0.12       |
| (1,1004) | 1:82:A:TRP:HA   | 1:86:A:TYR:HD2   | 9                   | 0.12     | 0.01                | 0.12       |
| (1,4091) | 1:65:A:ASN:HD22 | 1:20:A:LYS:HA    | 8                   | 0.79     | 0.26                | 0.74       |
| (1,4045) | 1:21:A:LEU:HD13 | 1:23:A:SER:H     | 8                   | 0.48     | 0.23                | 0.38       |
| (1,4045) | 1:21:A:LEU:HD11 | 1:23:A:SER:H     | 8                   | 0.48     | 0.23                | 0.38       |
| (1,4045) | 1:21:A:LEU:HD12 | 1:23:A:SER:H     | 8                   | 0.48     | 0.23                | 0.38       |
| (1,3418) | 1:117:A:LEU:HB2 | 1:117:A:LEU:HD13 | 8                   | 0.44     | 0.02                | 0.43       |
| (1,3418) | 1:117:A:LEU:HB2 | 1:117:A:LEU:HD11 | 8                   | 0.44     | 0.02                | 0.43       |
| (1,3418) | 1:117:A:LEU:HB2 | 1:117:A:LEU:HD12 | 8                   | 0.44     | 0.02                | 0.43       |
| (1,3309) | 1:117:A:LEU:HA  | 1:117:A:LEU:HG   | 8                   | 0.4      | 0.01                | 0.4        |
| (3,119)  | 1:98:A:ASP:HB3  | 1:99:A:GLY:HA2   | 8                   | 0.38     | 0.15                | 0.32       |

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| Key      | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,2408) | 1:52:A:ILE:HD11 | 1:96:A:ASP:HA    | 8                   | 0.34     | 0.1                 | 0.39       |
| (1,2408) | 1:52:A:ILE:HD13 | 1:96:A:ASP:HA    | 8                   | 0.34     | 0.1                 | 0.39       |
| (1,2408) | 1:52:A:ILE:HD12 | 1:96:A:ASP:HA    | 8                   | 0.34     | 0.1                 | 0.39       |
| (1,3610) | 1:121:A:LYS:HG3 | 1:117:A:LEU:HD12 | 8                   | 0.3      | 0.05                | 0.3        |
| (1,3610) | 1:121:A:LYS:HG3 | 1:117:A:LEU:HD13 | 8                   | 0.3      | 0.05                | 0.3        |
| (1,3610) | 1:121:A:LYS:HG3 | 1:117:A:LEU:HD11 | 8                   | 0.3      | 0.05                | 0.3        |
| (1,1303) | 1:97:A:LEU:HD13 | 1:35:A:PHE:HE2   | 8                   | 0.21     | 0.07                | 0.2        |
| (1,1303) | 1:97:A:LEU:HD11 | 1:35:A:PHE:HE2   | 8                   | 0.21     | 0.07                | 0.2        |
| (1,1303) | 1:97:A:LEU:HD12 | 1:35:A:PHE:HE1   | 8                   | 0.21     | 0.07                | 0.2        |
| (1,1303) | 1:97:A:LEU:HD12 | 1:35:A:PHE:HE2   | 8                   | 0.21     | 0.07                | 0.2        |
| (1,1303) | 1:97:A:LEU:HD13 | 1:35:A:PHE:HE1   | 8                   | 0.21     | 0.07                | 0.2        |
| (1,2559) | 1:86:A:TYR:HE1  | 1:86:A:TYR:HB2   | 8                   | 0.2      | 0.04                | 0.2        |
| (1,2559) | 1:86:A:TYR:HE2  | 1:86:A:TYR:HB2   | 8                   | 0.2      | 0.04                | 0.2        |
| (1,3771) | 1:126:A:ALA:HB2 | 1:126:A:ALA:H    | 8                   | 0.19     | 0.04                | 0.19       |
| (1,3771) | 1:126:A:ALA:HB1 | 1:126:A:ALA:H    | 8                   | 0.19     | 0.04                | 0.19       |
| (1,3771) | 1:126:A:ALA:HB3 | 1:126:A:ALA:H    | 8                   | 0.19     | 0.04                | 0.19       |
| (1,3516) | 1:21:A:LEU:HG   | 1:65:A:ASN:HB3   | 8                   | 0.18     | 0.05                | 0.18       |
| (1,2932) | 1:95:A:VAL:HG21 | 1:95:A:VAL:H     | 8                   | 0.17     | 0.04                | 0.18       |
| (1,2932) | 1:95:A:VAL:HG23 | 1:95:A:VAL:H     | 8                   | 0.17     | 0.04                | 0.18       |
| (1,2932) | 1:95:A:VAL:HG22 | 1:95:A:VAL:H     | 8                   | 0.17     | 0.04                | 0.18       |
| (1,2761) | 1:76:A:ARG:HA   | 1:76:A:ARG:HD2   | 8                   | 0.17     | 0.07                | 0.15       |
| (1,1167) | 1:34:A:ARG:HB3  | 1:30:A:PHE:HD2   | 8                   | 0.17     | 0.02                | 0.17       |
| (1,1167) | 1:34:A:ARG:HB3  | 1:30:A:PHE:HD1   | 8                   | 0.17     | 0.02                | 0.17       |
| (1,4127) | 1:34:A:ARG:HE   | 1:30:A:PHE:HD2   | 8                   | 0.16     | 0.04                | 0.16       |
| (1,4127) | 1:34:A:ARG:HE   | 1:30:A:PHE:HD1   | 8                   | 0.16     | 0.04                | 0.16       |
| (1,156)  | 1:126:A:ALA:HB2 | 1:126:A:ALA:H    | 8                   | 0.16     | 0.04                | 0.16       |
| (1,156)  | 1:126:A:ALA:HB1 | 1:126:A:ALA:H    | 8                   | 0.16     | 0.04                | 0.16       |
| (1,156)  | 1:126:A:ALA:HB3 | 1:126:A:ALA:H    | 8                   | 0.16     | 0.04                | 0.16       |
| (1,1876) | 1:27:A:VAL:HG22 | 1:31:A:LEU:HD12  | 8                   | 0.16     | 0.03                | 0.15       |
| (1,1876) | 1:27:A:VAL:HG23 | 1:31:A:LEU:HD11  | 8                   | 0.16     | 0.03                | 0.15       |
| (1,1876) | 1:27:A:VAL:HG22 | 1:31:A:LEU:HD11  | 8                   | 0.16     | 0.03                | 0.15       |
| (1,1876) | 1:27:A:VAL:HG23 | 1:31:A:LEU:HD12  | 8                   | 0.16     | 0.03                | 0.15       |
| (1,1845) | 1:95:A:VAL:HG22 | 1:96:A:ASP:HA    | 8                   | 0.15     | 0.03                | 0.15       |
| (1,1845) | 1:95:A:VAL:HG23 | 1:96:A:ASP:HA    | 8                   | 0.15     | 0.03                | 0.15       |
| (1,1845) | 1:95:A:VAL:HG21 | 1:96:A:ASP:HA    | 8                   | 0.15     | 0.03                | 0.15       |
| (1,4326) | 1:65:A:ASN:HA   | 1:66:A:LEU:H     | 8                   | 0.15     | 0.03                | 0.15       |
| (1,1720) | 1:117:A:LEU:HG  | 1:117:A:LEU:HD13 | 8                   | 0.14     | 0.04                | 0.13       |
| (1,1720) | 1:117:A:LEU:HG  | 1:117:A:LEU:HD11 | 8                   | 0.14     | 0.04                | 0.13       |
| (1,1720) | 1:117:A:LEU:HG  | 1:117:A:LEU:HD12 | 8                   | 0.14     | 0.04                | 0.13       |
| (1,4170) | 1:49:A:LYS:HB2  | 1:49:A:LYS:H     | 8                   | 0.14     | 0.02                | 0.14       |
| (1,4273) | 1:73:A:SER:HA   | 1:75:A:LEU:H     | 8                   | 0.14     | 0.01                | 0.14       |
| (1,3929) | 1:68:A:LYS:HD2  | 1:68:A:LYS:H     | 8                   | 0.13     | 0.01                | 0.13       |

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| Key      | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,4165) | 1:40:A:SER:HA   | 1:43:A:GLY:H     | 8                   | 0.13     | 0.04                | 0.12       |
| (1,1047) | 1:124:A:VAL:HA  | 1:124:A:VAL:HG21 | 8                   | 0.13     | 0.02                | 0.13       |
| (1,1047) | 1:124:A:VAL:HA  | 1:124:A:VAL:HG23 | 8                   | 0.13     | 0.02                | 0.13       |
| (1,1047) | 1:124:A:VAL:HA  | 1:124:A:VAL:HG22 | 8                   | 0.13     | 0.02                | 0.13       |
| (1,4271) | 1:78:A:TYR:HE2  | 1:75:A:LEU:H     | 8                   | 0.12     | 0.01                | 0.12       |
| (1,4271) | 1:78:A:TYR:HE1  | 1:75:A:LEU:H     | 8                   | 0.12     | 0.01                | 0.12       |
| (1,1536) | 1:53:A:PHE:HA   | 1:56:A:LEU:HB3   | 8                   | 0.11     | 0.01                | 0.12       |
| (1,2236) | 1:54:A:GLN:HB2  | 1:54:A:GLN:HG2   | 8                   | 0.11     | 0.01                | 0.11       |
| (1,2070) | 1:48:A:LEU:H    | 1:84:A:TYR:HE1   | 8                   | 0.11     | 0.01                | 0.11       |
| (1,2070) | 1:48:A:LEU:H    | 1:84:A:TYR:HE2   | 8                   | 0.11     | 0.01                | 0.11       |
| (1,488)  | 1:21:A:LEU:HD13 | 1:23:A:SER:H     | 7                   | 0.48     | 0.19                | 0.34       |
| (1,488)  | 1:21:A:LEU:HD12 | 1:23:A:SER:H     | 7                   | 0.48     | 0.19                | 0.34       |
| (1,488)  | 1:21:A:LEU:HD11 | 1:23:A:SER:H     | 7                   | 0.48     | 0.19                | 0.34       |
| (1,4112) | 1:54:A:GLN:HE22 | 1:57:A:VAL:H     | 7                   | 0.37     | 0.11                | 0.41       |
| (1,1478) | 1:64:A:MET:HE1  | 1:66:A:LEU:H     | 7                   | 0.28     | 0.11                | 0.23       |
| (1,1478) | 1:64:A:MET:HE2  | 1:66:A:LEU:H     | 7                   | 0.28     | 0.11                | 0.23       |
| (1,1478) | 1:64:A:MET:HE3  | 1:66:A:LEU:H     | 7                   | 0.28     | 0.11                | 0.23       |
| (1,172)  | 1:27:A:VAL:HG12 | 1:21:A:LEU:H     | 7                   | 0.22     | 0.05                | 0.23       |
| (1,172)  | 1:27:A:VAL:HG11 | 1:21:A:LEU:H     | 7                   | 0.22     | 0.05                | 0.23       |
| (1,3019) | 1:64:A:MET:HE1  | 1:66:A:LEU:H     | 7                   | 0.22     | 0.11                | 0.17       |
| (1,3019) | 1:64:A:MET:HE2  | 1:66:A:LEU:H     | 7                   | 0.22     | 0.11                | 0.17       |
| (1,3019) | 1:64:A:MET:HE3  | 1:66:A:LEU:H     | 7                   | 0.22     | 0.11                | 0.17       |
| (1,2881) | 1:74:A:ALA:HB3  | 1:31:A:LEU:HD12  | 7                   | 0.2      | 0.05                | 0.2        |
| (1,2881) | 1:74:A:ALA:HB2  | 1:31:A:LEU:HD11  | 7                   | 0.2      | 0.05                | 0.2        |
| (1,2881) | 1:74:A:ALA:HB3  | 1:31:A:LEU:HD11  | 7                   | 0.2      | 0.05                | 0.2        |
| (1,2881) | 1:74:A:ALA:HB2  | 1:31:A:LEU:HD12  | 7                   | 0.2      | 0.05                | 0.2        |
| (1,2881) | 1:74:A:ALA:HB2  | 1:31:A:LEU:HD13  | 7                   | 0.2      | 0.05                | 0.2        |
| (1,2955) | 1:74:A:ALA:HB3  | 1:75:A:LEU:HD13  | 7                   | 0.17     | 0.07                | 0.12       |
| (1,2955) | 1:74:A:ALA:HB2  | 1:75:A:LEU:HD11  | 7                   | 0.17     | 0.07                | 0.12       |
| (1,2955) | 1:74:A:ALA:HB3  | 1:75:A:LEU:HD11  | 7                   | 0.17     | 0.07                | 0.12       |
| (1,2955) | 1:74:A:ALA:HB2  | 1:75:A:LEU:HD13  | 7                   | 0.17     | 0.07                | 0.12       |
| (1,2955) | 1:74:A:ALA:HB3  | 1:75:A:LEU:HD12  | 7                   | 0.17     | 0.07                | 0.12       |
| (1,2955) | 1:74:A:ALA:HB2  | 1:75:A:LEU:HD12  | 7                   | 0.17     | 0.07                | 0.12       |
| (1,2021) | 1:53:A:PHE:HE1  | 1:57:A:VAL:HG13  | 7                   | 0.16     | 0.05                | 0.14       |
| (1,2021) | 1:53:A:PHE:HE2  | 1:57:A:VAL:HG12  | 7                   | 0.16     | 0.05                | 0.14       |
| (1,2021) | 1:53:A:PHE:HE2  | 1:57:A:VAL:HG11  | 7                   | 0.16     | 0.05                | 0.14       |
| (1,1567) | 1:68:A:LYS:HB2  | 1:68:A:LYS:HA    | 7                   | 0.15     | 0.04                | 0.13       |
| (1,3255) | 1:40:A:SER:HA   | 1:41:A:ALA:HB1   | 7                   | 0.15     | 0.03                | 0.15       |
| (1,3255) | 1:40:A:SER:HA   | 1:41:A:ALA:HB3   | 7                   | 0.15     | 0.03                | 0.15       |
| (1,3767) | 1:129:A:ALA:HA  | 1:129:A:ALA:H    | 7                   | 0.14     | 0.03                | 0.14       |
| (1,3500) | 1:27:A:VAL:HG23 | 1:31:A:LEU:HD11  | 7                   | 0.13     | 0.03                | 0.12       |
| (1,3500) | 1:27:A:VAL:HG22 | 1:31:A:LEU:HD11  | 7                   | 0.13     | 0.03                | 0.12       |

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| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,3500) | 1:27:A:VAL:HG23  | 1:31:A:LEU:HD12 | 7                   | 0.13     | 0.03                | 0.12       |
| (1,959)  | 1:30:A:PHE:HD1   | 1:31:A:LEU:HA   | 7                   | 0.13     | 0.02                | 0.12       |
| (1,959)  | 1:30:A:PHE:HD2   | 1:31:A:LEU:HA   | 7                   | 0.13     | 0.02                | 0.12       |
| (1,1074) | 1:34:A:ARG:HG2   | 1:35:A:PHE:HD2  | 7                   | 0.13     | 0.03                | 0.11       |
| (1,1074) | 1:34:A:ARG:HG2   | 1:35:A:PHE:HD1  | 7                   | 0.13     | 0.03                | 0.11       |
| (1,707)  | 1:75:A:LEU:HB3   | 1:74:A:ALA:H    | 7                   | 0.13     | 0.01                | 0.12       |
| (1,351)  | 1:63:A:GLU:HB3   | 1:65:A:ASN:H    | 7                   | 0.12     | 0.02                | 0.12       |
| (1,287)  | 1:127:A:GLN:H    | 1:127:A:GLN:HG2 | 7                   | 0.12     | 0.02                | 0.12       |
| (1,1009) | 1:37:A:HIS:HD2   | 1:38:A:CYS:HA   | 7                   | 0.12     | 0.01                | 0.12       |
| (1,1052) | 1:69:A:THR:HG22  | 1:69:A:THR:HA   | 7                   | 0.12     | 0.01                | 0.12       |
| (1,1052) | 1:69:A:THR:HG21  | 1:69:A:THR:HA   | 7                   | 0.12     | 0.01                | 0.12       |
| (1,3667) | 1:37:A:HIS:H     | 1:37:A:HIS:HD2  | 7                   | 0.12     | 0.01                | 0.12       |
| (1,609)  | 1:49:A:LYS:HB2   | 1:49:A:LYS:H    | 7                   | 0.11     | 0.01                | 0.11       |
| (1,2270) | 1:113:A:ALA:HA   | 1:114:A:ARG:H   | 7                   | 0.11     | 0.01                | 0.11       |
| (1,3443) | 1:123:A:ARG:HG2  | 1:123:A:ARG:HD3 | 7                   | 0.11     | 0.01                | 0.11       |
| (1,4302) | 1:94:A:ARG:H     | 1:94:A:ARG:HB3  | 7                   | 0.11     | 0.01                | 0.1        |
| (1,280)  | 1:86:A:TYR:H     | 1:86:A:TYR:HB2  | 7                   | 0.11     | 0.01                | 0.1        |
| (1,1946) | 1:110:A:VAL:HG21 | 1:110:A:VAL:HB  | 7                   | 0.1      | 0.0                 | 0.1        |
| (1,1946) | 1:110:A:VAL:HG22 | 1:110:A:VAL:HB  | 7                   | 0.1      | 0.0                 | 0.1        |
| (1,1946) | 1:110:A:VAL:HG23 | 1:110:A:VAL:HB  | 7                   | 0.1      | 0.0                 | 0.1        |
| (3,102)  | 1:65:A:ASN:HB2   | 1:64:A:MET:HG2  | 6                   | 0.5      | 0.15                | 0.5        |
| (1,2411) | 1:45:A:ALA:HB3   | 1:84:A:TYR:HB3  | 6                   | 0.28     | 0.14                | 0.24       |
| (1,2411) | 1:45:A:ALA:HB2   | 1:84:A:TYR:HB3  | 6                   | 0.28     | 0.14                | 0.24       |
| (1,2411) | 1:45:A:ALA:HB1   | 1:84:A:TYR:HB3  | 6                   | 0.28     | 0.14                | 0.24       |
| (1,557)  | 1:66:A:LEU:HB2   | 1:70:A:GLN:HE22 | 6                   | 0.27     | 0.1                 | 0.24       |
| (3,29)   | 1:48:A:LEU:HD22  | 1:39:A:PHE:HD1  | 6                   | 0.23     | 0.12                | 0.22       |
| (3,29)   | 1:48:A:LEU:HD23  | 1:39:A:PHE:HD2  | 6                   | 0.23     | 0.12                | 0.22       |
| (3,29)   | 1:48:A:LEU:HD22  | 1:39:A:PHE:HD2  | 6                   | 0.23     | 0.12                | 0.22       |
| (3,29)   | 1:48:A:LEU:HD21  | 1:39:A:PHE:HD2  | 6                   | 0.23     | 0.12                | 0.22       |
| (1,1793) | 1:88:A:VAL:HG22  | 1:84:A:TYR:HA   | 6                   | 0.22     | 0.1                 | 0.18       |
| (1,1793) | 1:88:A:VAL:HG23  | 1:84:A:TYR:HA   | 6                   | 0.22     | 0.1                 | 0.18       |
| (1,1683) | 1:48:A:LEU:HD12  | 1:38:A:CYS:HA   | 6                   | 0.21     | 0.07                | 0.22       |
| (1,1683) | 1:48:A:LEU:HD11  | 1:38:A:CYS:HA   | 6                   | 0.21     | 0.07                | 0.22       |
| (1,1683) | 1:48:A:LEU:HD13  | 1:38:A:CYS:HA   | 6                   | 0.21     | 0.07                | 0.22       |
| (1,4113) | 1:22:A:ASN:H     | 1:22:A:ASN:HD22 | 6                   | 0.21     | 0.06                | 0.22       |
| (1,2819) | 1:97:A:LEU:HD13  | 1:35:A:PHE:HE2  | 6                   | 0.2      | 0.05                | 0.18       |
| (1,2819) | 1:97:A:LEU:HD11  | 1:35:A:PHE:HE2  | 6                   | 0.2      | 0.05                | 0.18       |
| (1,2819) | 1:97:A:LEU:HD12  | 1:35:A:PHE:HE1  | 6                   | 0.2      | 0.05                | 0.18       |
| (1,2819) | 1:97:A:LEU:HD12  | 1:35:A:PHE:HE2  | 6                   | 0.2      | 0.05                | 0.18       |
| (1,1753) | 1:113:A:ALA:HB3  | 1:89:A:LYS:H    | 6                   | 0.19     | 0.03                | 0.18       |
| (1,1753) | 1:113:A:ALA:HB2  | 1:89:A:LYS:H    | 6                   | 0.19     | 0.03                | 0.18       |
| (1,1753) | 1:113:A:ALA:HB1  | 1:89:A:LYS:H    | 6                   | 0.19     | 0.03                | 0.18       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,3273) | 1:42:A:GLU:HG2  | 1:43:A:GLY:H    | 6                   | 0.18     | 0.09                | 0.12       |
| (1,1329) | 1:73:A:SER:HB3  | 1:74:A:ALA:H    | 6                   | 0.16     | 0.0                 | 0.16       |
| (1,1801) | 1:117:A:LEU:HA  | 1:120:A:ALA:HB3 | 6                   | 0.16     | 0.03                | 0.17       |
| (1,1801) | 1:117:A:LEU:HA  | 1:120:A:ALA:HB2 | 6                   | 0.16     | 0.03                | 0.17       |
| (1,1801) | 1:117:A:LEU:HA  | 1:120:A:ALA:HB1 | 6                   | 0.16     | 0.03                | 0.17       |
| (1,2417) | 1:129:A:ALA:HB1 | 1:127:A:GLN:HB3 | 6                   | 0.15     | 0.08                | 0.12       |
| (1,2417) | 1:129:A:ALA:HB3 | 1:127:A:GLN:HB3 | 6                   | 0.15     | 0.08                | 0.12       |
| (1,3344) | 1:113:A:ALA:HB3 | 1:89:A:LYS:H    | 6                   | 0.15     | 0.03                | 0.15       |
| (1,3344) | 1:113:A:ALA:HB2 | 1:89:A:LYS:H    | 6                   | 0.15     | 0.03                | 0.15       |
| (1,3344) | 1:113:A:ALA:HB1 | 1:89:A:LYS:H    | 6                   | 0.15     | 0.03                | 0.15       |
| (1,3270) | 1:42:A:GLU:HG2  | 1:41:A:ALA:HB2  | 6                   | 0.15     | 0.04                | 0.15       |
| (1,3270) | 1:42:A:GLU:HG2  | 1:41:A:ALA:HB1  | 6                   | 0.15     | 0.04                | 0.15       |
| (1,1580) | 1:97:A:LEU:HA   | 1:97:A:LEU:H    | 6                   | 0.15     | 0.02                | 0.16       |
| (1,755)  | 1:95:A:VAL:H    | 1:94:A:ARG:HB3  | 6                   | 0.14     | 0.02                | 0.13       |
| (1,1939) | 1:33:A:GLU:HB3  | 1:30:A:PHE:HA   | 6                   | 0.14     | 0.02                | 0.13       |
| (1,1053) | 1:93:A:THR:HG23 | 1:102:A:CYS:HA  | 6                   | 0.13     | 0.02                | 0.14       |
| (1,1053) | 1:93:A:THR:HG21 | 1:102:A:CYS:HA  | 6                   | 0.13     | 0.02                | 0.14       |
| (1,1053) | 1:93:A:THR:HG22 | 1:102:A:CYS:HA  | 6                   | 0.13     | 0.02                | 0.14       |
| (1,4143) | 1:37:A:HIS:HA   | 1:39:A:PHE:H    | 6                   | 0.13     | 0.02                | 0.13       |
| (1,762)  | 1:65:A:ASN:HA   | 1:66:A:LEU:H    | 6                   | 0.13     | 0.02                | 0.13       |
| (1,2306) | 1:38:A:CYS:H    | 1:97:A:LEU:HA   | 6                   | 0.13     | 0.01                | 0.12       |
| (1,3603) | 1:97:A:LEU:HA   | 1:97:A:LEU:HG   | 6                   | 0.13     | 0.01                | 0.14       |
| (1,4110) | 1:40:A:SER:HA   | 1:42:A:GLU:H    | 6                   | 0.13     | 0.02                | 0.13       |
| (1,3884) | 1:83:A:ARG:H    | 1:83:A:ARG:HB2  | 6                   | 0.13     | 0.01                | 0.12       |
| (1,2689) | 1:34:A:ARG:HB3  | 1:30:A:PHE:HD1  | 6                   | 0.12     | 0.02                | 0.13       |
| (1,2689) | 1:34:A:ARG:HB3  | 1:30:A:PHE:HD2  | 6                   | 0.12     | 0.02                | 0.13       |
| (1,2811) | 1:97:A:LEU:HD13 | 1:97:A:LEU:HB3  | 6                   | 0.12     | 0.02                | 0.12       |
| (1,2811) | 1:97:A:LEU:HD12 | 1:97:A:LEU:HB3  | 6                   | 0.12     | 0.02                | 0.12       |
| (1,1111) | 1:75:A:LEU:HB3  | 1:75:A:LEU:H    | 6                   | 0.12     | 0.01                | 0.12       |
| (1,1847) | 1:36:A:PRO:HB2  | 1:36:A:PRO:HD2  | 6                   | 0.12     | 0.02                | 0.12       |
| (1,1327) | 1:73:A:SER:HB2  | 1:73:A:SER:H    | 6                   | 0.12     | 0.01                | 0.12       |
| (1,2986) | 1:115:A:LYS:HB3 | 1:115:A:LYS:H   | 6                   | 0.12     | 0.01                | 0.12       |
| (1,2849) | 1:73:A:SER:HB3  | 1:74:A:ALA:H    | 6                   | 0.12     | 0.0                 | 0.12       |
| (1,3169) | 1:53:A:PHE:HB3  | 1:75:A:LEU:HD23 | 6                   | 0.12     | 0.02                | 0.12       |
| (1,3169) | 1:53:A:PHE:HB3  | 1:75:A:LEU:HD21 | 6                   | 0.12     | 0.02                | 0.12       |
| (1,847)  | 1:49:A:LYS:HB2  | 1:102:A:CYS:HB3 | 6                   | 0.12     | 0.01                | 0.11       |
| (1,3736) | 1:41:A:ALA:HA   | 1:29:A:ALA:H    | 6                   | 0.11     | 0.01                | 0.11       |
| (1,1768) | 1:72:A:ARG:HA   | 1:75:A:LEU:H    | 6                   | 0.11     | 0.01                | 0.11       |
| (1,3029) | 1:25:A:LYS:HG3  | 1:26:A:GLU:HA   | 6                   | 0.11     | 0.0                 | 0.11       |
| (1,3991) | 1:85:A:LEU:H    | 1:84:A:TYR:HA   | 6                   | 0.11     | 0.0                 | 0.11       |
| (1,3542) | 1:105:A:LEU:HB3 | 1:101:A:PRO:HB3 | 6                   | 0.1      | 0.0                 | 0.1        |
| (1,3031) | 1:25:A:LYS:HG3  | 1:25:A:LYS:HD2  | 6                   | 0.1      | 0.0                 | 0.1        |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1882) | 1:64:A:MET:HE3  | 1:65:A:ASN:HD22 | 5                   | 0.75     | 0.05                | 0.74       |
| (1,1882) | 1:64:A:MET:HE2  | 1:65:A:ASN:HD22 | 5                   | 0.75     | 0.05                | 0.74       |
| (1,1882) | 1:64:A:MET:HE1  | 1:65:A:ASN:HD22 | 5                   | 0.75     | 0.05                | 0.74       |
| (1,3509) | 1:64:A:MET:HE3  | 1:65:A:ASN:HD22 | 5                   | 0.69     | 0.05                | 0.68       |
| (1,3509) | 1:64:A:MET:HE2  | 1:65:A:ASN:HD22 | 5                   | 0.69     | 0.05                | 0.68       |
| (1,3509) | 1:64:A:MET:HE1  | 1:65:A:ASN:HD22 | 5                   | 0.69     | 0.05                | 0.68       |
| (1,4195) | 1:61:A:ALA:HB1  | 1:67:A:SER:H    | 5                   | 0.25     | 0.04                | 0.27       |
| (1,4195) | 1:61:A:ALA:HB2  | 1:67:A:SER:H    | 5                   | 0.25     | 0.04                | 0.27       |
| (1,1273) | 1:45:A:ALA:HB3  | 1:84:A:TYR:HB3  | 5                   | 0.24     | 0.12                | 0.19       |
| (1,1273) | 1:45:A:ALA:HB2  | 1:84:A:TYR:HB3  | 5                   | 0.24     | 0.12                | 0.19       |
| (1,1273) | 1:45:A:ALA:HB1  | 1:84:A:TYR:HB3  | 5                   | 0.24     | 0.12                | 0.19       |
| (1,1872) | 1:56:A:LEU:HD21 | 1:55:A:ASP:HB3  | 5                   | 0.23     | 0.04                | 0.25       |
| (1,1872) | 1:56:A:LEU:HD23 | 1:55:A:ASP:HB3  | 5                   | 0.23     | 0.04                | 0.25       |
| (1,3600) | 1:113:A:ALA:HB1 | 1:92:A:ALA:HA   | 5                   | 0.21     | 0.08                | 0.18       |
| (1,3600) | 1:113:A:ALA:HB3 | 1:92:A:ALA:HA   | 5                   | 0.21     | 0.08                | 0.18       |
| (1,630)  | 1:61:A:ALA:HB1  | 1:67:A:SER:H    | 5                   | 0.2      | 0.04                | 0.21       |
| (1,630)  | 1:61:A:ALA:HB2  | 1:67:A:SER:H    | 5                   | 0.2      | 0.04                | 0.21       |
| (1,3511) | 1:50:A:ILE:HG13 | 1:49:A:LYS:HA   | 5                   | 0.16     | 0.04                | 0.15       |
| (1,3766) | 1:128:A:ARG:HB3 | 1:129:A:ALA:H   | 5                   | 0.16     | 0.04                | 0.15       |
| (1,3398) | 1:117:A:LEU:HA  | 1:120:A:ALA:HB3 | 5                   | 0.14     | 0.02                | 0.14       |
| (1,3398) | 1:117:A:LEU:HA  | 1:120:A:ALA:HB2 | 5                   | 0.14     | 0.02                | 0.14       |
| (1,3398) | 1:117:A:LEU:HA  | 1:120:A:ALA:HB1 | 5                   | 0.14     | 0.02                | 0.14       |
| (1,3456) | 1:95:A:VAL:HG22 | 1:96:A:ASP:HA   | 5                   | 0.14     | 0.02                | 0.14       |
| (1,3456) | 1:95:A:VAL:HG23 | 1:96:A:ASP:HA   | 5                   | 0.14     | 0.02                | 0.14       |
| (1,1591) | 1:120:A:ALA:HB1 | 1:120:A:ALA:H   | 5                   | 0.13     | 0.0                 | 0.13       |
| (1,1591) | 1:120:A:ALA:HB3 | 1:120:A:ALA:H   | 5                   | 0.13     | 0.0                 | 0.13       |
| (1,3269) | 1:33:A:GLU:HB3  | 1:17:A:ASN:HB2  | 5                   | 0.13     | 0.03                | 0.13       |
| (1,1952) | 1:112:A:HIS:HA  | 1:115:A:LYS:HB3 | 5                   | 0.13     | 0.02                | 0.12       |
| (1,1358) | 1:32:A:ALA:HB3  | 1:33:A:GLU:H    | 5                   | 0.13     | 0.02                | 0.12       |
| (1,1358) | 1:32:A:ALA:HB1  | 1:33:A:GLU:H    | 5                   | 0.13     | 0.02                | 0.12       |
| (1,3151) | 1:97:A:LEU:HA   | 1:97:A:LEU:H    | 5                   | 0.13     | 0.0                 | 0.13       |
| (1,319)  | 1:76:A:ARG:HD2  | 1:77:A:LEU:H    | 5                   | 0.12     | 0.01                | 0.13       |
| (1,2665) | 1:86:A:TYR:HE1  | 1:86:A:TYR:HB3  | 5                   | 0.12     | 0.01                | 0.12       |
| (1,2665) | 1:86:A:TYR:HE2  | 1:86:A:TYR:HB3  | 5                   | 0.12     | 0.01                | 0.12       |
| (1,4041) | 1:21:A:LEU:HA   | 1:23:A:SER:H    | 5                   | 0.12     | 0.01                | 0.12       |
| (1,3122) | 1:11:A:SER:HB2  | 1:11:A:SER:HA   | 5                   | 0.12     | 0.01                | 0.12       |
| (1,3291) | 1:72:A:ARG:HB3  | 1:53:A:PHE:HE1  | 5                   | 0.12     | 0.01                | 0.12       |
| (1,3291) | 1:72:A:ARG:HB3  | 1:53:A:PHE:HE2  | 5                   | 0.12     | 0.01                | 0.12       |
| (1,1590) | 1:61:A:ALA:HB2  | 1:61:A:ALA:H    | 5                   | 0.12     | 0.02                | 0.11       |
| (1,1590) | 1:61:A:ALA:HB3  | 1:61:A:ALA:H    | 5                   | 0.12     | 0.02                | 0.11       |
| (1,2695) | 1:78:A:TYR:HA   | 1:81:A:SER:H    | 5                   | 0.12     | 0.01                | 0.12       |
| (1,2859) | 1:86:A:TYR:HE1  | 1:85:A:LEU:H    | 5                   | 0.12     | 0.01                | 0.12       |

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| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1887) | 1:65:A:ASN:HB2   | 1:66:A:LEU:H    | 5                   | 0.11     | 0.01                | 0.11       |
| (1,3147) | 1:23:A:SER:HB2   | 1:70:A:GLN:HB3  | 5                   | 0.11     | 0.0                 | 0.11       |
| (1,3164) | 1:120:A:ALA:HB1  | 1:120:A:ALA:H   | 5                   | 0.11     | 0.01                | 0.11       |
| (1,3164) | 1:120:A:ALA:HB3  | 1:120:A:ALA:H   | 5                   | 0.11     | 0.01                | 0.11       |
| (1,1504) | 1:121:A:LYS:HD3  | 1:121:A:LYS:H   | 5                   | 0.11     | 0.0                 | 0.11       |
| (1,1121) | 1:101:A:PRO:HD2  | 1:100:A:ASN:HA  | 5                   | 0.1      | 0.0                 | 0.1        |
| (1,3489) | 1:21:A:LEU:HD22  | 1:20:A:LYS:HA   | 4                   | 0.54     | 0.22                | 0.55       |
| (1,3489) | 1:21:A:LEU:HD21  | 1:20:A:LYS:HA   | 4                   | 0.54     | 0.22                | 0.55       |
| (1,3489) | 1:21:A:LEU:HD23  | 1:20:A:LYS:HA   | 4                   | 0.54     | 0.22                | 0.55       |
| (1,2228) | 1:25:A:LYS:HD3   | 1:25:A:LYS:HG3  | 4                   | 0.39     | 0.17                | 0.48       |
| (1,1512) | 1:52:A:ILE:HG23  | 1:53:A:PHE:HB2  | 4                   | 0.32     | 0.13                | 0.39       |
| (1,1512) | 1:52:A:ILE:HG21  | 1:53:A:PHE:HB2  | 4                   | 0.32     | 0.13                | 0.39       |
| (1,790)  | 1:50:A:ILE:HG22  | 1:50:A:ILE:H    | 4                   | 0.31     | 0.01                | 0.32       |
| (1,790)  | 1:50:A:ILE:HG21  | 1:50:A:ILE:H    | 4                   | 0.31     | 0.01                | 0.32       |
| (1,1510) | 1:52:A:ILE:HG23  | 1:50:A:ILE:H    | 4                   | 0.29     | 0.13                | 0.26       |
| (1,3390) | 1:88:A:VAL:HG23  | 1:84:A:TYR:HA   | 4                   | 0.22     | 0.1                 | 0.21       |
| (1,3390) | 1:88:A:VAL:HG22  | 1:84:A:TYR:HA   | 4                   | 0.22     | 0.1                 | 0.21       |
| (3,41)   | 1:52:A:ILE:HD11  | 1:56:A:LEU:HA   | 4                   | 0.22     | 0.05                | 0.22       |
| (1,3257) | 1:48:A:LEU:HD12  | 1:38:A:CYS:HA   | 4                   | 0.2      | 0.05                | 0.19       |
| (1,3257) | 1:48:A:LEU:HD11  | 1:38:A:CYS:HA   | 4                   | 0.2      | 0.05                | 0.19       |
| (1,3257) | 1:48:A:LEU:HD13  | 1:38:A:CYS:HA   | 4                   | 0.2      | 0.05                | 0.19       |
| (1,3494) | 1:56:A:LEU:HD21  | 1:55:A:ASP:HB3  | 4                   | 0.2      | 0.0                 | 0.2        |
| (1,3494) | 1:56:A:LEU:HD23  | 1:55:A:ASP:HB3  | 4                   | 0.2      | 0.0                 | 0.2        |
| (1,1668) | 1:52:A:ILE:HG13  | 1:48:A:LEU:HD12 | 4                   | 0.2      | 0.04                | 0.2        |
| (1,1883) | 1:64:A:MET:HE3   | 1:21:A:LEU:H    | 4                   | 0.19     | 0.01                | 0.18       |
| (1,1883) | 1:64:A:MET:HE1   | 1:21:A:LEU:H    | 4                   | 0.19     | 0.01                | 0.18       |
| (1,3898) | 1:79:A:THR:HG21  | 1:80:A:SER:H    | 4                   | 0.18     | 0.05                | 0.19       |
| (1,3898) | 1:79:A:THR:HG22  | 1:80:A:SER:H    | 4                   | 0.18     | 0.05                | 0.19       |
| (1,818)  | 1:28:A:ILE:HD11  | 1:78:A:TYR:HB3  | 4                   | 0.17     | 0.09                | 0.12       |
| (1,818)  | 1:28:A:ILE:HD12  | 1:78:A:TYR:HB3  | 4                   | 0.17     | 0.09                | 0.12       |
| (1,3539) | 1:63:A:GLU:HG3   | 1:63:A:GLU:H    | 4                   | 0.16     | 0.02                | 0.16       |
| (1,2943) | 1:110:A:VAL:HG22 | 1:108:A:GLN:H   | 4                   | 0.14     | 0.02                | 0.15       |
| (1,2943) | 1:110:A:VAL:HG21 | 1:108:A:GLN:H   | 4                   | 0.14     | 0.02                | 0.15       |
| (3,81)   | 1:77:A:LEU:HA    | 1:77:A:LEU:HD13 | 4                   | 0.14     | 0.02                | 0.14       |
| (3,81)   | 1:77:A:LEU:HA    | 1:77:A:LEU:HD11 | 4                   | 0.14     | 0.02                | 0.14       |
| (3,81)   | 1:74:A:ALA:HA    | 1:77:A:LEU:HD13 | 4                   | 0.14     | 0.02                | 0.14       |
| (1,1247) | 1:42:A:GLU:HB3   | 1:43:A:GLY:HA2  | 4                   | 0.14     | 0.04                | 0.12       |
| (1,2961) | 1:56:A:LEU:HD22  | 1:52:A:ILE:HB   | 4                   | 0.14     | 0.01                | 0.14       |
| (1,2961) | 1:56:A:LEU:HD21  | 1:52:A:ILE:HB   | 4                   | 0.14     | 0.01                | 0.14       |
| (1,153)  | 1:129:A:ALA:HA   | 1:129:A:ALA:H   | 4                   | 0.14     | 0.02                | 0.13       |
| (1,2587) | 1:68:A:LYS:HB2   | 1:69:A:THR:HG22 | 4                   | 0.13     | 0.02                | 0.12       |
| (1,2587) | 1:68:A:LYS:HB2   | 1:69:A:THR:HG23 | 4                   | 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) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,2587) | 1:68:A:LYS:HB2  | 1:69:A:THR:HG21 | 4                   | 0.13     | 0.02                | 0.12       |
| (1,3731) | 1:66:A:LEU:HB3  | 1:66:A:LEU:H    | 4                   | 0.13     | 0.02                | 0.14       |
| (1,3687) | 1:85:A:LEU:H    | 1:82:A:TRP:HD1  | 4                   | 0.13     | 0.01                | 0.12       |
| (1,1013) | 1:11:A:SER:HA   | 1:12:A:GLN:H    | 4                   | 0.12     | 0.02                | 0.12       |
| (1,1787) | 1:93:A:THR:HB   | 1:49:A:LYS:HB3  | 4                   | 0.12     | 0.01                | 0.12       |
| (1,3510) | 1:64:A:MET:HE3  | 1:21:A:LEU:H    | 4                   | 0.12     | 0.01                | 0.12       |
| (1,3510) | 1:64:A:MET:HE1  | 1:21:A:LEU:H    | 4                   | 0.12     | 0.01                | 0.12       |
| (1,1835) | 1:20:A:LYS:H    | 1:20:A:LYS:HG2  | 4                   | 0.12     | 0.01                | 0.12       |
| (1,2089) | 1:49:A:LYS:HB2  | 1:52:A:ILE:H    | 4                   | 0.12     | 0.02                | 0.11       |
| (1,1640) | 1:33:A:GLU:HG3  | 1:33:A:GLU:H    | 4                   | 0.12     | 0.01                | 0.12       |
| (1,3316) | 1:66:A:LEU:HD12 | 1:30:A:PHE:HD2  | 4                   | 0.12     | 0.01                | 0.12       |
| (1,3316) | 1:66:A:LEU:HD13 | 1:30:A:PHE:HD1  | 4                   | 0.12     | 0.01                | 0.12       |
| (1,3316) | 1:66:A:LEU:HD11 | 1:30:A:PHE:HD2  | 4                   | 0.12     | 0.01                | 0.12       |
| (1,709)  | 1:73:A:SER:HA   | 1:75:A:LEU:H    | 4                   | 0.12     | 0.0                 | 0.12       |
| (1,4238) | 1:97:A:LEU:H    | 1:96:A:ASP:H    | 4                   | 0.12     | 0.0                 | 0.12       |
| (1,925)  | 1:28:A:ILE:HB   | 1:25:A:LYS:HA   | 4                   | 0.11     | 0.0                 | 0.11       |
| (1,2627) | 1:112:A:HIS:HA  | 1:112:A:HIS:HB2 | 4                   | 0.11     | 0.01                | 0.11       |
| (1,1143) | 1:86:A:TYR:HE1  | 1:86:A:TYR:HD1  | 4                   | 0.11     | 0.0                 | 0.11       |
| (1,1143) | 1:86:A:TYR:HE2  | 1:86:A:TYR:HD2  | 4                   | 0.11     | 0.0                 | 0.11       |
| (1,2257) | 1:69:A:THR:HB   | 1:72:A:ARG:HB3  | 4                   | 0.11     | 0.01                | 0.11       |
| (1,2519) | 1:55:A:ASP:HB3  | 1:55:A:ASP:HA   | 4                   | 0.11     | 0.01                | 0.11       |
| (1,158)  | 1:126:A:ALA:HA  | 1:126:A:ALA:H   | 4                   | 0.11     | 0.0                 | 0.11       |
| (1,1711) | 1:25:A:LYS:HD3  | 1:25:A:LYS:HA   | 4                   | 0.11     | 0.0                 | 0.11       |
| (1,1583) | 1:36:A:PRO:HD2  | 1:34:A:ARG:HA   | 4                   | 0.1      | 0.0                 | 0.11       |
| (1,2348) | 1:30:A:PHE:HD2  | 1:21:A:LEU:HD13 | 3                   | 0.54     | 0.23                | 0.62       |
| (1,2348) | 1:30:A:PHE:HD2  | 1:21:A:LEU:HD11 | 3                   | 0.54     | 0.23                | 0.62       |
| (1,2348) | 1:30:A:PHE:HD1  | 1:21:A:LEU:HD13 | 3                   | 0.54     | 0.23                | 0.62       |
| (1,3892) | 1:45:A:ALA:HB2  | 1:81:A:SER:H    | 3                   | 0.52     | 0.27                | 0.69       |
| (1,3892) | 1:45:A:ALA:HB1  | 1:81:A:SER:H    | 3                   | 0.52     | 0.27                | 0.69       |
| (1,1077) | 1:21:A:LEU:HA   | 1:21:A:LEU:HD23 | 3                   | 0.5      | 0.04                | 0.52       |
| (1,1077) | 1:21:A:LEU:HA   | 1:21:A:LEU:HD22 | 3                   | 0.5      | 0.04                | 0.52       |
| (1,2616) | 1:21:A:LEU:HA   | 1:21:A:LEU:HD23 | 3                   | 0.45     | 0.04                | 0.47       |
| (1,2616) | 1:21:A:LEU:HA   | 1:21:A:LEU:HD22 | 3                   | 0.45     | 0.04                | 0.47       |
| (1,2923) | 1:21:A:LEU:HD22 | 1:30:A:PHE:H    | 3                   | 0.41     | 0.0                 | 0.41       |
| (1,2923) | 1:21:A:LEU:HD21 | 1:30:A:PHE:H    | 3                   | 0.41     | 0.0                 | 0.41       |
| (1,1514) | 1:52:A:ILE:HG21 | 1:48:A:LEU:HG   | 3                   | 0.34     | 0.01                | 0.33       |
| (1,1514) | 1:52:A:ILE:HG23 | 1:48:A:LEU:HG   | 3                   | 0.34     | 0.01                | 0.33       |
| (1,1514) | 1:52:A:ILE:HG22 | 1:48:A:LEU:HG   | 3                   | 0.34     | 0.01                | 0.33       |
| (1,3330) | 1:25:A:LYS:HE3  | 1:77:A:LEU:HD12 | 3                   | 0.34     | 0.03                | 0.32       |
| (1,3330) | 1:25:A:LYS:HE3  | 1:77:A:LEU:HD11 | 3                   | 0.34     | 0.03                | 0.32       |
| (1,1483) | 1:21:A:LEU:HG   | 1:64:A:MET:HE3  | 3                   | 0.33     | 0.03                | 0.33       |
| (1,1483) | 1:21:A:LEU:HG   | 1:64:A:MET:HE1  | 3                   | 0.33     | 0.03                | 0.33       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1483) | 1:21:A:LEU:HG   | 1:64:A:MET:HE2  | 3                   | 0.33     | 0.03                | 0.33       |
| (1,2782) | 1:61:A:ALA:HB2  | 1:62:A:GLY:HA2  | 3                   | 0.32     | 0.02                | 0.31       |
| (1,2782) | 1:61:A:ALA:HB1  | 1:62:A:GLY:HA2  | 3                   | 0.32     | 0.02                | 0.31       |
| (1,3058) | 1:52:A:ILE:HG21 | 1:48:A:LEU:HG   | 3                   | 0.29     | 0.01                | 0.29       |
| (1,3058) | 1:52:A:ILE:HG23 | 1:48:A:LEU:HG   | 3                   | 0.29     | 0.01                | 0.29       |
| (1,3058) | 1:52:A:ILE:HG22 | 1:48:A:LEU:HG   | 3                   | 0.29     | 0.01                | 0.29       |
| (1,3055) | 1:52:A:ILE:HG23 | 1:50:A:ILE:H    | 3                   | 0.29     | 0.11                | 0.22       |
| (1,3025) | 1:21:A:LEU:HG   | 1:64:A:MET:HE3  | 3                   | 0.28     | 0.03                | 0.28       |
| (1,3025) | 1:21:A:LEU:HG   | 1:64:A:MET:HE1  | 3                   | 0.28     | 0.03                | 0.28       |
| (1,3025) | 1:21:A:LEU:HG   | 1:64:A:MET:HE2  | 3                   | 0.28     | 0.03                | 0.28       |
| (3,130)  | 1:52:A:ILE:HG22 | 1:50:A:ILE:HA   | 3                   | 0.28     | 0.08                | 0.27       |
| (3,130)  | 1:52:A:ILE:HG21 | 1:50:A:ILE:HA   | 3                   | 0.28     | 0.08                | 0.27       |
| (3,31)   | 1:22:A:ASN:HD21 | 1:22:A:ASN:HB2  | 3                   | 0.27     | 0.04                | 0.25       |
| (1,2075) | 1:61:A:ALA:HB3  | 1:62:A:GLY:H    | 3                   | 0.25     | 0.03                | 0.24       |
| (1,2075) | 1:61:A:ALA:HB2  | 1:62:A:GLY:H    | 3                   | 0.25     | 0.03                | 0.24       |
| (1,1826) | 1:64:A:MET:HE3  | 1:21:A:LEU:HD11 | 3                   | 0.23     | 0.03                | 0.24       |
| (1,1826) | 1:64:A:MET:HE1  | 1:21:A:LEU:HD12 | 3                   | 0.23     | 0.03                | 0.24       |
| (1,1826) | 1:64:A:MET:HE2  | 1:21:A:LEU:HD13 | 3                   | 0.23     | 0.03                | 0.24       |
| (1,838)  | 1:64:A:MET:HE1  | 1:30:A:PHE:HD2  | 3                   | 0.21     | 0.03                | 0.21       |
| (1,838)  | 1:64:A:MET:HE1  | 1:30:A:PHE:HD1  | 3                   | 0.21     | 0.03                | 0.21       |
| (1,2253) | 1:44:A:GLU:HB3  | 1:44:A:GLU:H    | 3                   | 0.21     | 0.05                | 0.24       |
| (1,1353) | 1:61:A:ALA:HB3  | 1:62:A:GLY:H    | 3                   | 0.21     | 0.02                | 0.2        |
| (1,1353) | 1:61:A:ALA:HB2  | 1:62:A:GLY:H    | 3                   | 0.21     | 0.02                | 0.2        |
| (1,3784) | 1:21:A:LEU:HG   | 1:21:A:LEU:H    | 3                   | 0.21     | 0.08                | 0.23       |
| (1,3436) | 1:64:A:MET:HE3  | 1:21:A:LEU:HD11 | 3                   | 0.2      | 0.02                | 0.21       |
| (1,3436) | 1:64:A:MET:HE1  | 1:21:A:LEU:HD12 | 3                   | 0.2      | 0.02                | 0.21       |
| (1,3436) | 1:64:A:MET:HE2  | 1:21:A:LEU:HD13 | 3                   | 0.2      | 0.02                | 0.21       |
| (1,1660) | 1:27:A:VAL:HA   | 1:27:A:VAL:HG11 | 3                   | 0.19     | 0.01                | 0.19       |
| (1,1660) | 1:27:A:VAL:HA   | 1:27:A:VAL:HG12 | 3                   | 0.19     | 0.01                | 0.19       |
| (1,1824) | 1:27:A:VAL:HA   | 1:21:A:LEU:HD13 | 3                   | 0.19     | 0.02                | 0.19       |
| (1,1824) | 1:27:A:VAL:HA   | 1:21:A:LEU:HD11 | 3                   | 0.19     | 0.02                | 0.19       |
| (1,1078) | 1:48:A:LEU:HD22 | 1:84:A:TYR:HE2  | 3                   | 0.18     | 0.03                | 0.17       |
| (1,1078) | 1:48:A:LEU:HD23 | 1:84:A:TYR:HE1  | 3                   | 0.18     | 0.03                | 0.17       |
| (1,2424) | 1:64:A:MET:HE1  | 1:30:A:PHE:HD2  | 3                   | 0.18     | 0.03                | 0.18       |
| (1,2424) | 1:64:A:MET:HE1  | 1:30:A:PHE:HD1  | 3                   | 0.18     | 0.03                | 0.18       |
| (1,2876) | 1:61:A:ALA:HB3  | 1:62:A:GLY:H    | 3                   | 0.18     | 0.02                | 0.16       |
| (1,2876) | 1:61:A:ALA:HB2  | 1:62:A:GLY:H    | 3                   | 0.18     | 0.02                | 0.16       |
| (1,1963) | 1:120:A:ALA:HB1 | 1:82:A:TRP:HE1  | 3                   | 0.17     | 0.02                | 0.16       |
| (1,1963) | 1:120:A:ALA:HB2 | 1:82:A:TRP:HE1  | 3                   | 0.17     | 0.02                | 0.16       |
| (1,308)  | 1:79:A:THR:HG21 | 1:80:A:SER:H    | 3                   | 0.17     | 0.02                | 0.15       |
| (1,308)  | 1:79:A:THR:HG22 | 1:80:A:SER:H    | 3                   | 0.17     | 0.02                | 0.15       |
| (1,4325) | 1:62:A:GLY:HA3  | 1:66:A:LEU:H    | 3                   | 0.16     | 0.02                | 0.17       |

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| Key      | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,152)  | 1:128:A:ARG:HB3 | 1:129:A:ALA:H    | 3                   | 0.15     | 0.03                | 0.14       |
| (1,3240) | 1:52:A:ILE:HG13 | 1:48:A:LEU:HD12  | 3                   | 0.15     | 0.03                | 0.17       |
| (1,3433) | 1:27:A:VAL:HA   | 1:21:A:LEU:HD13  | 3                   | 0.15     | 0.02                | 0.16       |
| (1,3433) | 1:27:A:VAL:HA   | 1:21:A:LEU:HD11  | 3                   | 0.15     | 0.02                | 0.16       |
| (1,2619) | 1:48:A:LEU:HD22 | 1:84:A:TYR:HE2   | 3                   | 0.15     | 0.02                | 0.14       |
| (1,2619) | 1:48:A:LEU:HD23 | 1:84:A:TYR:HE1   | 3                   | 0.15     | 0.02                | 0.14       |
| (1,3348) | 1:79:A:THR:HG22 | 1:84:A:TYR:HE2   | 3                   | 0.15     | 0.03                | 0.16       |
| (1,3348) | 1:79:A:THR:HG23 | 1:84:A:TYR:HE1   | 3                   | 0.15     | 0.03                | 0.16       |
| (1,3348) | 1:79:A:THR:HG22 | 1:84:A:TYR:HE1   | 3                   | 0.15     | 0.03                | 0.16       |
| (1,1885) | 1:83:A:ARG:HG3  | 1:84:A:TYR:H     | 3                   | 0.15     | 0.02                | 0.14       |
| (1,605)  | 1:40:A:SER:HA   | 1:43:A:GLY:H     | 3                   | 0.14     | 0.02                | 0.15       |
| (1,1818) | 1:118:A:GLU:HA  | 1:122:A:ALA:H    | 3                   | 0.14     | 0.02                | 0.15       |
| (1,856)  | 1:13:A:ASP:HB3  | 1:14:A:PRO:HD3   | 3                   | 0.14     | 0.02                | 0.13       |
| (1,2042) | 1:15:A:MET:H    | 1:16:A:GLU:H     | 3                   | 0.14     | 0.02                | 0.13       |
| (1,2436) | 1:13:A:ASP:HB3  | 1:33:A:GLU:HB3   | 3                   | 0.13     | 0.02                | 0.13       |
| (1,3994) | 1:45:A:ALA:H    | 1:83:A:ARG:HB2   | 3                   | 0.12     | 0.02                | 0.12       |
| (1,297)  | 1:81:A:SER:HB2  | 1:82:A:TRP:H     | 3                   | 0.12     | 0.02                | 0.12       |
| (1,2575) | 1:124:A:VAL:HA  | 1:124:A:VAL:HG22 | 3                   | 0.12     | 0.0                 | 0.12       |
| (1,2575) | 1:124:A:VAL:HA  | 1:124:A:VAL:HG21 | 3                   | 0.12     | 0.0                 | 0.12       |
| (1,3104) | 1:56:A:LEU:HD13 | 1:52:A:ILE:HG13  | 3                   | 0.12     | 0.0                 | 0.12       |
| (1,3803) | 1:108:A:GLN:HB3 | 1:108:A:GLN:H    | 3                   | 0.12     | 0.02                | 0.11       |
| (1,3685) | 1:81:A:SER:H    | 1:84:A:TYR:H     | 3                   | 0.12     | 0.01                | 0.11       |
| (1,550)  | 1:40:A:SER:HA   | 1:42:A:GLU:H     | 3                   | 0.11     | 0.01                | 0.11       |
| (1,1454) | 1:60:A:VAL:HB   | 1:61:A:ALA:H     | 3                   | 0.11     | 0.01                | 0.1        |
| (1,1457) | 1:60:A:VAL:HG13 | 1:60:A:VAL:HB    | 3                   | 0.11     | 0.01                | 0.11       |
| (1,1457) | 1:60:A:VAL:HG11 | 1:60:A:VAL:HB    | 3                   | 0.11     | 0.01                | 0.11       |
| (1,3931) | 1:67:A:SER:H    | 1:66:A:LEU:H     | 3                   | 0.11     | 0.01                | 0.11       |
| (1,1389) | 1:68:A:LYS:HD3  | 1:53:A:PHE:HZ    | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,1391) | 1:54:A:GLN:HB3  | 1:53:A:PHE:HD1   | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,3779) | 1:121:A:LYS:HB2 | 1:120:A:ALA:H    | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,3647) | 1:59:A:ARG:H    | 1:61:A:ALA:H     | 3                   | 0.1      | 0.0                 | 0.1        |
| (1,303)  | 1:45:A:ALA:HB1  | 1:81:A:SER:H     | 2                   | 0.66     | 0.02                | 0.66       |
| (1,303)  | 1:45:A:ALA:HB2  | 1:81:A:SER:H     | 2                   | 0.66     | 0.02                | 0.66       |
| (1,1912) | 1:64:A:MET:HE1  | 1:65:A:ASN:HB2   | 2                   | 0.36     | 0.01                | 0.36       |
| (1,1912) | 1:64:A:MET:HE3  | 1:65:A:ASN:HB2   | 2                   | 0.36     | 0.01                | 0.36       |
| (1,3548) | 1:64:A:MET:HE1  | 1:65:A:ASN:HB2   | 2                   | 0.29     | 0.01                | 0.29       |
| (1,3548) | 1:64:A:MET:HE3  | 1:65:A:ASN:HB2   | 2                   | 0.29     | 0.01                | 0.29       |
| (1,4083) | 1:21:A:LEU:HA   | 1:22:A:ASN:HD22  | 2                   | 0.28     | 0.05                | 0.28       |
| (3,93)   | 1:21:A:LEU:HB3  | 1:21:A:LEU:HD13  | 2                   | 0.28     | 0.04                | 0.28       |
| (3,93)   | 1:21:A:LEU:HB3  | 1:21:A:LEU:HD12  | 2                   | 0.28     | 0.04                | 0.28       |
| (1,1949) | 1:92:A:ALA:HB1  | 1:110:A:VAL:HG12 | 2                   | 0.26     | 0.15                | 0.26       |
| (1,1949) | 1:92:A:ALA:HB3  | 1:110:A:VAL:HG11 | 2                   | 0.26     | 0.15                | 0.26       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,523)  | 1:21:A:LEU:HA   | 1:22:A:ASN:HD22 | 2                   | 0.22     | 0.05                | 0.22       |
| (1,1568) | 1:68:A:LYS:HB2  | 1:57:A:VAL:HG12 | 2                   | 0.22     | 0.02                | 0.22       |
| (1,1568) | 1:68:A:LYS:HB2  | 1:57:A:VAL:HG11 | 2                   | 0.22     | 0.02                | 0.22       |
| (1,2476) | 1:50:A:ILE:HD12 | 1:50:A:ILE:HB   | 2                   | 0.22     | 0.03                | 0.22       |
| (1,2108) | 1:40:A:SER:H    | 1:41:A:ALA:H    | 2                   | 0.2      | 0.06                | 0.2        |
| (1,2740) | 1:57:A:VAL:HG21 | 1:58:A:ASP:HB2  | 2                   | 0.19     | 0.01                | 0.19       |
| (1,2740) | 1:57:A:VAL:HG22 | 1:58:A:ASP:HB2  | 2                   | 0.19     | 0.01                | 0.19       |
| (1,4144) | 1:21:A:LEU:H    | 1:65:A:ASN:HB3  | 2                   | 0.19     | 0.03                | 0.19       |
| (1,2946) | 1:88:A:VAL:HG11 | 1:84:A:TYR:HE2  | 2                   | 0.18     | 0.04                | 0.18       |
| (1,2946) | 1:88:A:VAL:HG12 | 1:84:A:TYR:HE1  | 2                   | 0.18     | 0.04                | 0.18       |
| (1,3933) | 1:65:A:ASN:HB2  | 1:65:A:ASN:H    | 2                   | 0.18     | 0.02                | 0.18       |
| (1,4154) | 1:17:A:ASN:HA   | 1:18:A:GLN:H    | 2                   | 0.18     | 0.02                | 0.18       |
| (1,1285) | 1:48:A:LEU:HD23 | 1:48:A:LEU:HB3  | 2                   | 0.17     | 0.05                | 0.17       |
| (1,3136) | 1:68:A:LYS:HB2  | 1:57:A:VAL:HG12 | 2                   | 0.17     | 0.02                | 0.17       |
| (1,3136) | 1:68:A:LYS:HB2  | 1:57:A:VAL:HG11 | 2                   | 0.17     | 0.02                | 0.17       |
| (1,1224) | 1:13:A:ASP:HB2  | 1:16:A:GLU:H    | 2                   | 0.16     | 0.0                 | 0.16       |
| (1,1776) | 1:88:A:VAL:HA   | 1:88:A:VAL:HG13 | 2                   | 0.16     | 0.01                | 0.16       |
| (1,1776) | 1:88:A:VAL:HA   | 1:88:A:VAL:HG12 | 2                   | 0.16     | 0.01                | 0.16       |
| (1,1366) | 1:50:A:ILE:HG12 | 1:50:A:ILE:HG22 | 2                   | 0.16     | 0.02                | 0.16       |
| (1,4278) | 1:12:A:GLN:HA   | 1:13:A:ASP:H    | 2                   | 0.16     | 0.01                | 0.16       |
| (1,2979) | 1:53:A:PHE:HZ   | 1:68:A:LYS:HB2  | 2                   | 0.15     | 0.02                | 0.15       |
| (1,3798) | 1:43:A:GLY:HA3  | 1:44:A:GLU:H    | 2                   | 0.15     | 0.02                | 0.15       |
| (1,4260) | 1:38:A:CYS:H    | 1:35:A:PHE:HD2  | 2                   | 0.15     | 0.0                 | 0.15       |
| (1,4260) | 1:38:A:CYS:H    | 1:35:A:PHE:HD1  | 2                   | 0.15     | 0.0                 | 0.15       |
| (1,348)  | 1:65:A:ASN:HB2  | 1:65:A:ASN:H    | 2                   | 0.15     | 0.02                | 0.15       |
| (1,593)  | 1:17:A:ASN:HA   | 1:18:A:GLN:H    | 2                   | 0.15     | 0.02                | 0.15       |
| (3,38)   | 1:32:A:ALA:HB3  | 1:33:A:GLU:HG2  | 2                   | 0.14     | 0.03                | 0.14       |
| (3,38)   | 1:32:A:ALA:HB2  | 1:33:A:GLU:HG2  | 2                   | 0.14     | 0.03                | 0.14       |
| (1,761)  | 1:62:A:GLY:HA3  | 1:66:A:LEU:H    | 2                   | 0.14     | 0.01                | 0.14       |
| (1,1351) | 1:127:A:GLN:H   | 1:126:A:ALA:HB3 | 2                   | 0.14     | 0.02                | 0.14       |
| (1,1351) | 1:127:A:GLN:H   | 1:126:A:ALA:HB1 | 2                   | 0.14     | 0.02                | 0.14       |
| (1,3374) | 1:88:A:VAL:HA   | 1:88:A:VAL:HG13 | 2                   | 0.13     | 0.01                | 0.13       |
| (1,3374) | 1:88:A:VAL:HA   | 1:88:A:VAL:HG12 | 2                   | 0.13     | 0.01                | 0.13       |
| (1,3708) | 1:62:A:GLY:H    | 1:62:A:GLY:HA3  | 2                   | 0.13     | 0.01                | 0.13       |
| (1,435)  | 1:42:A:GLU:HB2  | 1:43:A:GLY:H    | 2                   | 0.12     | 0.02                | 0.12       |
| (1,714)  | 1:12:A:GLN:HA   | 1:13:A:ASP:H    | 2                   | 0.12     | 0.01                | 0.12       |
| (1,1589) | 1:120:A:ALA:HB3 | 1:121:A:LYS:H   | 2                   | 0.12     | 0.01                | 0.12       |
| (1,2435) | 1:33:A:GLU:HB3  | 1:13:A:ASP:HB2  | 2                   | 0.12     | 0.02                | 0.12       |
| (1,2791) | 1:84:A:TYR:HE1  | 1:84:A:TYR:HB3  | 2                   | 0.12     | 0.02                | 0.12       |
| (1,2791) | 1:84:A:TYR:HE2  | 1:84:A:TYR:HB3  | 2                   | 0.12     | 0.02                | 0.12       |
| (1,3579) | 1:33:A:GLU:HB3  | 1:30:A:PHE:HA   | 2                   | 0.12     | 0.01                | 0.12       |
| (1,3596) | 1:112:A:HIS:HA  | 1:115:A:LYS:HB3 | 2                   | 0.12     | 0.01                | 0.12       |

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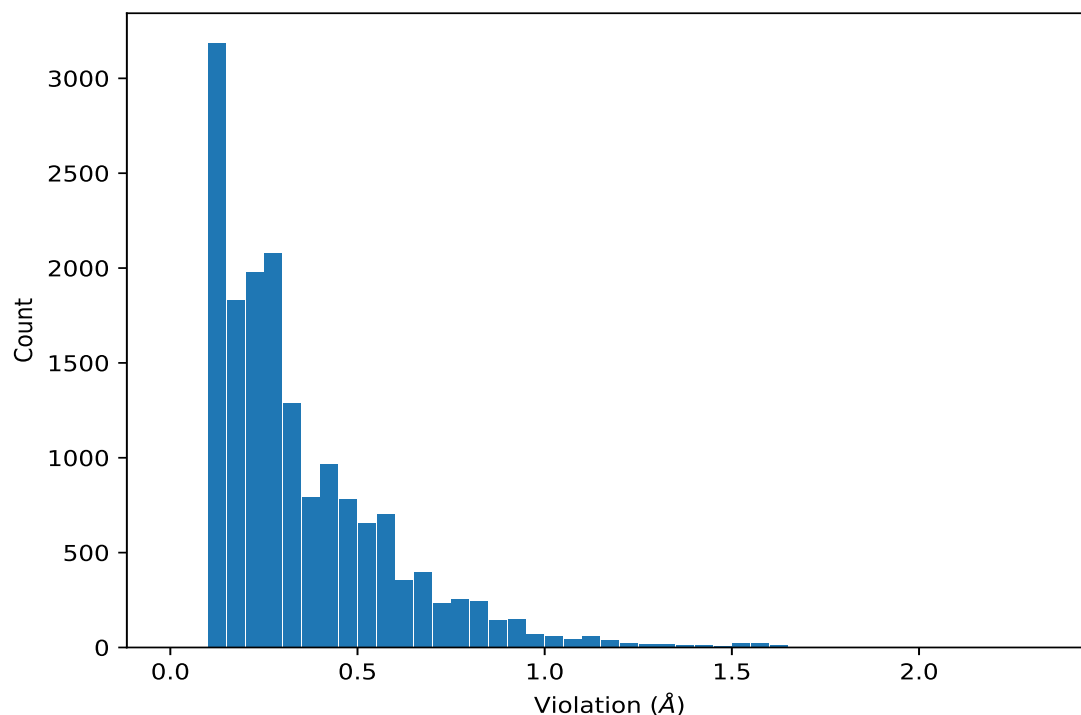
| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,3699) | 1:88:A:VAL:HA   | 1:89:A:LYS:H    | 2                   | 0.12     | 0.02                | 0.12       |
| (1,184)  | 1:43:A:GLY:HA3  | 1:44:A:GLU:H    | 2                   | 0.12     | 0.02                | 0.12       |
| (1,1214) | 1:17:A:ASN:HB3  | 1:17:A:ASN:H    | 2                   | 0.12     | 0.02                | 0.12       |
| (1,1441) | 1:42:A:GLU:HB2  | 1:43:A:GLY:H    | 2                   | 0.12     | 0.02                | 0.12       |
| (1,1910) | 1:128:A:ARG:HB3 | 1:128:A:ARG:HD2 | 2                   | 0.12     | 0.02                | 0.12       |
| (1,4000) | 1:42:A:GLU:HB2  | 1:43:A:GLY:H    | 2                   | 0.12     | 0.02                | 0.12       |
| (1,1445) | 1:15:A:MET:H    | 1:15:A:MET:HB2  | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,2561) | 1:85:A:LEU:H    | 1:84:A:TYR:HE1  | 2                   | 0.12     | 0.01                | 0.12       |
| (1,2561) | 1:85:A:LEU:H    | 1:84:A:TYR:HE2  | 2                   | 0.12     | 0.01                | 0.12       |
| (1,2915) | 1:38:A:CYS:HB2  | 1:39:A:PHE:HE1  | 2                   | 0.12     | 0.01                | 0.12       |
| (1,2915) | 1:38:A:CYS:HB2  | 1:39:A:PHE:HE2  | 2                   | 0.12     | 0.01                | 0.12       |
| (1,3424) | 1:118:A:GLU:HA  | 1:122:A:ALA:H   | 2                   | 0.12     | 0.01                | 0.12       |
| (1,4128) | 1:34:A:ARG:HE   | 1:34:A:ARG:HA   | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,773)  | 1:116:A:GLN:HG3 | 1:115:A:LYS:H   | 2                   | 0.12     | 0.02                | 0.12       |
| (1,1997) | 1:107:A:GLU:HG2 | 1:107:A:GLU:H   | 2                   | 0.12     | 0.02                | 0.12       |
| (1,2765) | 1:79:A:THR:H    | 1:78:A:TYR:HE1  | 2                   | 0.12     | 0.02                | 0.12       |
| (1,2586) | 1:93:A:THR:HG23 | 1:102:A:CYS:HA  | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,2586) | 1:93:A:THR:HG21 | 1:102:A:CYS:HA  | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,2613) | 1:34:A:ARG:HG2  | 1:35:A:PHE:HD1  | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,2613) | 1:34:A:ARG:HG2  | 1:35:A:PHE:HD2  | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,2707) | 1:35:A:PHE:HB2  | 1:97:A:LEU:HD21 | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,2707) | 1:35:A:PHE:HB2  | 1:97:A:LEU:HD22 | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,2743) | 1:34:A:ARG:HD3  | 1:30:A:PHE:HD2  | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,2743) | 1:34:A:ARG:HD3  | 1:30:A:PHE:HD1  | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,2988) | 1:68:A:LYS:HB2  | 1:68:A:LYS:H    | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,3880) | 1:83:A:ARG:HB3  | 1:84:A:TYR:H    | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,4151) | 1:18:A:GLN:HG2  | 1:18:A:GLN:H    | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,294)  | 1:83:A:ARG:H    | 1:83:A:ARG:HB2  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,917)  | 1:15:A:MET:HG3  | 1:15:A:MET:H    | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,982)  | 1:20:A:LYS:HA   | 1:20:A:LYS:HG2  | 2                   | 0.11     | 0.01                | 0.11       |
| (1,1911) | 1:114:A:ARG:HB2 | 1:111:A:GLU:HA  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,2301) | 1:92:A:ALA:HA   | 1:93:A:THR:H    | 2                   | 0.11     | 0.01                | 0.11       |
| (1,2744) | 1:13:A:ASP:HB2  | 1:16:A:GLU:H    | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,3335) | 1:71:A:LEU:HA   | 1:71:A:LEU:HD23 | 2                   | 0.11     | 0.01                | 0.11       |
| (1,3335) | 1:71:A:LEU:HA   | 1:71:A:LEU:HD22 | 2                   | 0.11     | 0.01                | 0.11       |
| (1,3934) | 1:65:A:ASN:H    | 1:64:A:MET:HG2  | 2                   | 0.11     | 0.01                | 0.11       |
| (1,4281) | 1:118:A:GLU:HA  | 1:119:A:GLU:H   | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,734)  | 1:116:A:GLN:HA  | 1:117:A:LEU:H   | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1549) | 1:107:A:GLU:H   | 1:107:A:GLU:HB3 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,2501) | 1:42:A:GLU:HA   | 1:42:A:GLU:HB3  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1716) | 1:84:A:TYR:H    | 1:83:A:ARG:HB2  | 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) |
|----------|------------------|-----------------|----------|---------------|
| (1,4095) | 1:116:A:GLN:HE22 | 1:85:A:LEU:HD13 | 4        | 2.33          |
| (1,4095) | 1:116:A:GLN:HE22 | 1:85:A:LEU:HD13 | 9        | 2.25          |
| (1,4095) | 1:116:A:GLN:HE22 | 1:85:A:LEU:HD13 | 2        | 2.23          |
| (1,4095) | 1:116:A:GLN:HE22 | 1:85:A:LEU:HD13 | 1        | 2.21          |
| (1,4095) | 1:116:A:GLN:HE22 | 1:85:A:LEU:HD11 | 15       | 2.21          |
| (1,4095) | 1:116:A:GLN:HE22 | 1:85:A:LEU:HD11 | 7        | 2.2           |
| (1,4095) | 1:116:A:GLN:HE22 | 1:85:A:LEU:HD13 | 12       | 2.2           |
| (1,4095) | 1:116:A:GLN:HE22 | 1:85:A:LEU:HD13 | 11       | 2.18          |
| (1,4095) | 1:116:A:GLN:HE22 | 1:85:A:LEU:HD12 | 17       | 2.16          |
| (1,4095) | 1:116:A:GLN:HE22 | 1:85:A:LEU:HD11 | 3        | 2.15          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,4095) | 1:116:A:GLN:HE22 | 1:85:A:LEU:HD12 | 5        | 2.14          |
| (1,4095) | 1:116:A:GLN:HE22 | 1:85:A:LEU:HD12 | 13       | 2.14          |
| (1,4095) | 1:116:A:GLN:HE22 | 1:85:A:LEU:HD11 | 14       | 2.13          |
| (1,4095) | 1:116:A:GLN:HE22 | 1:85:A:LEU:HD11 | 6        | 2.12          |
| (1,4095) | 1:116:A:GLN:HE22 | 1:85:A:LEU:HD12 | 8        | 2.07          |
| (1,4095) | 1:116:A:GLN:HE22 | 1:85:A:LEU:HD13 | 10       | 2.07          |
| (1,4095) | 1:116:A:GLN:HE22 | 1:85:A:LEU:HD11 | 16       | 2.06          |
| (3,17)   | 1:60:A:VAL:HG12  | 1:62:A:GLY:H    | 1        | 1.82          |
| (3,17)   | 1:60:A:VAL:HG11  | 1:62:A:GLY:H    | 8        | 1.69          |
| (3,17)   | 1:60:A:VAL:HG11  | 1:62:A:GLY:H    | 12       | 1.69          |
| (3,17)   | 1:60:A:VAL:HG11  | 1:62:A:GLY:H    | 13       | 1.66          |
| (3,17)   | 1:60:A:VAL:HG13  | 1:62:A:GLY:H    | 2        | 1.65          |
| (3,128)  | 1:97:A:LEU:HD23  | 1:75:A:LEU:HD11 | 7        | 1.64          |
| (3,17)   | 1:60:A:VAL:HG13  | 1:62:A:GLY:H    | 15       | 1.64          |
| (3,128)  | 1:57:A:VAL:HG11  | 1:75:A:LEU:HD11 | 17       | 1.62          |
| (3,17)   | 1:60:A:VAL:HG13  | 1:62:A:GLY:H    | 16       | 1.62          |
| (3,128)  | 1:97:A:LEU:HD23  | 1:75:A:LEU:HD11 | 10       | 1.61          |
| (3,17)   | 1:60:A:VAL:HG11  | 1:62:A:GLY:H    | 4        | 1.61          |
| (3,17)   | 1:60:A:VAL:HG13  | 1:62:A:GLY:H    | 6        | 1.61          |
| (3,17)   | 1:60:A:VAL:HG12  | 1:62:A:GLY:H    | 10       | 1.61          |
| (3,17)   | 1:60:A:VAL:HG11  | 1:62:A:GLY:H    | 17       | 1.61          |
| (3,128)  | 1:97:A:LEU:HD21  | 1:75:A:LEU:HD13 | 8        | 1.6           |
| (3,128)  | 1:97:A:LEU:HD23  | 1:75:A:LEU:HD12 | 14       | 1.6           |
| (3,120)  | 1:48:A:LEU:HD21  | 1:49:A:LYS:HB2  | 4        | 1.6           |
| (1,1386) | 1:56:A:LEU:HB3   | 1:53:A:PHE:HD2  | 12       | 1.6           |
| (1,1386) | 1:56:A:LEU:HB3   | 1:53:A:PHE:HD2  | 17       | 1.6           |
| (3,120)  | 1:50:A:ILE:HG21  | 1:49:A:LYS:HB2  | 12       | 1.59          |
| (3,17)   | 1:60:A:VAL:HG13  | 1:62:A:GLY:H    | 14       | 1.59          |
| (1,1386) | 1:56:A:LEU:HB3   | 1:53:A:PHE:HD2  | 10       | 1.59          |
| (1,1386) | 1:56:A:LEU:HB3   | 1:53:A:PHE:HD2  | 11       | 1.59          |
| (3,128)  | 1:57:A:VAL:HG11  | 1:75:A:LEU:HD13 | 2        | 1.58          |
| (3,128)  | 1:97:A:LEU:HD23  | 1:75:A:LEU:HD11 | 5        | 1.58          |
| (3,17)   | 1:60:A:VAL:HG11  | 1:62:A:GLY:H    | 9        | 1.58          |
| (1,1386) | 1:56:A:LEU:HB3   | 1:53:A:PHE:HD1  | 1        | 1.58          |
| (1,1386) | 1:56:A:LEU:HB3   | 1:53:A:PHE:HD1  | 8        | 1.58          |
| (1,1386) | 1:56:A:LEU:HB3   | 1:53:A:PHE:HD2  | 13       | 1.58          |
| (1,1386) | 1:56:A:LEU:HB3   | 1:53:A:PHE:HD1  | 15       | 1.58          |
| (3,128)  | 1:97:A:LEU:HD21  | 1:75:A:LEU:HD13 | 4        | 1.57          |
| (3,128)  | 1:97:A:LEU:HD22  | 1:75:A:LEU:HD13 | 16       | 1.57          |
| (3,120)  | 1:50:A:ILE:HG23  | 1:49:A:LYS:HB2  | 8        | 1.57          |
| (1,1386) | 1:56:A:LEU:HB3   | 1:53:A:PHE:HD1  | 16       | 1.57          |
| (1,2917) | 1:56:A:LEU:HB3   | 1:53:A:PHE:HD2  | 12       | 1.56          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2917) | 1:56:A:LEU:HB3  | 1:53:A:PHE:HD2  | 17       | 1.56          |
| (1,1386) | 1:56:A:LEU:HB3  | 1:53:A:PHE:HD2  | 3        | 1.56          |
| (1,1386) | 1:56:A:LEU:HB3  | 1:53:A:PHE:HD2  | 4        | 1.56          |
| (1,1386) | 1:56:A:LEU:HB3  | 1:53:A:PHE:HD2  | 7        | 1.56          |
| (3,120)  | 1:50:A:ILE:HG21 | 1:49:A:LYS:HB2  | 7        | 1.55          |
| (1,2917) | 1:56:A:LEU:HB3  | 1:53:A:PHE:HD2  | 10       | 1.55          |
| (1,1386) | 1:56:A:LEU:HB3  | 1:53:A:PHE:HD2  | 6        | 1.55          |
| (1,1386) | 1:56:A:LEU:HB3  | 1:53:A:PHE:HD2  | 9        | 1.55          |
| (3,128)  | 1:97:A:LEU:HD23 | 1:75:A:LEU:HD12 | 6        | 1.54          |
| (3,120)  | 1:49:A:LYS:HB2  | 1:52:A:ILE:HD13 | 2        | 1.54          |
| (1,2917) | 1:56:A:LEU:HB3  | 1:53:A:PHE:HD1  | 1        | 1.54          |
| (1,2917) | 1:56:A:LEU:HB3  | 1:53:A:PHE:HD1  | 8        | 1.54          |
| (1,2917) | 1:56:A:LEU:HB3  | 1:53:A:PHE:HD2  | 11       | 1.54          |
| (1,2917) | 1:56:A:LEU:HB3  | 1:53:A:PHE:HD2  | 13       | 1.54          |
| (1,1386) | 1:56:A:LEU:HB3  | 1:53:A:PHE:HD1  | 2        | 1.54          |
| (1,1386) | 1:56:A:LEU:HB3  | 1:53:A:PHE:HD1  | 14       | 1.54          |
| (3,128)  | 1:97:A:LEU:HD21 | 1:75:A:LEU:HD13 | 13       | 1.53          |
| (1,2917) | 1:56:A:LEU:HB3  | 1:53:A:PHE:HD1  | 15       | 1.53          |
| (1,1386) | 1:56:A:LEU:HB3  | 1:53:A:PHE:HD1  | 5        | 1.53          |
| (3,128)  | 1:97:A:LEU:HD23 | 1:75:A:LEU:HD13 | 15       | 1.52          |
| (1,2917) | 1:56:A:LEU:HB3  | 1:53:A:PHE:HD2  | 3        | 1.52          |
| (1,2917) | 1:56:A:LEU:HB3  | 1:53:A:PHE:HD2  | 4        | 1.52          |
| (1,2917) | 1:56:A:LEU:HB3  | 1:53:A:PHE:HD2  | 7        | 1.52          |
| (1,2917) | 1:56:A:LEU:HB3  | 1:53:A:PHE:HD1  | 16       | 1.52          |
| (3,128)  | 1:97:A:LEU:HD22 | 1:75:A:LEU:HD12 | 1        | 1.51          |
| (3,128)  | 1:97:A:LEU:HD23 | 1:75:A:LEU:HD12 | 3        | 1.51          |
| (3,128)  | 1:97:A:LEU:HD23 | 1:75:A:LEU:HD11 | 12       | 1.51          |
| (3,120)  | 1:50:A:ILE:HG23 | 1:49:A:LYS:HB2  | 13       | 1.51          |
| (3,39)   | 1:31:A:LEU:HD21 | 1:32:A:ALA:HB3  | 12       | 1.51          |
| (3,17)   | 1:60:A:VAL:HG12 | 1:62:A:GLY:H    | 7        | 1.51          |
| (1,2917) | 1:56:A:LEU:HB3  | 1:53:A:PHE:HD2  | 6        | 1.51          |
| (1,2917) | 1:56:A:LEU:HB3  | 1:53:A:PHE:HD2  | 9        | 1.51          |
| (1,2917) | 1:56:A:LEU:HB3  | 1:53:A:PHE:HD1  | 2        | 1.5           |
| (1,2917) | 1:56:A:LEU:HB3  | 1:53:A:PHE:HD1  | 14       | 1.5           |
| (3,128)  | 1:97:A:LEU:HD21 | 1:75:A:LEU:HD12 | 9        | 1.49          |
| (3,120)  | 1:49:A:LYS:HB2  | 1:52:A:ILE:HD12 | 10       | 1.49          |
| (1,2917) | 1:56:A:LEU:HB3  | 1:53:A:PHE:HD1  | 5        | 1.49          |
| (3,39)   | 1:31:A:LEU:HD22 | 1:32:A:ALA:HB3  | 10       | 1.48          |
| (3,39)   | 1:31:A:LEU:HD22 | 1:32:A:ALA:HB3  | 14       | 1.47          |
| (3,39)   | 1:31:A:LEU:HD22 | 1:32:A:ALA:HB2  | 17       | 1.47          |
| (3,120)  | 1:50:A:ILE:HG23 | 1:49:A:LYS:HB2  | 16       | 1.46          |
| (3,39)   | 1:31:A:LEU:HD22 | 1:32:A:ALA:HB2  | 16       | 1.46          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (3,39)   | 1:31:A:LEU:HD23  | 1:32:A:ALA:HB1  | 2        | 1.45          |
| (3,39)   | 1:31:A:LEU:HD22  | 1:32:A:ALA:HB1  | 6        | 1.45          |
| (3,39)   | 1:31:A:LEU:HD23  | 1:32:A:ALA:HB3  | 15       | 1.44          |
| (3,128)  | 1:97:A:LEU:HD21  | 1:75:A:LEU:HD11 | 11       | 1.42          |
| (3,95)   | 1:75:A:LEU:HD13  | 1:78:A:TYR:H    | 5        | 1.42          |
| (3,95)   | 1:75:A:LEU:HD13  | 1:78:A:TYR:H    | 7        | 1.42          |
| (3,95)   | 1:75:A:LEU:HD13  | 1:78:A:TYR:H    | 11       | 1.42          |
| (3,39)   | 1:31:A:LEU:HD21  | 1:32:A:ALA:HB1  | 7        | 1.42          |
| (3,39)   | 1:31:A:LEU:HD22  | 1:32:A:ALA:HB2  | 13       | 1.42          |
| (1,836)  | 1:64:A:MET:HE1   | 1:60:A:VAL:HG13 | 11       | 1.42          |
| (3,39)   | 1:31:A:LEU:HD23  | 1:32:A:ALA:HB1  | 3        | 1.41          |
| (3,39)   | 1:31:A:LEU:HD23  | 1:32:A:ALA:HB2  | 9        | 1.41          |
| (3,120)  | 1:49:A:LYS:HB2   | 1:52:A:ILE:HD11 | 3        | 1.4           |
| (3,95)   | 1:75:A:LEU:HD11  | 1:78:A:TYR:H    | 1        | 1.4           |
| (3,95)   | 1:75:A:LEU:HD11  | 1:78:A:TYR:H    | 3        | 1.4           |
| (3,95)   | 1:75:A:LEU:HD11  | 1:78:A:TYR:H    | 14       | 1.4           |
| (3,39)   | 1:31:A:LEU:HD21  | 1:32:A:ALA:HB3  | 1        | 1.39          |
| (3,39)   | 1:31:A:LEU:HD23  | 1:32:A:ALA:HB2  | 8        | 1.39          |
| (3,39)   | 1:31:A:LEU:HD23  | 1:32:A:ALA:HB2  | 11       | 1.39          |
| (3,120)  | 1:49:A:LYS:HB2   | 1:52:A:ILE:HD11 | 9        | 1.38          |
| (3,39)   | 1:31:A:LEU:HD22  | 1:32:A:ALA:HB1  | 5        | 1.38          |
| (1,4121) | 1:116:A:GLN:HE21 | 1:116:A:GLN:HA  | 2        | 1.38          |
| (3,39)   | 1:31:A:LEU:HD22  | 1:32:A:ALA:HB2  | 4        | 1.37          |
| (1,4121) | 1:116:A:GLN:HE21 | 1:116:A:GLN:HA  | 11       | 1.36          |
| (1,2421) | 1:64:A:MET:HE1   | 1:60:A:VAL:HG13 | 11       | 1.36          |
| (3,120)  | 1:49:A:LYS:HB2   | 1:52:A:ILE:HD11 | 11       | 1.34          |
| (3,104)  | 1:66:A:LEU:HD11  | 1:70:A:GLN:H    | 7        | 1.34          |
| (1,4121) | 1:116:A:GLN:HE21 | 1:116:A:GLN:HA  | 12       | 1.34          |
| (3,95)   | 1:75:A:LEU:HD13  | 1:78:A:TYR:H    | 10       | 1.33          |
| (1,4121) | 1:116:A:GLN:HE21 | 1:116:A:GLN:HA  | 3        | 1.33          |
| (1,558)  | 1:116:A:GLN:HE21 | 1:116:A:GLN:HA  | 2        | 1.33          |
| (3,120)  | 1:49:A:LYS:HB2   | 1:52:A:ILE:HD11 | 1        | 1.32          |
| (3,120)  | 1:50:A:ILE:HG23  | 1:49:A:LYS:HB2  | 17       | 1.32          |
| (3,104)  | 1:66:A:LEU:HD12  | 1:70:A:GLN:H    | 10       | 1.32          |
| (1,4121) | 1:116:A:GLN:HE21 | 1:116:A:GLN:HA  | 7        | 1.32          |
| (3,95)   | 1:75:A:LEU:HD12  | 1:78:A:TYR:H    | 13       | 1.31          |
| (1,4121) | 1:116:A:GLN:HE21 | 1:116:A:GLN:HA  | 15       | 1.31          |
| (1,4121) | 1:116:A:GLN:HE21 | 1:116:A:GLN:HA  | 17       | 1.31          |
| (1,558)  | 1:116:A:GLN:HE21 | 1:116:A:GLN:HA  | 11       | 1.31          |
| (3,120)  | 1:50:A:ILE:HG21  | 1:49:A:LYS:HB2  | 15       | 1.3           |
| (3,104)  | 1:66:A:LEU:HD12  | 1:57:A:VAL:H    | 3        | 1.3           |
| (3,104)  | 1:66:A:LEU:HD13  | 1:70:A:GLN:H    | 14       | 1.3           |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,4121) | 1:116:A:GLN:HE21 | 1:116:A:GLN:HA  | 9        | 1.3           |
| (1,558)  | 1:116:A:GLN:HE21 | 1:116:A:GLN:HA  | 12       | 1.3           |
| (1,558)  | 1:116:A:GLN:HE21 | 1:116:A:GLN:HA  | 3        | 1.29          |
| (1,4121) | 1:116:A:GLN:HE21 | 1:116:A:GLN:HA  | 13       | 1.28          |
| (1,836)  | 1:64:A:MET:HE1   | 1:60:A:VAL:HG13 | 7        | 1.28          |
| (1,558)  | 1:116:A:GLN:HE21 | 1:116:A:GLN:HA  | 7        | 1.27          |
| (1,558)  | 1:116:A:GLN:HE21 | 1:116:A:GLN:HA  | 15       | 1.27          |
| (1,558)  | 1:116:A:GLN:HE21 | 1:116:A:GLN:HA  | 17       | 1.27          |
| (3,104)  | 1:66:A:LEU:HD12  | 1:70:A:GLN:H    | 5        | 1.26          |
| (3,104)  | 1:66:A:LEU:HD13  | 1:70:A:GLN:H    | 11       | 1.26          |
| (1,4121) | 1:116:A:GLN:HE21 | 1:116:A:GLN:HA  | 1        | 1.26          |
| (1,836)  | 1:64:A:MET:HE2   | 1:60:A:VAL:HG11 | 16       | 1.26          |
| (1,558)  | 1:116:A:GLN:HE21 | 1:116:A:GLN:HA  | 9        | 1.26          |
| (3,117)  | 1:48:A:LEU:HD23  | 1:39:A:PHE:HD2  | 8        | 1.25          |
| (3,104)  | 1:66:A:LEU:HD13  | 1:70:A:GLN:H    | 16       | 1.25          |
| (3,104)  | 1:66:A:LEU:HD13  | 1:70:A:GLN:H    | 17       | 1.25          |
| (1,4121) | 1:116:A:GLN:HE21 | 1:116:A:GLN:HA  | 8        | 1.25          |
| (1,1758) | 1:79:A:THR:HG22  | 1:48:A:LEU:HD11 | 1        | 1.25          |
| (3,104)  | 1:66:A:LEU:HD12  | 1:70:A:GLN:H    | 4        | 1.24          |
| (1,3486) | 1:97:A:LEU:HD13  | 1:31:A:LEU:HD13 | 10       | 1.24          |
| (1,3486) | 1:97:A:LEU:HD12  | 1:31:A:LEU:HD12 | 12       | 1.24          |
| (1,3486) | 1:97:A:LEU:HD11  | 1:31:A:LEU:HD11 | 17       | 1.24          |
| (3,104)  | 1:66:A:LEU:HD12  | 1:70:A:GLN:H    | 2        | 1.23          |
| (3,104)  | 1:66:A:LEU:HD13  | 1:70:A:GLN:H    | 13       | 1.23          |
| (3,5)    | 1:28:A:ILE:HD13  | 1:25:A:LYS:HA   | 8        | 1.23          |
| (1,4121) | 1:116:A:GLN:HE21 | 1:116:A:GLN:HA  | 16       | 1.23          |
| (1,558)  | 1:116:A:GLN:HE21 | 1:116:A:GLN:HA  | 13       | 1.23          |
| (3,95)   | 1:75:A:LEU:HD11  | 1:78:A:TYR:H    | 6        | 1.22          |
| (3,52)   | 1:99:A:GLY:HA3   | 1:95:A:VAL:HG21 | 6        | 1.22          |
| (1,4121) | 1:116:A:GLN:HE21 | 1:116:A:GLN:HA  | 4        | 1.22          |
| (1,4084) | 1:20:A:LYS:HB3   | 1:22:A:ASN:HD22 | 2        | 1.22          |
| (1,3486) | 1:97:A:LEU:HD11  | 1:31:A:LEU:HD11 | 8        | 1.22          |
| (3,127)  | 1:31:A:LEU:HD23  | 1:97:A:LEU:HD22 | 15       | 1.21          |
| (3,107)  | 1:95:A:VAL:HG23  | 1:102:A:CYS:HB3 | 3        | 1.21          |
| (3,107)  | 1:95:A:VAL:HG22  | 1:102:A:CYS:HB3 | 11       | 1.21          |
| (3,104)  | 1:66:A:LEU:HD12  | 1:70:A:GLN:H    | 12       | 1.21          |
| (3,95)   | 1:75:A:LEU:HD12  | 1:78:A:TYR:H    | 16       | 1.21          |
| (3,5)    | 1:28:A:ILE:HD12  | 1:25:A:LYS:HA   | 2        | 1.21          |
| (1,4121) | 1:116:A:GLN:HE21 | 1:116:A:GLN:HA  | 10       | 1.21          |
| (1,4121) | 1:116:A:GLN:HE21 | 1:116:A:GLN:HA  | 14       | 1.21          |
| (1,2421) | 1:64:A:MET:HE1   | 1:60:A:VAL:HG13 | 7        | 1.21          |
| (1,2191) | 1:32:A:ALA:HB3   | 1:39:A:PHE:HE1  | 10       | 1.21          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,558)  | 1:116:A:GLN:HE21 | 1:116:A:GLN:HA  | 1        | 1.21          |
| (3,104)  | 1:66:A:LEU:HD11  | 1:70:A:GLN:H    | 6        | 1.2           |
| (1,4121) | 1:116:A:GLN:HE21 | 1:116:A:GLN:HA  | 5        | 1.2           |
| (1,4121) | 1:116:A:GLN:HE21 | 1:116:A:GLN:HA  | 6        | 1.2           |
| (1,4091) | 1:65:A:ASN:HD22  | 1:20:A:LYS:HA   | 11       | 1.2           |
| (1,3486) | 1:97:A:LEU:HD12  | 1:31:A:LEU:HD13 | 5        | 1.2           |
| (1,3352) | 1:79:A:THR:HG22  | 1:48:A:LEU:HD11 | 1        | 1.2           |
| (1,2421) | 1:64:A:MET:HE2   | 1:60:A:VAL:HG11 | 16       | 1.2           |
| (1,2191) | 1:32:A:ALA:HB2   | 1:39:A:PHE:HE1  | 16       | 1.2           |
| (1,558)  | 1:116:A:GLN:HE21 | 1:116:A:GLN:HA  | 8        | 1.2           |
| (3,127)  | 1:31:A:LEU:HD23  | 1:97:A:LEU:HD23 | 9        | 1.19          |
| (1,558)  | 1:116:A:GLN:HE21 | 1:116:A:GLN:HA  | 16       | 1.19          |
| (3,127)  | 1:31:A:LEU:HD22  | 1:97:A:LEU:HD22 | 5        | 1.18          |
| (3,127)  | 1:31:A:LEU:HD23  | 1:97:A:LEU:HD21 | 8        | 1.18          |
| (3,104)  | 1:66:A:LEU:HD11  | 1:70:A:GLN:H    | 9        | 1.18          |
| (1,3486) | 1:97:A:LEU:HD12  | 1:31:A:LEU:HD12 | 14       | 1.18          |
| (1,2191) | 1:32:A:ALA:HB3   | 1:39:A:PHE:HE2  | 12       | 1.18          |
| (1,2191) | 1:32:A:ALA:HB3   | 1:39:A:PHE:HE1  | 15       | 1.18          |
| (1,558)  | 1:116:A:GLN:HE21 | 1:116:A:GLN:HA  | 4        | 1.18          |
| (3,127)  | 1:31:A:LEU:HD21  | 1:97:A:LEU:HD22 | 7        | 1.17          |
| (3,5)    | 1:28:A:ILE:HD13  | 1:25:A:LYS:HA   | 14       | 1.17          |
| (1,2617) | 1:21:A:LEU:HD21  | 1:30:A:PHE:HD1  | 8        | 1.17          |
| (1,2191) | 1:32:A:ALA:HB1   | 1:39:A:PHE:HE1  | 2        | 1.17          |
| (1,1758) | 1:79:A:THR:HG21  | 1:48:A:LEU:HD13 | 5        | 1.17          |
| (1,558)  | 1:116:A:GLN:HE21 | 1:116:A:GLN:HA  | 10       | 1.17          |
| (1,558)  | 1:116:A:GLN:HE21 | 1:116:A:GLN:HA  | 14       | 1.17          |
| (1,524)  | 1:20:A:LYS:HB3   | 1:22:A:ASN:HD22 | 2        | 1.17          |
| (3,127)  | 1:31:A:LEU:HD22  | 1:97:A:LEU:HD22 | 6        | 1.16          |
| (3,127)  | 1:31:A:LEU:HD22  | 1:97:A:LEU:HD22 | 10       | 1.16          |
| (3,127)  | 1:31:A:LEU:HD21  | 1:97:A:LEU:HD22 | 12       | 1.16          |
| (3,127)  | 1:31:A:LEU:HD22  | 1:97:A:LEU:HD22 | 17       | 1.16          |
| (3,95)   | 1:75:A:LEU:HD11  | 1:78:A:TYR:H    | 9        | 1.16          |
| (3,52)   | 1:99:A:GLY:HA3   | 1:95:A:VAL:HG21 | 17       | 1.16          |
| (1,4080) | 1:54:A:GLN:HE22  | 1:57:A:VAL:HG22 | 3        | 1.16          |
| (1,3486) | 1:97:A:LEU:HD12  | 1:31:A:LEU:HD13 | 15       | 1.16          |
| (1,3486) | 1:97:A:LEU:HD12  | 1:31:A:LEU:HD11 | 16       | 1.16          |
| (1,2191) | 1:32:A:ALA:HB1   | 1:39:A:PHE:HE1  | 7        | 1.16          |
| (1,558)  | 1:116:A:GLN:HE21 | 1:116:A:GLN:HA  | 6        | 1.16          |
| (3,127)  | 1:31:A:LEU:HD23  | 1:97:A:LEU:HD23 | 3        | 1.15          |
| (3,127)  | 1:31:A:LEU:HD22  | 1:97:A:LEU:HD23 | 4        | 1.15          |
| (3,104)  | 1:66:A:LEU:HD13  | 1:70:A:GLN:H    | 15       | 1.15          |
| (3,82)   | 1:57:A:VAL:HG13  | 1:71:A:LEU:HD23 | 12       | 1.15          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,4120) | 1:116:A:GLN:HE21 | 1:119:A:GLU:HB2  | 12       | 1.15          |
| (1,4080) | 1:54:A:GLN:HE22  | 1:57:A:VAL:HG22  | 1        | 1.15          |
| (1,4080) | 1:54:A:GLN:HE22  | 1:57:A:VAL:HG21  | 2        | 1.15          |
| (1,3486) | 1:97:A:LEU:HD12  | 1:31:A:LEU:HD13  | 2        | 1.15          |
| (1,2191) | 1:32:A:ALA:HB3   | 1:39:A:PHE:HE2   | 1        | 1.15          |
| (1,1758) | 1:79:A:THR:HG23  | 1:48:A:LEU:HD12  | 14       | 1.15          |
| (1,558)  | 1:116:A:GLN:HE21 | 1:116:A:GLN:HA   | 5        | 1.15          |
| (1,4080) | 1:54:A:GLN:HE22  | 1:57:A:VAL:HG23  | 4        | 1.14          |
| (1,4080) | 1:54:A:GLN:HE22  | 1:57:A:VAL:HG23  | 11       | 1.14          |
| (1,3486) | 1:97:A:LEU:HD13  | 1:31:A:LEU:HD12  | 6        | 1.14          |
| (1,3486) | 1:97:A:LEU:HD12  | 1:31:A:LEU:HD12  | 13       | 1.14          |
| (1,1758) | 1:79:A:THR:HG21  | 1:48:A:LEU:HD13  | 3        | 1.14          |
| (1,836)  | 1:64:A:MET:HE2   | 1:60:A:VAL:HG12  | 9        | 1.14          |
| (3,127)  | 1:31:A:LEU:HD21  | 1:97:A:LEU:HD21  | 1        | 1.13          |
| (3,52)   | 1:99:A:GLY:HA3   | 1:95:A:VAL:HG23  | 8        | 1.13          |
| (3,52)   | 1:99:A:GLY:HA3   | 1:95:A:VAL:HG23  | 12       | 1.13          |
| (1,4091) | 1:65:A:ASN:HD22  | 1:20:A:LYS:HA    | 5        | 1.13          |
| (1,4080) | 1:54:A:GLN:HE22  | 1:57:A:VAL:HG23  | 9        | 1.13          |
| (1,3486) | 1:97:A:LEU:HD12  | 1:31:A:LEU:HD13  | 1        | 1.13          |
| (1,3486) | 1:97:A:LEU:HD12  | 1:31:A:LEU:HD12  | 4        | 1.13          |
| (1,3486) | 1:97:A:LEU:HD12  | 1:31:A:LEU:HD12  | 7        | 1.13          |
| (1,2191) | 1:32:A:ALA:HB1   | 1:39:A:PHE:HE1   | 6        | 1.13          |
| (1,2191) | 1:32:A:ALA:HB2   | 1:39:A:PHE:HE1   | 11       | 1.13          |
| (1,2191) | 1:32:A:ALA:HB2   | 1:39:A:PHE:HE1   | 13       | 1.13          |
| (3,104)  | 1:66:A:LEU:HD11  | 1:70:A:GLN:H     | 8        | 1.12          |
| (3,52)   | 1:99:A:GLY:HA3   | 1:95:A:VAL:HG23  | 4        | 1.12          |
| (3,20)   | 1:93:A:THR:HG23  | 1:110:A:VAL:HG13 | 7        | 1.12          |
| (3,5)    | 1:28:A:ILE:HD11  | 1:25:A:LYS:HA    | 10       | 1.12          |
| (3,5)    | 1:28:A:ILE:HD13  | 1:25:A:LYS:HA    | 17       | 1.12          |
| (1,3486) | 1:97:A:LEU:HD13  | 1:31:A:LEU:HD13  | 11       | 1.12          |
| (1,3352) | 1:79:A:THR:HG21  | 1:48:A:LEU:HD13  | 5        | 1.12          |
| (1,2191) | 1:32:A:ALA:HB1   | 1:39:A:PHE:HE1   | 5        | 1.12          |
| (1,2191) | 1:32:A:ALA:HB2   | 1:39:A:PHE:HE2   | 9        | 1.12          |
| (1,1503) | 1:52:A:ILE:HG12  | 1:54:A:GLN:HE21  | 10       | 1.12          |
| (1,836)  | 1:64:A:MET:HE3   | 1:60:A:VAL:HG12  | 4        | 1.12          |
| (1,522)  | 1:54:A:GLN:HE22  | 1:57:A:VAL:HG22  | 3        | 1.12          |
| (3,127)  | 1:31:A:LEU:HD23  | 1:97:A:LEU:HD22  | 2        | 1.11          |
| (3,127)  | 1:31:A:LEU:HD23  | 1:97:A:LEU:HD21  | 11       | 1.11          |
| (3,127)  | 1:31:A:LEU:HD22  | 1:97:A:LEU:HD21  | 16       | 1.11          |
| (3,107)  | 1:95:A:VAL:HG22  | 1:102:A:CYS:HB3  | 17       | 1.11          |
| (3,104)  | 1:66:A:LEU:HD11  | 1:70:A:GLN:H     | 1        | 1.11          |
| (3,95)   | 1:75:A:LEU:HD13  | 1:78:A:TYR:H     | 12       | 1.11          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3486) | 1:97:A:LEU:HD12 | 1:31:A:LEU:HD12  | 3        | 1.11          |
| (1,2191) | 1:32:A:ALA:HB2  | 1:39:A:PHE:HE1   | 4        | 1.11          |
| (1,2191) | 1:32:A:ALA:HB3  | 1:39:A:PHE:HE2   | 14       | 1.11          |
| (1,522)  | 1:54:A:GLN:HE22 | 1:57:A:VAL:HG22  | 1        | 1.11          |
| (1,522)  | 1:54:A:GLN:HE22 | 1:57:A:VAL:HG21  | 2        | 1.11          |
| (3,127)  | 1:31:A:LEU:HD22 | 1:97:A:LEU:HD22  | 14       | 1.1           |
| (3,82)   | 1:57:A:VAL:HG13 | 1:71:A:LEU:HD22  | 10       | 1.1           |
| (3,82)   | 1:57:A:VAL:HG11 | 1:71:A:LEU:HD23  | 17       | 1.1           |
| (3,52)   | 1:99:A:GLY:HA3  | 1:95:A:VAL:HG22  | 10       | 1.1           |
| (1,4084) | 1:20:A:LYS:HB3  | 1:22:A:ASN:HD22  | 12       | 1.1           |
| (1,3486) | 1:97:A:LEU:HD11 | 1:31:A:LEU:HD13  | 9        | 1.1           |
| (1,3352) | 1:79:A:THR:HG23 | 1:48:A:LEU:HD12  | 14       | 1.1           |
| (1,522)  | 1:54:A:GLN:HE22 | 1:57:A:VAL:HG23  | 4        | 1.1           |
| (1,522)  | 1:54:A:GLN:HE22 | 1:57:A:VAL:HG23  | 11       | 1.1           |
| (3,127)  | 1:31:A:LEU:HD22 | 1:97:A:LEU:HD23  | 13       | 1.09          |
| (3,95)   | 1:75:A:LEU:HD12 | 1:78:A:TYR:H     | 15       | 1.09          |
| (3,82)   | 1:57:A:VAL:HG12 | 1:71:A:LEU:HD21  | 6        | 1.09          |
| (3,82)   | 1:57:A:VAL:HG11 | 1:71:A:LEU:HD22  | 14       | 1.09          |
| (3,17)   | 1:60:A:VAL:HG13 | 1:62:A:GLY:H     | 5        | 1.09          |
| (3,5)    | 1:28:A:ILE:HD12 | 1:25:A:LYS:HA    | 1        | 1.09          |
| (1,1534) | 1:56:A:LEU:HB2  | 1:35:A:PHE:HE1   | 11       | 1.09          |
| (1,522)  | 1:54:A:GLN:HE22 | 1:57:A:VAL:HG23  | 9        | 1.09          |
| (3,107)  | 1:95:A:VAL:HG21 | 1:102:A:CYS:HB3  | 1        | 1.08          |
| (3,82)   | 1:57:A:VAL:HG13 | 1:71:A:LEU:HD21  | 8        | 1.08          |
| (1,3412) | 1:82:A:TRP:HZ3  | 1:117:A:LEU:HD11 | 2        | 1.08          |
| (1,3352) | 1:79:A:THR:HG21 | 1:48:A:LEU:HD13  | 3        | 1.08          |
| (1,2191) | 1:32:A:ALA:HB2  | 1:39:A:PHE:HE1   | 8        | 1.08          |
| (1,1758) | 1:79:A:THR:HG22 | 1:48:A:LEU:HD12  | 7        | 1.08          |
| (3,82)   | 1:57:A:VAL:HG11 | 1:71:A:LEU:HD22  | 7        | 1.07          |
| (3,52)   | 1:99:A:GLY:HA3  | 1:95:A:VAL:HG22  | 13       | 1.07          |
| (3,20)   | 1:93:A:THR:HG23 | 1:110:A:VAL:HG12 | 13       | 1.07          |
| (1,3046) | 1:52:A:ILE:HG12 | 1:54:A:GLN:HE21  | 10       | 1.07          |
| (1,2421) | 1:64:A:MET:HE2  | 1:60:A:VAL:HG12  | 9        | 1.07          |
| (1,2191) | 1:32:A:ALA:HB1  | 1:39:A:PHE:HE1   | 3        | 1.07          |
| (1,1758) | 1:79:A:THR:HG21 | 1:48:A:LEU:HD13  | 10       | 1.07          |
| (3,116)  | 1:95:A:VAL:H    | 1:48:A:LEU:HD11  | 12       | 1.06          |
| (3,82)   | 1:57:A:VAL:HG12 | 1:71:A:LEU:HD21  | 1        | 1.06          |
| (3,82)   | 1:57:A:VAL:HG12 | 1:71:A:LEU:HD23  | 2        | 1.06          |
| (3,82)   | 1:57:A:VAL:HG13 | 1:71:A:LEU:HD23  | 11       | 1.06          |
| (3,82)   | 1:57:A:VAL:HG12 | 1:71:A:LEU:HD21  | 16       | 1.06          |
| (3,17)   | 1:60:A:VAL:HG12 | 1:62:A:GLY:H     | 3        | 1.06          |
| (3,17)   | 1:60:A:VAL:HG12 | 1:62:A:GLY:H     | 11       | 1.06          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (3,5)    | 1:28:A:ILE:HD12  | 1:25:A:LYS:HA    | 7        | 1.06          |
| (1,4084) | 1:20:A:LYS:HB3   | 1:22:A:ASN:HD22  | 9        | 1.06          |
| (1,2421) | 1:64:A:MET:HE3   | 1:60:A:VAL:HG12  | 4        | 1.06          |
| (1,1758) | 1:79:A:THR:HG23  | 1:48:A:LEU:HD12  | 13       | 1.06          |
| (3,82)   | 1:57:A:VAL:HG12  | 1:71:A:LEU:HD21  | 4        | 1.05          |
| (3,82)   | 1:57:A:VAL:HG13  | 1:71:A:LEU:HD22  | 5        | 1.05          |
| (3,20)   | 1:93:A:THR:HG23  | 1:110:A:VAL:HG11 | 2        | 1.05          |
| (3,20)   | 1:93:A:THR:HG22  | 1:110:A:VAL:HG13 | 5        | 1.05          |
| (3,5)    | 1:28:A:ILE:HD12  | 1:25:A:LYS:HA    | 3        | 1.05          |
| (1,3412) | 1:82:A:TRP:HZ3   | 1:117:A:LEU:HD12 | 7        | 1.05          |
| (1,2617) | 1:21:A:LEU:HD21  | 1:30:A:PHE:HD2   | 2        | 1.05          |
| (1,1758) | 1:79:A:THR:HG23  | 1:48:A:LEU:HD12  | 8        | 1.05          |
| (1,1758) | 1:79:A:THR:HG23  | 1:48:A:LEU:HD13  | 11       | 1.05          |
| (1,1503) | 1:52:A:ILE:HG12  | 1:54:A:GLN:HE21  | 12       | 1.05          |
| (1,524)  | 1:20:A:LYS:HB3   | 1:22:A:ASN:HD22  | 12       | 1.05          |
| (3,116)  | 1:95:A:VAL:H     | 1:48:A:LEU:HD11  | 16       | 1.04          |
| (3,82)   | 1:57:A:VAL:HG12  | 1:71:A:LEU:HD21  | 9        | 1.04          |
| (3,5)    | 1:28:A:ILE:HD11  | 1:25:A:LYS:HA    | 15       | 1.04          |
| (1,4120) | 1:116:A:GLN:HE21 | 1:119:A:GLU:HB2  | 9        | 1.04          |
| (1,4026) | 1:32:A:ALA:H     | 1:29:A:ALA:HB1   | 1        | 1.04          |
| (1,1503) | 1:52:A:ILE:HG12  | 1:54:A:GLN:HE21  | 8        | 1.04          |
| (3,117)  | 1:48:A:LEU:HD22  | 1:39:A:PHE:HD2   | 10       | 1.03          |
| (3,82)   | 1:57:A:VAL:HG12  | 1:71:A:LEU:HD21  | 13       | 1.03          |
| (3,52)   | 1:99:A:GLY:HA3   | 1:95:A:VAL:HG21  | 16       | 1.03          |
| (3,30)   | 1:64:A:MET:HE1   | 1:34:A:ARG:HB3   | 1        | 1.03          |
| (3,20)   | 1:93:A:THR:HG21  | 1:110:A:VAL:HG12 | 17       | 1.03          |
| (1,4124) | 1:116:A:GLN:HE21 | 1:120:A:ALA:H    | 7        | 1.03          |
| (1,4026) | 1:32:A:ALA:H     | 1:29:A:ALA:HB1   | 5        | 1.03          |
| (1,3412) | 1:82:A:TRP:HZ3   | 1:117:A:LEU:HD13 | 17       | 1.03          |
| (1,3352) | 1:79:A:THR:HG22  | 1:48:A:LEU:HD12  | 7        | 1.03          |
| (1,3088) | 1:56:A:LEU:HB2   | 1:35:A:PHE:HE1   | 11       | 1.03          |
| (1,2617) | 1:21:A:LEU:HD21  | 1:30:A:PHE:HD2   | 11       | 1.03          |
| (1,1415) | 1:48:A:LEU:HD13  | 1:75:A:LEU:HD12  | 11       | 1.03          |
| (3,134)  | 1:75:A:LEU:HD21  | 1:97:A:LEU:HD23  | 14       | 1.02          |
| (3,117)  | 1:48:A:LEU:HD21  | 1:39:A:PHE:HD2   | 13       | 1.02          |
| (3,116)  | 1:95:A:VAL:H     | 1:48:A:LEU:HD11  | 7        | 1.02          |
| (3,116)  | 1:95:A:VAL:H     | 1:48:A:LEU:HD12  | 15       | 1.02          |
| (3,107)  | 1:95:A:VAL:HG23  | 1:102:A:CYS:HB3  | 15       | 1.02          |
| (3,20)   | 1:93:A:THR:HG23  | 1:110:A:VAL:HG11 | 8        | 1.02          |
| (3,20)   | 1:93:A:THR:HG23  | 1:110:A:VAL:HG12 | 12       | 1.02          |
| (1,4283) | 1:120:A:ALA:H    | 1:85:A:LEU:HD21  | 2        | 1.02          |
| (1,4120) | 1:116:A:GLN:HE21 | 1:119:A:GLU:HB2  | 2        | 1.02          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,4118) | 1:71:A:LEU:H     | 1:70:A:GLN:HE21  | 3        | 1.02          |
| (1,4026) | 1:32:A:ALA:H     | 1:29:A:ALA:HB1   | 6        | 1.02          |
| (1,4026) | 1:32:A:ALA:H     | 1:29:A:ALA:HB2   | 15       | 1.02          |
| (1,3352) | 1:79:A:THR:HG21  | 1:48:A:LEU:HD13  | 10       | 1.02          |
| (1,2617) | 1:21:A:LEU:HD22  | 1:30:A:PHE:HD1   | 14       | 1.02          |
| (1,2157) | 1:99:A:GLY:HA3   | 1:95:A:VAL:HG22  | 15       | 1.02          |
| (1,1415) | 1:48:A:LEU:HD13  | 1:75:A:LEU:HD11  | 17       | 1.02          |
| (3,134)  | 1:75:A:LEU:HD21  | 1:97:A:LEU:HD23  | 5        | 1.01          |
| (3,107)  | 1:95:A:VAL:HG22  | 1:102:A:CYS:HB3  | 9        | 1.01          |
| (3,5)    | 1:28:A:ILE:HD12  | 1:25:A:LYS:HA    | 6        | 1.01          |
| (1,4118) | 1:71:A:LEU:H     | 1:70:A:GLN:HE21  | 12       | 1.01          |
| (1,4026) | 1:32:A:ALA:H     | 1:29:A:ALA:HB1   | 2        | 1.01          |
| (1,4026) | 1:32:A:ALA:H     | 1:29:A:ALA:HB3   | 8        | 1.01          |
| (1,4026) | 1:32:A:ALA:H     | 1:29:A:ALA:HB1   | 13       | 1.01          |
| (1,4026) | 1:32:A:ALA:H     | 1:29:A:ALA:HB1   | 14       | 1.01          |
| (1,3412) | 1:82:A:TRP:HZ3   | 1:117:A:LEU:HD11 | 3        | 1.01          |
| (1,3412) | 1:82:A:TRP:HZ3   | 1:117:A:LEU:HD12 | 12       | 1.01          |
| (1,3352) | 1:79:A:THR:HG23  | 1:48:A:LEU:HD12  | 13       | 1.01          |
| (1,2617) | 1:21:A:LEU:HD22  | 1:30:A:PHE:HD1   | 3        | 1.01          |
| (1,2191) | 1:32:A:ALA:HB2   | 1:39:A:PHE:HE1   | 17       | 1.01          |
| (1,1758) | 1:79:A:THR:HG22  | 1:48:A:LEU:HD12  | 9        | 1.01          |
| (1,836)  | 1:64:A:MET:HE1   | 1:60:A:VAL:HG13  | 1        | 1.01          |
| (1,524)  | 1:20:A:LYS:HB3   | 1:22:A:ASN:HD22  | 9        | 1.01          |
| (3,82)   | 1:57:A:VAL:HG12  | 1:71:A:LEU:HD22  | 3        | 1.0           |
| (3,82)   | 1:57:A:VAL:HG12  | 1:71:A:LEU:HD22  | 15       | 1.0           |
| (1,4026) | 1:32:A:ALA:H     | 1:29:A:ALA:HB1   | 4        | 1.0           |
| (1,4026) | 1:32:A:ALA:H     | 1:29:A:ALA:HB2   | 9        | 1.0           |
| (1,4026) | 1:32:A:ALA:H     | 1:29:A:ALA:HB3   | 11       | 1.0           |
| (1,3352) | 1:79:A:THR:HG23  | 1:48:A:LEU:HD12  | 8        | 1.0           |
| (1,3352) | 1:79:A:THR:HG23  | 1:48:A:LEU:HD13  | 11       | 1.0           |
| (1,3060) | 1:52:A:ILE:HG21  | 1:97:A:LEU:HD23  | 12       | 1.0           |
| (1,2308) | 1:82:A:TRP:HB2   | 1:117:A:LEU:HD13 | 8        | 1.0           |
| (1,836)  | 1:64:A:MET:HE3   | 1:60:A:VAL:HG13  | 10       | 1.0           |
| (3,134)  | 1:75:A:LEU:HD23  | 1:97:A:LEU:HD23  | 7        | 0.99          |
| (3,134)  | 1:75:A:LEU:HD23  | 1:97:A:LEU:HD21  | 13       | 0.99          |
| (3,20)   | 1:93:A:THR:HG21  | 1:110:A:VAL:HG13 | 10       | 0.99          |
| (3,20)   | 1:93:A:THR:HG22  | 1:110:A:VAL:HG11 | 16       | 0.99          |
| (1,4124) | 1:116:A:GLN:HE21 | 1:120:A:ALA:H    | 17       | 0.99          |
| (1,4116) | 1:70:A:GLN:HA    | 1:70:A:GLN:HE21  | 3        | 0.99          |
| (1,4084) | 1:20:A:LYS:HB3   | 1:22:A:ASN:HD22  | 5        | 0.99          |
| (1,4026) | 1:32:A:ALA:H     | 1:29:A:ALA:HB2   | 3        | 0.99          |
| (1,4026) | 1:32:A:ALA:H     | 1:29:A:ALA:HB2   | 7        | 0.99          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,4026) | 1:32:A:ALA:H     | 1:29:A:ALA:HB3   | 12       | 0.99          |
| (1,4026) | 1:32:A:ALA:H     | 1:29:A:ALA:HB1   | 16       | 0.99          |
| (1,4026) | 1:32:A:ALA:H     | 1:29:A:ALA:HB3   | 17       | 0.99          |
| (1,3412) | 1:82:A:TRP:HZ3   | 1:117:A:LEU:HD11 | 9        | 0.99          |
| (1,3412) | 1:82:A:TRP:HZ3   | 1:117:A:LEU:HD13 | 15       | 0.99          |
| (1,3046) | 1:52:A:ILE:HG12  | 1:54:A:GLN:HE21  | 8        | 0.99          |
| (1,3046) | 1:52:A:ILE:HG12  | 1:54:A:GLN:HE21  | 12       | 0.99          |
| (1,2883) | 1:32:A:ALA:HB2   | 1:39:A:PHE:H     | 17       | 0.99          |
| (1,2617) | 1:21:A:LEU:HD22  | 1:30:A:PHE:HD1   | 17       | 0.99          |
| (1,1415) | 1:48:A:LEU:HD12  | 1:75:A:LEU:HD11  | 7        | 0.99          |
| (1,836)  | 1:64:A:MET:HE3   | 1:60:A:VAL:HG12  | 12       | 0.99          |
| (1,836)  | 1:64:A:MET:HE1   | 1:60:A:VAL:HG11  | 14       | 0.99          |
| (3,30)   | 1:64:A:MET:HE3   | 1:34:A:ARG:HB3   | 16       | 0.98          |
| (3,20)   | 1:88:A:VAL:HG13  | 1:93:A:THR:HG23  | 15       | 0.98          |
| (1,4120) | 1:116:A:GLN:HE21 | 1:119:A:GLU:HB2  | 11       | 0.98          |
| (1,4118) | 1:71:A:LEU:H     | 1:70:A:GLN:HE21  | 1        | 0.98          |
| (1,4118) | 1:71:A:LEU:H     | 1:70:A:GLN:HE21  | 2        | 0.98          |
| (1,4026) | 1:32:A:ALA:H     | 1:29:A:ALA:HB2   | 10       | 0.98          |
| (1,2956) | 1:48:A:LEU:HD13  | 1:75:A:LEU:HD12  | 11       | 0.98          |
| (1,2883) | 1:32:A:ALA:HB1   | 1:39:A:PHE:H     | 10       | 0.98          |
| (1,1758) | 1:79:A:THR:HG21  | 1:48:A:LEU:HD12  | 16       | 0.98          |
| (1,1503) | 1:52:A:ILE:HG12  | 1:54:A:GLN:HE21  | 17       | 0.98          |
| (1,1415) | 1:48:A:LEU:HD12  | 1:75:A:LEU:HD12  | 6        | 0.98          |
| (1,836)  | 1:64:A:MET:HE2   | 1:60:A:VAL:HG13  | 3        | 0.98          |
| (1,836)  | 1:64:A:MET:HE2   | 1:60:A:VAL:HG11  | 6        | 0.98          |
| (3,107)  | 1:95:A:VAL:HG23  | 1:102:A:CYS:HB3  | 6        | 0.97          |
| (3,70)   | 1:58:A:ASP:HA    | 1:57:A:VAL:HG13  | 11       | 0.97          |
| (3,51)   | 1:95:A:VAL:HG23  | 1:35:A:PHE:HB2   | 9        | 0.97          |
| (3,20)   | 1:93:A:THR:HG22  | 1:110:A:VAL:HG12 | 4        | 0.97          |
| (3,20)   | 1:88:A:VAL:HG12  | 1:93:A:THR:HG22  | 14       | 0.97          |
| (3,5)    | 1:28:A:ILE:HD13  | 1:25:A:LYS:HA    | 5        | 0.97          |
| (3,5)    | 1:28:A:ILE:HD12  | 1:25:A:LYS:HA    | 11       | 0.97          |
| (1,4118) | 1:71:A:LEU:H     | 1:70:A:GLN:HE21  | 6        | 0.97          |
| (1,4118) | 1:71:A:LEU:H     | 1:70:A:GLN:HE21  | 8        | 0.97          |
| (1,4116) | 1:70:A:GLN:HA    | 1:70:A:GLN:HE21  | 5        | 0.97          |
| (1,2956) | 1:48:A:LEU:HD13  | 1:75:A:LEU:HD11  | 17       | 0.97          |
| (1,2883) | 1:32:A:ALA:HB3   | 1:39:A:PHE:H     | 11       | 0.97          |
| (1,1758) | 1:79:A:THR:HG23  | 1:48:A:LEU:HD13  | 15       | 0.97          |
| (1,836)  | 1:64:A:MET:HE3   | 1:60:A:VAL:HG12  | 17       | 0.97          |
| (1,720)  | 1:120:A:ALA:H    | 1:85:A:LEU:HD21  | 2        | 0.97          |
| (1,561)  | 1:116:A:GLN:HE21 | 1:120:A:ALA:H    | 7        | 0.97          |
| (3,134)  | 1:75:A:LEU:HD23  | 1:97:A:LEU:HD23  | 2        | 0.96          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (3,134)  | 1:75:A:LEU:HD21  | 1:97:A:LEU:HD23  | 3        | 0.96          |
| (3,134)  | 1:75:A:LEU:HD22  | 1:97:A:LEU:HD21  | 8        | 0.96          |
| (3,117)  | 1:48:A:LEU:HD22  | 1:39:A:PHE:HD1   | 7        | 0.96          |
| (3,116)  | 1:95:A:VAL:H     | 1:48:A:LEU:HD12  | 10       | 0.96          |
| (3,116)  | 1:95:A:VAL:H     | 1:48:A:LEU:HD11  | 13       | 0.96          |
| (3,107)  | 1:95:A:VAL:HG21  | 1:102:A:CYS:HB3  | 8        | 0.96          |
| (3,51)   | 1:95:A:VAL:HG23  | 1:49:A:LYS:HA    | 6        | 0.96          |
| (3,5)    | 1:28:A:ILE:HD13  | 1:25:A:LYS:HA    | 13       | 0.96          |
| (3,5)    | 1:28:A:ILE:HD12  | 1:25:A:LYS:HA    | 16       | 0.96          |
| (1,4283) | 1:120:A:ALA:H    | 1:85:A:LEU:HD22  | 11       | 0.96          |
| (1,4120) | 1:116:A:GLN:HE21 | 1:119:A:GLU:HB2  | 7        | 0.96          |
| (1,3352) | 1:79:A:THR:HG22  | 1:48:A:LEU:HD12  | 9        | 0.96          |
| (1,3060) | 1:52:A:ILE:HG22  | 1:97:A:LEU:HD21  | 4        | 0.96          |
| (1,3060) | 1:52:A:ILE:HG21  | 1:97:A:LEU:HD21  | 13       | 0.96          |
| (1,2617) | 1:21:A:LEU:HD23  | 1:30:A:PHE:HD2   | 15       | 0.96          |
| (1,1158) | 1:120:A:ALA:HB1  | 1:82:A:TRP:HD1   | 12       | 0.96          |
| (1,1065) | 1:21:A:LEU:HD12  | 1:21:A:LEU:H     | 1        | 0.96          |
| (1,836)  | 1:64:A:MET:HE1   | 1:60:A:VAL:HG12  | 8        | 0.96          |
| (1,836)  | 1:64:A:MET:HE2   | 1:60:A:VAL:HG11  | 15       | 0.96          |
| (1,556)  | 1:71:A:LEU:H     | 1:70:A:GLN:HE21  | 3        | 0.96          |
| (1,556)  | 1:71:A:LEU:H     | 1:70:A:GLN:HE21  | 12       | 0.96          |
| (3,134)  | 1:75:A:LEU:HD22  | 1:97:A:LEU:HD23  | 15       | 0.95          |
| (3,70)   | 1:58:A:ASP:HA    | 1:57:A:VAL:HG12  | 15       | 0.95          |
| (3,52)   | 1:95:A:VAL:HG23  | 1:37:A:HIS:HB2   | 7        | 0.95          |
| (3,5)    | 1:28:A:ILE:HD11  | 1:25:A:LYS:HA    | 9        | 0.95          |
| (1,4124) | 1:116:A:GLN:HE21 | 1:120:A:ALA:H    | 2        | 0.95          |
| (1,3412) | 1:82:A:TRP:HZ3   | 1:117:A:LEU:HD13 | 11       | 0.95          |
| (1,3060) | 1:52:A:ILE:HG22  | 1:97:A:LEU:HD21  | 8        | 0.95          |
| (1,3060) | 1:52:A:ILE:HG22  | 1:97:A:LEU:HD23  | 15       | 0.95          |
| (1,2883) | 1:32:A:ALA:HB3   | 1:39:A:PHE:H     | 13       | 0.95          |
| (1,2617) | 1:21:A:LEU:HD23  | 1:30:A:PHE:HD1   | 1        | 0.95          |
| (1,2617) | 1:21:A:LEU:HD23  | 1:30:A:PHE:HD1   | 5        | 0.95          |
| (1,2308) | 1:82:A:TRP:HB2   | 1:117:A:LEU:HD11 | 5        | 0.95          |
| (1,1534) | 1:56:A:LEU:HB2   | 1:35:A:PHE:HE1   | 8        | 0.95          |
| (1,1503) | 1:52:A:ILE:HG12  | 1:54:A:GLN:HE21  | 15       | 0.95          |
| (1,1415) | 1:48:A:LEU:HD12  | 1:75:A:LEU:HD13  | 16       | 0.95          |
| (1,1158) | 1:120:A:ALA:HB2  | 1:82:A:TRP:HD1   | 9        | 0.95          |
| (1,1158) | 1:120:A:ALA:HB3  | 1:82:A:TRP:HD1   | 11       | 0.95          |
| (3,142)  | 1:59:A:ARG:H     | 1:57:A:VAL:HG13  | 11       | 0.94          |
| (3,134)  | 1:75:A:LEU:HD21  | 1:97:A:LEU:HD22  | 1        | 0.94          |
| (3,134)  | 1:75:A:LEU:HD21  | 1:97:A:LEU:HD23  | 10       | 0.94          |
| (3,134)  | 1:75:A:LEU:HD22  | 1:97:A:LEU:HD21  | 11       | 0.94          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (3,116)  | 1:95:A:VAL:H     | 1:48:A:LEU:HD12  | 5        | 0.94          |
| (3,86)   | 1:84:A:TYR:HE2   | 1:47:A:PRO:HB3   | 1        | 0.94          |
| (3,30)   | 1:64:A:MET:HE2   | 1:34:A:ARG:HB3   | 6        | 0.94          |
| (3,30)   | 1:64:A:MET:HE2   | 1:34:A:ARG:HB3   | 15       | 0.94          |
| (1,4283) | 1:120:A:ALA:H    | 1:85:A:LEU:HD23  | 12       | 0.94          |
| (1,4118) | 1:71:A:LEU:H     | 1:70:A:GLN:HE21  | 14       | 0.94          |
| (1,4084) | 1:20:A:LYS:HB3   | 1:22:A:ASN:HD22  | 8        | 0.94          |
| (1,2956) | 1:48:A:LEU:HD12  | 1:75:A:LEU:HD11  | 7        | 0.94          |
| (1,2883) | 1:32:A:ALA:HB2   | 1:39:A:PHE:H     | 2        | 0.94          |
| (1,2883) | 1:32:A:ALA:HB3   | 1:39:A:PHE:H     | 4        | 0.94          |
| (1,2883) | 1:32:A:ALA:HB3   | 1:39:A:PHE:H     | 14       | 0.94          |
| (1,2421) | 1:64:A:MET:HE1   | 1:60:A:VAL:HG13  | 1        | 0.94          |
| (1,2421) | 1:64:A:MET:HE3   | 1:60:A:VAL:HG13  | 10       | 0.94          |
| (1,2326) | 1:31:A:LEU:HD12  | 1:27:A:VAL:HG13  | 9        | 0.94          |
| (1,2308) | 1:82:A:TRP:HB2   | 1:117:A:LEU:HD12 | 1        | 0.94          |
| (1,2308) | 1:82:A:TRP:HB2   | 1:117:A:LEU:HD13 | 10       | 0.94          |
| (1,2308) | 1:82:A:TRP:HB2   | 1:117:A:LEU:HD13 | 13       | 0.94          |
| (1,836)  | 1:64:A:MET:HE2   | 1:60:A:VAL:HG12  | 13       | 0.94          |
| (1,561)  | 1:116:A:GLN:HE21 | 1:120:A:ALA:H    | 17       | 0.94          |
| (1,554)  | 1:70:A:GLN:HA    | 1:70:A:GLN:HE21  | 3        | 0.94          |
| (1,524)  | 1:20:A:LYS:HB3   | 1:22:A:ASN:HD22  | 5        | 0.94          |
| (3,146)  | 1:52:A:ILE:H     | 1:52:A:ILE:HD13  | 9        | 0.93          |
| (3,70)   | 1:58:A:ASP:HA    | 1:57:A:VAL:HG13  | 5        | 0.93          |
| (3,62)   | 1:52:A:ILE:HG23  | 1:56:A:LEU:H     | 6        | 0.93          |
| (3,52)   | 1:95:A:VAL:HG21  | 1:37:A:HIS:HB2   | 15       | 0.93          |
| (3,20)   | 1:88:A:VAL:HG13  | 1:93:A:THR:HG21  | 11       | 0.93          |
| (1,4283) | 1:120:A:ALA:H    | 1:85:A:LEU:HD22  | 9        | 0.93          |
| (1,4116) | 1:70:A:GLN:HA    | 1:70:A:GLN:HE21  | 10       | 0.93          |
| (1,4116) | 1:70:A:GLN:HA    | 1:70:A:GLN:HE21  | 17       | 0.93          |
| (1,3352) | 1:79:A:THR:HG21  | 1:48:A:LEU:HD12  | 16       | 0.93          |
| (1,3060) | 1:52:A:ILE:HG23  | 1:97:A:LEU:HD23  | 3        | 0.93          |
| (1,3046) | 1:52:A:ILE:HG12  | 1:54:A:GLN:HE21  | 17       | 0.93          |
| (1,2956) | 1:48:A:LEU:HD12  | 1:75:A:LEU:HD12  | 6        | 0.93          |
| (1,2421) | 1:64:A:MET:HE3   | 1:60:A:VAL:HG12  | 12       | 0.93          |
| (1,2326) | 1:31:A:LEU:HD11  | 1:27:A:VAL:HG13  | 6        | 0.93          |
| (1,2326) | 1:31:A:LEU:HD12  | 1:27:A:VAL:HG12  | 15       | 0.93          |
| (1,2308) | 1:82:A:TRP:HB2   | 1:117:A:LEU:HD11 | 14       | 0.93          |
| (1,2157) | 1:99:A:GLY:HA3   | 1:95:A:VAL:HG23  | 9        | 0.93          |
| (1,1862) | 1:32:A:ALA:HB3   | 1:31:A:LEU:HD13  | 14       | 0.93          |
| (1,1534) | 1:56:A:LEU:HB2   | 1:35:A:PHE:HE2   | 15       | 0.93          |
| (1,1415) | 1:48:A:LEU:HD13  | 1:75:A:LEU:HD11  | 10       | 0.93          |
| (1,836)  | 1:64:A:MET:HE3   | 1:60:A:VAL:HG11  | 2        | 0.93          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,836)  | 1:64:A:MET:HE3   | 1:60:A:VAL:HG11  | 5        | 0.93          |
| (1,556)  | 1:71:A:LEU:H     | 1:70:A:GLN:HE21  | 2        | 0.93          |
| (3,107)  | 1:95:A:VAL:HG23  | 1:102:A:CYS:HB3  | 10       | 0.92          |
| (3,70)   | 1:58:A:ASP:HA    | 1:57:A:VAL:HG11  | 7        | 0.92          |
| (3,5)    | 1:28:A:ILE:HD11  | 1:25:A:LYS:HA    | 12       | 0.92          |
| (1,4341) | 1:113:A:ALA:HB3  | 1:116:A:GLN:H    | 13       | 0.92          |
| (1,3352) | 1:79:A:THR:HG23  | 1:48:A:LEU:HD13  | 15       | 0.92          |
| (1,3060) | 1:52:A:ILE:HG23  | 1:97:A:LEU:HD23  | 2        | 0.92          |
| (1,2903) | 1:50:A:ILE:HD12  | 1:51:A:GLY:H     | 12       | 0.92          |
| (1,2883) | 1:32:A:ALA:HB2   | 1:39:A:PHE:H     | 7        | 0.92          |
| (1,2602) | 1:21:A:LEU:HD12  | 1:21:A:LEU:H     | 1        | 0.92          |
| (1,2421) | 1:64:A:MET:HE2   | 1:60:A:VAL:HG11  | 6        | 0.92          |
| (1,2421) | 1:64:A:MET:HE1   | 1:60:A:VAL:HG11  | 14       | 0.92          |
| (1,2326) | 1:31:A:LEU:HD12  | 1:27:A:VAL:HG11  | 5        | 0.92          |
| (1,2326) | 1:31:A:LEU:HD11  | 1:27:A:VAL:HG11  | 13       | 0.92          |
| (1,2308) | 1:82:A:TRP:HB2   | 1:117:A:LEU:HD13 | 16       | 0.92          |
| (1,1758) | 1:79:A:THR:HG21  | 1:48:A:LEU:HD12  | 12       | 0.92          |
| (1,1675) | 1:88:A:VAL:HG22  | 1:92:A:ALA:HB2   | 16       | 0.92          |
| (1,1534) | 1:56:A:LEU:HB2   | 1:35:A:PHE:HE1   | 6        | 0.92          |
| (1,1415) | 1:48:A:LEU:HD12  | 1:75:A:LEU:HD11  | 12       | 0.92          |
| (1,1158) | 1:120:A:ALA:HB3  | 1:82:A:TRP:HD1   | 3        | 0.92          |
| (1,556)  | 1:71:A:LEU:H     | 1:70:A:GLN:HE21  | 1        | 0.92          |
| (1,554)  | 1:70:A:GLN:HA    | 1:70:A:GLN:HE21  | 5        | 0.92          |
| (3,146)  | 1:52:A:ILE:H     | 1:52:A:ILE:HD11  | 3        | 0.91          |
| (3,146)  | 1:52:A:ILE:H     | 1:52:A:ILE:HD13  | 4        | 0.91          |
| (3,134)  | 1:75:A:LEU:HD21  | 1:97:A:LEU:HD21  | 9        | 0.91          |
| (3,112)  | 1:82:A:TRP:HA    | 1:117:A:LEU:HD13 | 1        | 0.91          |
| (3,76)   | 1:116:A:GLN:HE21 | 1:85:A:LEU:HD13  | 2        | 0.91          |
| (3,70)   | 1:58:A:ASP:HA    | 1:57:A:VAL:HG12  | 1        | 0.91          |
| (3,70)   | 1:58:A:ASP:HA    | 1:57:A:VAL:HG12  | 2        | 0.91          |
| (3,70)   | 1:58:A:ASP:HA    | 1:57:A:VAL:HG12  | 3        | 0.91          |
| (3,70)   | 1:58:A:ASP:HA    | 1:57:A:VAL:HG12  | 13       | 0.91          |
| (3,52)   | 1:99:A:GLY:HA3   | 1:95:A:VAL:HG22  | 2        | 0.91          |
| (3,51)   | 1:95:A:VAL:HG23  | 1:35:A:PHE:HB2   | 11       | 0.91          |
| (3,20)   | 1:88:A:VAL:HG12  | 1:93:A:THR:HG21  | 6        | 0.91          |
| (1,4341) | 1:113:A:ALA:HB1  | 1:116:A:GLN:H    | 4        | 0.91          |
| (1,4341) | 1:113:A:ALA:HB3  | 1:116:A:GLN:H    | 8        | 0.91          |
| (1,4283) | 1:120:A:ALA:H    | 1:85:A:LEU:HD21  | 3        | 0.91          |
| (1,4124) | 1:116:A:GLN:HE21 | 1:120:A:ALA:H    | 12       | 0.91          |
| (1,4120) | 1:116:A:GLN:HE21 | 1:119:A:GLU:HB2  | 17       | 0.91          |
| (1,4118) | 1:71:A:LEU:H     | 1:70:A:GLN:HE21  | 16       | 0.91          |
| (1,3060) | 1:52:A:ILE:HG21  | 1:97:A:LEU:HD22  | 16       | 0.91          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2903) | 1:50:A:ILE:HD13 | 1:51:A:GLY:H     | 16       | 0.91          |
| (1,2902) | 1:50:A:ILE:HD11 | 1:76:A:ARG:H     | 12       | 0.91          |
| (1,2883) | 1:32:A:ALA:HB3  | 1:39:A:PHE:H     | 12       | 0.91          |
| (1,2883) | 1:32:A:ALA:HB2  | 1:39:A:PHE:H     | 16       | 0.91          |
| (1,2421) | 1:64:A:MET:HE2  | 1:60:A:VAL:HG13  | 3        | 0.91          |
| (1,2398) | 1:50:A:ILE:HD13 | 1:50:A:ILE:H     | 4        | 0.91          |
| (1,2398) | 1:50:A:ILE:HD13 | 1:50:A:ILE:H     | 17       | 0.91          |
| (1,2308) | 1:82:A:TRP:HB2  | 1:117:A:LEU:HD13 | 6        | 0.91          |
| (1,2157) | 1:99:A:GLY:HA3  | 1:95:A:VAL:HG21  | 6        | 0.91          |
| (1,1862) | 1:32:A:ALA:HB3  | 1:31:A:LEU:HD11  | 10       | 0.91          |
| (1,1534) | 1:56:A:LEU:HB2  | 1:35:A:PHE:HE2   | 7        | 0.91          |
| (1,1415) | 1:48:A:LEU:HD11 | 1:75:A:LEU:HD13  | 4        | 0.91          |
| (1,720)  | 1:120:A:ALA:H   | 1:85:A:LEU:HD22  | 11       | 0.91          |
| (1,556)  | 1:71:A:LEU:H    | 1:70:A:GLN:HE21  | 6        | 0.91          |
| (1,556)  | 1:71:A:LEU:H    | 1:70:A:GLN:HE21  | 8        | 0.91          |
| (3,146)  | 1:52:A:ILE:H    | 1:52:A:ILE:HD13  | 8        | 0.9           |
| (3,146)  | 1:52:A:ILE:H    | 1:52:A:ILE:HD11  | 11       | 0.9           |
| (3,134)  | 1:75:A:LEU:HD21 | 1:97:A:LEU:HD23  | 6        | 0.9           |
| (3,117)  | 1:48:A:LEU:HD23 | 1:39:A:PHE:HD2   | 16       | 0.9           |
| (3,70)   | 1:58:A:ASP:HA   | 1:57:A:VAL:HG12  | 4        | 0.9           |
| (3,70)   | 1:58:A:ASP:HA   | 1:57:A:VAL:HG12  | 9        | 0.9           |
| (3,70)   | 1:58:A:ASP:HA   | 1:57:A:VAL:HG11  | 17       | 0.9           |
| (3,52)   | 1:99:A:GLY:HA3  | 1:95:A:VAL:HG21  | 14       | 0.9           |
| (3,51)   | 1:95:A:VAL:HG22 | 1:49:A:LYS:HA    | 17       | 0.9           |
| (1,4341) | 1:113:A:ALA:HB1 | 1:116:A:GLN:H    | 11       | 0.9           |
| (1,4341) | 1:113:A:ALA:HB2 | 1:116:A:GLN:H    | 12       | 0.9           |
| (1,4283) | 1:120:A:ALA:H   | 1:85:A:LEU:HD21  | 7        | 0.9           |
| (1,4118) | 1:71:A:LEU:H    | 1:70:A:GLN:HE21  | 9        | 0.9           |
| (1,4118) | 1:71:A:LEU:H    | 1:70:A:GLN:HE21  | 10       | 0.9           |
| (1,4118) | 1:71:A:LEU:H    | 1:70:A:GLN:HE21  | 13       | 0.9           |
| (1,4116) | 1:70:A:GLN:HA   | 1:70:A:GLN:HE21  | 13       | 0.9           |
| (1,4116) | 1:70:A:GLN:HA   | 1:70:A:GLN:HE21  | 15       | 0.9           |
| (1,3088) | 1:56:A:LEU:HB2  | 1:35:A:PHE:HE1   | 8        | 0.9           |
| (1,3060) | 1:52:A:ILE:HG23 | 1:97:A:LEU:HD21  | 9        | 0.9           |
| (1,3060) | 1:52:A:ILE:HG22 | 1:97:A:LEU:HD23  | 10       | 0.9           |
| (1,2956) | 1:48:A:LEU:HD12 | 1:75:A:LEU:HD13  | 16       | 0.9           |
| (1,2883) | 1:32:A:ALA:HB2  | 1:39:A:PHE:H     | 3        | 0.9           |
| (1,2681) | 1:120:A:ALA:HB1 | 1:82:A:TRP:HD1   | 12       | 0.9           |
| (1,2421) | 1:64:A:MET:HE1  | 1:60:A:VAL:HG12  | 8        | 0.9           |
| (1,2421) | 1:64:A:MET:HE2  | 1:60:A:VAL:HG11  | 15       | 0.9           |
| (1,2421) | 1:64:A:MET:HE3  | 1:60:A:VAL:HG12  | 17       | 0.9           |
| (1,1862) | 1:32:A:ALA:HB3  | 1:31:A:LEU:HD11  | 1        | 0.9           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1862) | 1:32:A:ALA:HB1   | 1:31:A:LEU:HD11  | 2        | 0.9           |
| (1,1675) | 1:88:A:VAL:HG23  | 1:92:A:ALA:HB1   | 14       | 0.9           |
| (1,1158) | 1:120:A:ALA:HB3  | 1:82:A:TRP:HD1   | 2        | 0.9           |
| (1,1158) | 1:120:A:ALA:HB1  | 1:82:A:TRP:HD1   | 17       | 0.9           |
| (1,1065) | 1:21:A:LEU:HD12  | 1:21:A:LEU:H     | 3        | 0.9           |
| (3,146)  | 1:52:A:ILE:H     | 1:52:A:ILE:HD13  | 1        | 0.89          |
| (3,142)  | 1:59:A:ARG:H     | 1:57:A:VAL:HG12  | 3        | 0.89          |
| (3,142)  | 1:59:A:ARG:H     | 1:57:A:VAL:HG13  | 5        | 0.89          |
| (3,117)  | 1:48:A:LEU:HD22  | 1:39:A:PHE:HD2   | 14       | 0.89          |
| (3,98)   | 1:64:A:MET:HE3   | 1:63:A:GLU:HG3   | 4        | 0.89          |
| (3,86)   | 1:84:A:TYR:HE1   | 1:47:A:PRO:HB3   | 13       | 0.89          |
| (3,70)   | 1:58:A:ASP:HA    | 1:57:A:VAL:HG13  | 8        | 0.89          |
| (3,51)   | 1:95:A:VAL:HG21  | 1:35:A:PHE:HB2   | 3        | 0.89          |
| (1,4341) | 1:113:A:ALA:HB1  | 1:116:A:GLN:H    | 2        | 0.89          |
| (1,4341) | 1:113:A:ALA:HB3  | 1:116:A:GLN:H    | 14       | 0.89          |
| (1,4283) | 1:120:A:ALA:H    | 1:85:A:LEU:HD21  | 15       | 0.89          |
| (1,4124) | 1:116:A:GLN:HE21 | 1:120:A:ALA:H    | 11       | 0.89          |
| (1,4120) | 1:116:A:GLN:HE21 | 1:119:A:GLU:HB2  | 13       | 0.89          |
| (1,4116) | 1:70:A:GLN:HA    | 1:70:A:GLN:HE21  | 16       | 0.89          |
| (1,3098) | 1:56:A:LEU:HD13  | 1:57:A:VAL:H     | 2        | 0.89          |
| (1,3098) | 1:56:A:LEU:HD11  | 1:57:A:VAL:H     | 6        | 0.89          |
| (1,3098) | 1:56:A:LEU:HD13  | 1:57:A:VAL:H     | 8        | 0.89          |
| (1,3046) | 1:52:A:ILE:HG12  | 1:54:A:GLN:HE21  | 15       | 0.89          |
| (1,2883) | 1:32:A:ALA:HB2   | 1:39:A:PHE:H     | 5        | 0.89          |
| (1,2883) | 1:32:A:ALA:HB2   | 1:39:A:PHE:H     | 6        | 0.89          |
| (1,2681) | 1:120:A:ALA:HB2  | 1:82:A:TRP:HD1   | 9        | 0.89          |
| (1,2681) | 1:120:A:ALA:HB3  | 1:82:A:TRP:HD1   | 11       | 0.89          |
| (1,2326) | 1:31:A:LEU:HD11  | 1:27:A:VAL:HG11  | 4        | 0.89          |
| (1,2308) | 1:82:A:TRP:HB2   | 1:117:A:LEU:HD13 | 4        | 0.89          |
| (1,1862) | 1:32:A:ALA:HB1   | 1:31:A:LEU:HD13  | 3        | 0.89          |
| (1,1862) | 1:32:A:ALA:HB2   | 1:31:A:LEU:HD13  | 13       | 0.89          |
| (1,1534) | 1:56:A:LEU:HB2   | 1:35:A:PHE:HE2   | 9        | 0.89          |
| (1,1415) | 1:48:A:LEU:HD12  | 1:75:A:LEU:HD13  | 8        | 0.89          |
| (1,1065) | 1:21:A:LEU:HD11  | 1:21:A:LEU:H     | 5        | 0.89          |
| (1,561)  | 1:116:A:GLN:HE21 | 1:120:A:ALA:H    | 2        | 0.89          |
| (1,524)  | 1:20:A:LYS:HB3   | 1:22:A:ASN:HD22  | 8        | 0.89          |
| (3,146)  | 1:52:A:ILE:H     | 1:52:A:ILE:HD11  | 15       | 0.88          |
| (3,142)  | 1:59:A:ARG:H     | 1:57:A:VAL:HG12  | 1        | 0.88          |
| (3,134)  | 1:75:A:LEU:HD23  | 1:97:A:LEU:HD21  | 4        | 0.88          |
| (3,5)    | 1:28:A:ILE:HD12  | 1:25:A:LYS:HA    | 4        | 0.88          |
| (1,4341) | 1:113:A:ALA:HB1  | 1:116:A:GLN:H    | 5        | 0.88          |
| (1,4341) | 1:113:A:ALA:HB1  | 1:116:A:GLN:H    | 17       | 0.88          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,4120) | 1:116:A:GLN:HE21 | 1:119:A:GLU:HB2 | 3        | 0.88          |
| (1,4120) | 1:116:A:GLN:HE21 | 1:119:A:GLU:HB2 | 15       | 0.88          |
| (1,4118) | 1:71:A:LEU:H     | 1:70:A:GLN:HE21 | 17       | 0.88          |
| (1,4116) | 1:70:A:GLN:HA    | 1:70:A:GLN:HE21 | 12       | 0.88          |
| (1,4091) | 1:65:A:ASN:HD22  | 1:20:A:LYS:HA   | 14       | 0.88          |
| (1,3893) | 1:79:A:THR:HG22  | 1:81:A:SER:H    | 4        | 0.88          |
| (1,3248) | 1:88:A:VAL:HG22  | 1:92:A:ALA:HB2  | 16       | 0.88          |
| (1,3098) | 1:56:A:LEU:HD12  | 1:57:A:VAL:H    | 15       | 0.88          |
| (1,2956) | 1:48:A:LEU:HD13  | 1:75:A:LEU:HD11 | 10       | 0.88          |
| (1,2903) | 1:50:A:ILE:HD13  | 1:51:A:GLY:H    | 7        | 0.88          |
| (1,2903) | 1:50:A:ILE:HD11  | 1:51:A:GLY:H    | 10       | 0.88          |
| (1,2903) | 1:50:A:ILE:HD11  | 1:51:A:GLY:H    | 15       | 0.88          |
| (1,2883) | 1:32:A:ALA:HB1   | 1:39:A:PHE:H    | 1        | 0.88          |
| (1,2883) | 1:32:A:ALA:HB1   | 1:39:A:PHE:H    | 15       | 0.88          |
| (1,2617) | 1:21:A:LEU:HD21  | 1:30:A:PHE:HD2  | 10       | 0.88          |
| (1,2192) | 1:55:A:ASP:HB2   | 1:52:A:ILE:HD13 | 6        | 0.88          |
| (1,2157) | 1:99:A:GLY:HA3   | 1:95:A:VAL:HG23 | 11       | 0.88          |
| (1,1862) | 1:32:A:ALA:HB3   | 1:31:A:LEU:HD13 | 12       | 0.88          |
| (1,1676) | 1:94:A:ARG:HD2   | 1:92:A:ALA:HB1  | 5        | 0.88          |
| (1,1675) | 1:88:A:VAL:HG23  | 1:92:A:ALA:HB3  | 10       | 0.88          |
| (1,1415) | 1:48:A:LEU:HD13  | 1:75:A:LEU:HD12 | 2        | 0.88          |
| (1,1415) | 1:48:A:LEU:HD13  | 1:75:A:LEU:HD11 | 5        | 0.88          |
| (1,1415) | 1:48:A:LEU:HD12  | 1:75:A:LEU:HD12 | 14       | 0.88          |
| (1,1137) | 1:97:A:LEU:HD11  | 1:35:A:PHE:HD1  | 6        | 0.88          |
| (1,1065) | 1:21:A:LEU:HD11  | 1:21:A:LEU:H    | 14       | 0.88          |
| (1,1065) | 1:21:A:LEU:HD12  | 1:21:A:LEU:H    | 15       | 0.88          |
| (1,1065) | 1:21:A:LEU:HD13  | 1:21:A:LEU:H    | 17       | 0.88          |
| (1,720)  | 1:120:A:ALA:H    | 1:85:A:LEU:HD23 | 12       | 0.88          |
| (1,556)  | 1:71:A:LEU:H     | 1:70:A:GLN:HE21 | 14       | 0.88          |
| (1,554)  | 1:70:A:GLN:HA    | 1:70:A:GLN:HE21 | 10       | 0.88          |
| (1,554)  | 1:70:A:GLN:HA    | 1:70:A:GLN:HE21 | 17       | 0.88          |
| (3,134)  | 1:75:A:LEU:HD22  | 1:97:A:LEU:HD22 | 16       | 0.87          |
| (3,116)  | 1:95:A:VAL:H     | 1:48:A:LEU:HD11 | 6        | 0.87          |
| (3,107)  | 1:95:A:VAL:HG21  | 1:102:A:CYS:HB3 | 12       | 0.87          |
| (3,70)   | 1:58:A:ASP:HA    | 1:57:A:VAL:HG13 | 10       | 0.87          |
| (1,4341) | 1:113:A:ALA:HB3  | 1:116:A:GLN:H   | 3        | 0.87          |
| (1,4341) | 1:113:A:ALA:HB3  | 1:116:A:GLN:H   | 10       | 0.87          |
| (1,4341) | 1:113:A:ALA:HB1  | 1:116:A:GLN:H   | 15       | 0.87          |
| (1,4283) | 1:120:A:ALA:H    | 1:85:A:LEU:HD21 | 17       | 0.87          |
| (1,4124) | 1:116:A:GLN:HE21 | 1:120:A:ALA:H   | 3        | 0.87          |
| (1,4116) | 1:70:A:GLN:HA    | 1:70:A:GLN:HE21 | 11       | 0.87          |
| (1,3893) | 1:79:A:THR:HG21  | 1:81:A:SER:H    | 1        | 0.87          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3893) | 1:79:A:THR:HG22  | 1:81:A:SER:H     | 2        | 0.87          |
| (1,3893) | 1:79:A:THR:HG22  | 1:81:A:SER:H     | 14       | 0.87          |
| (1,3474) | 1:32:A:ALA:HB3   | 1:31:A:LEU:HD13  | 14       | 0.87          |
| (1,3098) | 1:56:A:LEU:HD11  | 1:57:A:VAL:H     | 4        | 0.87          |
| (1,3098) | 1:56:A:LEU:HD13  | 1:57:A:VAL:H     | 5        | 0.87          |
| (1,3098) | 1:56:A:LEU:HD13  | 1:57:A:VAL:H     | 10       | 0.87          |
| (1,3098) | 1:56:A:LEU:HD13  | 1:57:A:VAL:H     | 12       | 0.87          |
| (1,3098) | 1:56:A:LEU:HD11  | 1:57:A:VAL:H     | 13       | 0.87          |
| (1,3098) | 1:56:A:LEU:HD11  | 1:57:A:VAL:H     | 14       | 0.87          |
| (1,3088) | 1:56:A:LEU:HB2   | 1:35:A:PHE:HE1   | 6        | 0.87          |
| (1,3088) | 1:56:A:LEU:HB2   | 1:35:A:PHE:HE2   | 15       | 0.87          |
| (1,2956) | 1:48:A:LEU:HD12  | 1:75:A:LEU:HD11  | 12       | 0.87          |
| (1,2617) | 1:21:A:LEU:HD23  | 1:30:A:PHE:HD1   | 12       | 0.87          |
| (1,2421) | 1:64:A:MET:HE3   | 1:60:A:VAL:HG11  | 2        | 0.87          |
| (1,2421) | 1:64:A:MET:HE3   | 1:60:A:VAL:HG11  | 5        | 0.87          |
| (1,2421) | 1:64:A:MET:HE2   | 1:60:A:VAL:HG12  | 13       | 0.87          |
| (1,2398) | 1:50:A:ILE:HD11  | 1:50:A:ILE:H     | 2        | 0.87          |
| (1,2338) | 1:61:A:ALA:HB3   | 1:66:A:LEU:HD12  | 3        | 0.87          |
| (1,2326) | 1:31:A:LEU:HD12  | 1:27:A:VAL:HG13  | 1        | 0.87          |
| (1,2157) | 1:99:A:GLY:HA3   | 1:95:A:VAL:HG21  | 3        | 0.87          |
| (1,1676) | 1:94:A:ARG:HD2   | 1:92:A:ALA:HB2   | 11       | 0.87          |
| (1,1534) | 1:56:A:LEU:HB2   | 1:35:A:PHE:HE2   | 3        | 0.87          |
| (1,1534) | 1:56:A:LEU:HB2   | 1:35:A:PHE:HE2   | 4        | 0.87          |
| (1,1065) | 1:21:A:LEU:HD12  | 1:21:A:LEU:H     | 10       | 0.87          |
| (1,720)  | 1:120:A:ALA:H    | 1:85:A:LEU:HD22  | 9        | 0.87          |
| (3,146)  | 1:52:A:ILE:H     | 1:52:A:ILE:HD13  | 2        | 0.86          |
| (3,142)  | 1:59:A:ARG:H     | 1:57:A:VAL:HG11  | 7        | 0.86          |
| (3,134)  | 1:75:A:LEU:HD23  | 1:97:A:LEU:HD23  | 17       | 0.86          |
| (3,116)  | 1:95:A:VAL:H     | 1:48:A:LEU:HD11  | 9        | 0.86          |
| (3,112)  | 1:82:A:TRP:HA    | 1:117:A:LEU:HD11 | 8        | 0.86          |
| (3,112)  | 1:82:A:TRP:HA    | 1:117:A:LEU:HD11 | 10       | 0.86          |
| (3,112)  | 1:82:A:TRP:HA    | 1:117:A:LEU:HD11 | 13       | 0.86          |
| (3,112)  | 1:82:A:TRP:HA    | 1:117:A:LEU:HD11 | 16       | 0.86          |
| (3,51)   | 1:95:A:VAL:HG23  | 1:49:A:LYS:HA    | 2        | 0.86          |
| (3,20)   | 1:88:A:VAL:HG13  | 1:93:A:THR:HG23  | 9        | 0.86          |
| (1,4341) | 1:113:A:ALA:HB2  | 1:116:A:GLN:H    | 7        | 0.86          |
| (1,4122) | 1:116:A:GLN:HE21 | 1:113:A:ALA:HA   | 1        | 0.86          |
| (1,3893) | 1:79:A:THR:HG21  | 1:81:A:SER:H     | 11       | 0.86          |
| (1,3352) | 1:79:A:THR:HG21  | 1:48:A:LEU:HD12  | 12       | 0.86          |
| (1,3248) | 1:88:A:VAL:HG23  | 1:92:A:ALA:HB1   | 14       | 0.86          |
| (1,3098) | 1:56:A:LEU:HD13  | 1:57:A:VAL:H     | 1        | 0.86          |
| (1,3098) | 1:56:A:LEU:HD11  | 1:57:A:VAL:H     | 7        | 0.86          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3098) | 1:56:A:LEU:HD13  | 1:57:A:VAL:H    | 9        | 0.86          |
| (1,3098) | 1:56:A:LEU:HD13  | 1:57:A:VAL:H    | 16       | 0.86          |
| (1,3098) | 1:56:A:LEU:HD13  | 1:57:A:VAL:H    | 17       | 0.86          |
| (1,2956) | 1:48:A:LEU:HD11  | 1:75:A:LEU:HD13 | 4        | 0.86          |
| (1,2681) | 1:120:A:ALA:HB3  | 1:82:A:TRP:HD1  | 3        | 0.86          |
| (1,2602) | 1:21:A:LEU:HD12  | 1:21:A:LEU:H    | 3        | 0.86          |
| (1,2338) | 1:61:A:ALA:HB3   | 1:66:A:LEU:HD12 | 5        | 0.86          |
| (1,2338) | 1:61:A:ALA:HB1   | 1:66:A:LEU:HD13 | 11       | 0.86          |
| (1,2326) | 1:31:A:LEU:HD11  | 1:27:A:VAL:HG11 | 14       | 0.86          |
| (1,1862) | 1:32:A:ALA:HB2   | 1:31:A:LEU:HD13 | 4        | 0.86          |
| (1,1862) | 1:32:A:ALA:HB1   | 1:31:A:LEU:HD13 | 6        | 0.86          |
| (1,1862) | 1:32:A:ALA:HB1   | 1:31:A:LEU:HD13 | 7        | 0.86          |
| (1,1862) | 1:32:A:ALA:HB2   | 1:31:A:LEU:HD12 | 16       | 0.86          |
| (1,1862) | 1:32:A:ALA:HB2   | 1:31:A:LEU:HD12 | 17       | 0.86          |
| (1,1676) | 1:94:A:ARG:HD2   | 1:92:A:ALA:HB1  | 4        | 0.86          |
| (1,1675) | 1:88:A:VAL:HG22  | 1:92:A:ALA:HB1  | 3        | 0.86          |
| (1,1534) | 1:56:A:LEU:HB2   | 1:35:A:PHE:HE1  | 13       | 0.86          |
| (1,1503) | 1:52:A:ILE:HG12  | 1:54:A:GLN:HE21 | 11       | 0.86          |
| (1,1415) | 1:48:A:LEU:HD13  | 1:75:A:LEU:HD13 | 15       | 0.86          |
| (1,1158) | 1:120:A:ALA:HB2  | 1:82:A:TRP:HD1  | 7        | 0.86          |
| (1,1137) | 1:97:A:LEU:HD12  | 1:35:A:PHE:HD2  | 9        | 0.86          |
| (1,1125) | 1:97:A:LEU:HD11  | 1:60:A:VAL:HG12 | 11       | 0.86          |
| (1,1065) | 1:21:A:LEU:HD11  | 1:21:A:LEU:H    | 11       | 0.86          |
| (1,720)  | 1:120:A:ALA:H    | 1:85:A:LEU:HD21 | 3        | 0.86          |
| (1,561)  | 1:116:A:GLN:HE21 | 1:120:A:ALA:H   | 12       | 0.86          |
| (1,556)  | 1:71:A:LEU:H     | 1:70:A:GLN:HE21 | 16       | 0.86          |
| (3,150)  | 1:77:A:LEU:HD23  | 1:77:A:LEU:H    | 3        | 0.85          |
| (3,146)  | 1:52:A:ILE:H     | 1:52:A:ILE:HD11 | 16       | 0.85          |
| (3,107)  | 1:95:A:VAL:HG21  | 1:102:A:CYS:HB3 | 4        | 0.85          |
| (3,98)   | 1:64:A:MET:HE2   | 1:63:A:GLU:HG3  | 9        | 0.85          |
| (3,86)   | 1:84:A:TYR:HE1   | 1:47:A:PRO:HB3  | 8        | 0.85          |
| (3,70)   | 1:58:A:ASP:HA    | 1:57:A:VAL:HG13 | 12       | 0.85          |
| (3,51)   | 1:95:A:VAL:HG22  | 1:35:A:PHE:HB2  | 1        | 0.85          |
| (3,18)   | 1:58:A:ASP:HB3   | 1:60:A:VAL:HG13 | 6        | 0.85          |
| (1,4341) | 1:113:A:ALA:HB1  | 1:116:A:GLN:H   | 1        | 0.85          |
| (1,4341) | 1:113:A:ALA:HB1  | 1:116:A:GLN:H   | 6        | 0.85          |
| (1,4122) | 1:116:A:GLN:HE21 | 1:113:A:ALA:HA  | 10       | 0.85          |
| (1,3893) | 1:79:A:THR:HG23  | 1:81:A:SER:H    | 16       | 0.85          |
| (1,3098) | 1:56:A:LEU:HD13  | 1:57:A:VAL:H    | 3        | 0.85          |
| (1,3088) | 1:56:A:LEU:HB2   | 1:35:A:PHE:HE2  | 7        | 0.85          |
| (1,2883) | 1:32:A:ALA:HB3   | 1:39:A:PHE:H    | 8        | 0.85          |
| (1,2883) | 1:32:A:ALA:HB3   | 1:39:A:PHE:H    | 9        | 0.85          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2617) | 1:21:A:LEU:HD21  | 1:30:A:PHE:HD1   | 6        | 0.85          |
| (1,2617) | 1:21:A:LEU:HD23  | 1:30:A:PHE:HD2   | 13       | 0.85          |
| (1,2602) | 1:21:A:LEU:HD11  | 1:21:A:LEU:H     | 5        | 0.85          |
| (1,2334) | 1:60:A:VAL:HG13  | 1:63:A:GLU:HG3   | 14       | 0.85          |
| (1,2192) | 1:55:A:ASP:HB2   | 1:52:A:ILE:HD11  | 5        | 0.85          |
| (1,2157) | 1:99:A:GLY:HA3   | 1:95:A:VAL:HG21  | 17       | 0.85          |
| (1,1862) | 1:32:A:ALA:HB2   | 1:31:A:LEU:HD11  | 9        | 0.85          |
| (1,1862) | 1:32:A:ALA:HB2   | 1:31:A:LEU:HD11  | 11       | 0.85          |
| (1,1675) | 1:88:A:VAL:HG21  | 1:92:A:ALA:HB1   | 7        | 0.85          |
| (1,1675) | 1:88:A:VAL:HG21  | 1:92:A:ALA:HB3   | 12       | 0.85          |
| (1,1534) | 1:56:A:LEU:HB2   | 1:35:A:PHE:HE1   | 12       | 0.85          |
| (1,1503) | 1:52:A:ILE:HG12  | 1:54:A:GLN:HE21  | 1        | 0.85          |
| (1,1503) | 1:52:A:ILE:HG12  | 1:54:A:GLN:HE21  | 3        | 0.85          |
| (1,1065) | 1:21:A:LEU:HD13  | 1:21:A:LEU:H     | 13       | 0.85          |
| (1,720)  | 1:120:A:ALA:H    | 1:85:A:LEU:HD21  | 7        | 0.85          |
| (1,556)  | 1:71:A:LEU:H     | 1:70:A:GLN:HE21  | 9        | 0.85          |
| (1,556)  | 1:71:A:LEU:H     | 1:70:A:GLN:HE21  | 13       | 0.85          |
| (3,146)  | 1:52:A:ILE:H     | 1:52:A:ILE:HD11  | 12       | 0.84          |
| (3,142)  | 1:59:A:ARG:H     | 1:57:A:VAL:HG12  | 2        | 0.84          |
| (3,142)  | 1:59:A:ARG:H     | 1:57:A:VAL:HG13  | 10       | 0.84          |
| (3,142)  | 1:59:A:ARG:H     | 1:57:A:VAL:HG13  | 12       | 0.84          |
| (3,142)  | 1:59:A:ARG:H     | 1:57:A:VAL:HG12  | 13       | 0.84          |
| (3,142)  | 1:59:A:ARG:H     | 1:57:A:VAL:HG12  | 15       | 0.84          |
| (3,142)  | 1:59:A:ARG:H     | 1:57:A:VAL:HG11  | 17       | 0.84          |
| (3,134)  | 1:75:A:LEU:HD22  | 1:97:A:LEU:HD23  | 12       | 0.84          |
| (3,120)  | 1:49:A:LYS:HB2   | 1:52:A:ILE:HD12  | 6        | 0.84          |
| (3,116)  | 1:95:A:VAL:H     | 1:48:A:LEU:HD11  | 14       | 0.84          |
| (3,112)  | 1:82:A:TRP:HA    | 1:117:A:LEU:HD12 | 14       | 0.84          |
| (3,86)   | 1:84:A:TYR:HE2   | 1:47:A:PRO:HB3   | 7        | 0.84          |
| (3,86)   | 1:84:A:TYR:HE1   | 1:47:A:PRO:HB3   | 14       | 0.84          |
| (3,76)   | 1:116:A:GLN:HE21 | 1:85:A:LEU:HD11  | 7        | 0.84          |
| (3,70)   | 1:58:A:ASP:HA    | 1:57:A:VAL:HG12  | 16       | 0.84          |
| (1,4122) | 1:116:A:GLN:HE21 | 1:113:A:ALA:HA   | 5        | 0.84          |
| (1,4122) | 1:116:A:GLN:HE21 | 1:113:A:ALA:HA   | 7        | 0.84          |
| (1,4122) | 1:116:A:GLN:HE21 | 1:113:A:ALA:HA   | 16       | 0.84          |
| (1,4122) | 1:116:A:GLN:HE21 | 1:113:A:ALA:HA   | 17       | 0.84          |
| (1,4120) | 1:116:A:GLN:HE21 | 1:119:A:GLU:HB2  | 14       | 0.84          |
| (1,4116) | 1:70:A:GLN:HA    | 1:70:A:GLN:HE21  | 2        | 0.84          |
| (1,4116) | 1:70:A:GLN:HA    | 1:70:A:GLN:HE21  | 4        | 0.84          |
| (1,4116) | 1:70:A:GLN:HA    | 1:70:A:GLN:HE21  | 6        | 0.84          |
| (1,4116) | 1:70:A:GLN:HA    | 1:70:A:GLN:HE21  | 7        | 0.84          |
| (1,3893) | 1:79:A:THR:HG23  | 1:81:A:SER:H     | 9        | 0.84          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3893) | 1:79:A:THR:HG23  | 1:81:A:SER:H     | 12       | 0.84          |
| (1,3474) | 1:32:A:ALA:HB3   | 1:31:A:LEU:HD11  | 1        | 0.84          |
| (1,3474) | 1:32:A:ALA:HB3   | 1:31:A:LEU:HD11  | 10       | 0.84          |
| (1,3248) | 1:88:A:VAL:HG23  | 1:92:A:ALA:HB3   | 10       | 0.84          |
| (1,3060) | 1:52:A:ILE:HG22  | 1:97:A:LEU:HD22  | 1        | 0.84          |
| (1,2956) | 1:48:A:LEU:HD12  | 1:75:A:LEU:HD13  | 8        | 0.84          |
| (1,2903) | 1:50:A:ILE:HD13  | 1:51:A:GLY:H     | 6        | 0.84          |
| (1,2903) | 1:50:A:ILE:HD12  | 1:51:A:GLY:H     | 9        | 0.84          |
| (1,2681) | 1:120:A:ALA:HB3  | 1:82:A:TRP:HD1   | 2        | 0.84          |
| (1,2681) | 1:120:A:ALA:HB1  | 1:82:A:TRP:HD1   | 17       | 0.84          |
| (1,2602) | 1:21:A:LEU:HD12  | 1:21:A:LEU:H     | 10       | 0.84          |
| (1,2602) | 1:21:A:LEU:HD11  | 1:21:A:LEU:H     | 14       | 0.84          |
| (1,2602) | 1:21:A:LEU:HD12  | 1:21:A:LEU:H     | 15       | 0.84          |
| (1,2602) | 1:21:A:LEU:HD13  | 1:21:A:LEU:H     | 17       | 0.84          |
| (1,2326) | 1:31:A:LEU:HD11  | 1:27:A:VAL:HG11  | 3        | 0.84          |
| (1,2157) | 1:99:A:GLY:HA3   | 1:95:A:VAL:HG22  | 1        | 0.84          |
| (1,1862) | 1:32:A:ALA:HB1   | 1:31:A:LEU:HD11  | 5        | 0.84          |
| (1,1862) | 1:32:A:ALA:HB3   | 1:31:A:LEU:HD11  | 15       | 0.84          |
| (1,1758) | 1:79:A:THR:HG23  | 1:48:A:LEU:HD12  | 6        | 0.84          |
| (1,1675) | 1:88:A:VAL:HG21  | 1:92:A:ALA:HB1   | 4        | 0.84          |
| (1,1534) | 1:56:A:LEU:HB2   | 1:35:A:PHE:HE1   | 2        | 0.84          |
| (1,1534) | 1:56:A:LEU:HB2   | 1:35:A:PHE:HE2   | 5        | 0.84          |
| (1,1534) | 1:56:A:LEU:HB2   | 1:35:A:PHE:HE1   | 16       | 0.84          |
| (1,1503) | 1:52:A:ILE:HG12  | 1:54:A:GLN:HE21  | 13       | 0.84          |
| (1,561)  | 1:116:A:GLN:HE21 | 1:120:A:ALA:H    | 11       | 0.84          |
| (1,556)  | 1:71:A:LEU:H     | 1:70:A:GLN:HE21  | 10       | 0.84          |
| (1,554)  | 1:70:A:GLN:HA    | 1:70:A:GLN:HE21  | 13       | 0.84          |
| (1,554)  | 1:70:A:GLN:HA    | 1:70:A:GLN:HE21  | 15       | 0.84          |
| (1,554)  | 1:70:A:GLN:HA    | 1:70:A:GLN:HE21  | 16       | 0.84          |
| (3,150)  | 1:77:A:LEU:HD21  | 1:77:A:LEU:H     | 10       | 0.83          |
| (3,150)  | 1:77:A:LEU:HD23  | 1:77:A:LEU:H     | 13       | 0.83          |
| (3,146)  | 1:52:A:ILE:H     | 1:52:A:ILE:HD12  | 17       | 0.83          |
| (3,117)  | 1:48:A:LEU:HD23  | 1:39:A:PHE:HD2   | 15       | 0.83          |
| (3,112)  | 1:82:A:TRP:HA    | 1:117:A:LEU:HD11 | 4        | 0.83          |
| (3,30)   | 1:64:A:MET:HE3   | 1:34:A:ARG:HB3   | 5        | 0.83          |
| (1,4341) | 1:113:A:ALA:HB2  | 1:116:A:GLN:H    | 9        | 0.83          |
| (1,4341) | 1:113:A:ALA:HB1  | 1:116:A:GLN:H    | 16       | 0.83          |
| (1,4124) | 1:116:A:GLN:HE21 | 1:120:A:ALA:H    | 15       | 0.83          |
| (1,4120) | 1:116:A:GLN:HE21 | 1:119:A:GLU:HB2  | 6        | 0.83          |
| (1,4118) | 1:71:A:LEU:H     | 1:70:A:GLN:HE21  | 4        | 0.83          |
| (1,3951) | 1:56:A:LEU:HB2   | 1:60:A:VAL:H     | 8        | 0.83          |
| (1,3951) | 1:56:A:LEU:HB2   | 1:60:A:VAL:H     | 10       | 0.83          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3951) | 1:56:A:LEU:HB2   | 1:60:A:VAL:H     | 17       | 0.83          |
| (1,3893) | 1:79:A:THR:HG23  | 1:81:A:SER:H     | 5        | 0.83          |
| (1,3893) | 1:79:A:THR:HG22  | 1:81:A:SER:H     | 13       | 0.83          |
| (1,3489) | 1:21:A:LEU:HD23  | 1:20:A:LYS:HA    | 7        | 0.83          |
| (1,3474) | 1:32:A:ALA:HB1   | 1:31:A:LEU:HD11  | 2        | 0.83          |
| (1,3474) | 1:32:A:ALA:HB1   | 1:31:A:LEU:HD13  | 3        | 0.83          |
| (1,3474) | 1:32:A:ALA:HB2   | 1:31:A:LEU:HD13  | 13       | 0.83          |
| (1,3249) | 1:94:A:ARG:HD2   | 1:92:A:ALA:HB1   | 5        | 0.83          |
| (1,3098) | 1:56:A:LEU:HD13  | 1:57:A:VAL:H     | 11       | 0.83          |
| (1,3088) | 1:56:A:LEU:HB2   | 1:35:A:PHE:HE2   | 9        | 0.83          |
| (1,2956) | 1:48:A:LEU:HD13  | 1:75:A:LEU:HD12  | 2        | 0.83          |
| (1,2956) | 1:48:A:LEU:HD13  | 1:75:A:LEU:HD11  | 5        | 0.83          |
| (1,2956) | 1:48:A:LEU:HD12  | 1:75:A:LEU:HD12  | 14       | 0.83          |
| (1,2903) | 1:50:A:ILE:HD11  | 1:51:A:GLY:H     | 11       | 0.83          |
| (1,2894) | 1:52:A:ILE:HD13  | 1:53:A:PHE:HB2   | 2        | 0.83          |
| (1,2820) | 1:97:A:LEU:HD13  | 1:52:A:ILE:H     | 6        | 0.83          |
| (1,2673) | 1:97:A:LEU:HD11  | 1:35:A:PHE:HD1   | 6        | 0.83          |
| (1,2192) | 1:55:A:ASP:HB2   | 1:52:A:ILE:HD13  | 14       | 0.83          |
| (1,1882) | 1:64:A:MET:HE2   | 1:65:A:ASN:HD22  | 5        | 0.83          |
| (1,1800) | 1:75:A:LEU:HA    | 1:31:A:LEU:HD11  | 10       | 0.83          |
| (1,1676) | 1:94:A:ARG:HD2   | 1:92:A:ALA:HB3   | 15       | 0.83          |
| (1,1675) | 1:88:A:VAL:HG23  | 1:92:A:ALA:HB3   | 6        | 0.83          |
| (1,1415) | 1:48:A:LEU:HD13  | 1:75:A:LEU:HD12  | 3        | 0.83          |
| (1,1415) | 1:48:A:LEU:HD12  | 1:75:A:LEU:HD12  | 9        | 0.83          |
| (1,1415) | 1:48:A:LEU:HD12  | 1:75:A:LEU:HD13  | 13       | 0.83          |
| (1,1158) | 1:120:A:ALA:HB3  | 1:82:A:TRP:HD1   | 15       | 0.83          |
| (1,1065) | 1:21:A:LEU:HD12  | 1:21:A:LEU:H     | 6        | 0.83          |
| (1,720)  | 1:120:A:ALA:H    | 1:85:A:LEU:HD21  | 15       | 0.83          |
| (1,556)  | 1:71:A:LEU:H     | 1:70:A:GLN:HE21  | 17       | 0.83          |
| (1,554)  | 1:70:A:GLN:HA    | 1:70:A:GLN:HE21  | 12       | 0.83          |
| (3,142)  | 1:59:A:ARG:H     | 1:57:A:VAL:HG12  | 9        | 0.82          |
| (3,142)  | 1:59:A:ARG:H     | 1:57:A:VAL:HG12  | 16       | 0.82          |
| (3,112)  | 1:82:A:TRP:HA    | 1:117:A:LEU:HD12 | 5        | 0.82          |
| (3,112)  | 1:82:A:TRP:HA    | 1:117:A:LEU:HD11 | 6        | 0.82          |
| (3,86)   | 1:84:A:TYR:HE1   | 1:47:A:PRO:HB3   | 12       | 0.82          |
| (3,76)   | 1:116:A:GLN:HE21 | 1:85:A:LEU:HD13  | 11       | 0.82          |
| (3,70)   | 1:58:A:ASP:HA    | 1:57:A:VAL:HG11  | 14       | 0.82          |
| (3,65)   | 1:52:A:ILE:HG13  | 1:52:A:ILE:HG23  | 2        | 0.82          |
| (3,62)   | 1:52:A:ILE:HG22  | 1:56:A:LEU:H     | 5        | 0.82          |
| (3,30)   | 1:64:A:MET:HE1   | 1:34:A:ARG:HB3   | 7        | 0.82          |
| (3,30)   | 1:64:A:MET:HE3   | 1:34:A:ARG:HB3   | 12       | 0.82          |
| (3,21)   | 1:22:A:ASN:H     | 1:21:A:LEU:HD11  | 7        | 0.82          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,4122) | 1:116:A:GLN:HE21 | 1:113:A:ALA:HA  | 2        | 0.82          |
| (1,3951) | 1:56:A:LEU:HB2   | 1:60:A:VAL:H    | 7        | 0.82          |
| (1,3893) | 1:79:A:THR:HG23  | 1:81:A:SER:H    | 3        | 0.82          |
| (1,3474) | 1:32:A:ALA:HB3   | 1:31:A:LEU:HD13 | 12       | 0.82          |
| (1,3249) | 1:94:A:ARG:HD2   | 1:92:A:ALA:HB2  | 11       | 0.82          |
| (1,3248) | 1:88:A:VAL:HG22  | 1:92:A:ALA:HB1  | 3        | 0.82          |
| (1,2903) | 1:50:A:ILE:HD13  | 1:51:A:GLY:H    | 13       | 0.82          |
| (1,2664) | 1:97:A:LEU:HD11  | 1:60:A:VAL:HG12 | 11       | 0.82          |
| (1,2602) | 1:21:A:LEU:HD11  | 1:21:A:LEU:H    | 11       | 0.82          |
| (1,2398) | 1:50:A:ILE:HD12  | 1:50:A:ILE:H    | 8        | 0.82          |
| (1,2337) | 1:66:A:LEU:HD13  | 1:31:A:LEU:HD11 | 6        | 0.82          |
| (1,2326) | 1:31:A:LEU:HD13  | 1:27:A:VAL:HG13 | 8        | 0.82          |
| (1,2157) | 1:99:A:GLY:HA3   | 1:95:A:VAL:HG23 | 8        | 0.82          |
| (1,2157) | 1:99:A:GLY:HA3   | 1:95:A:VAL:HG23 | 12       | 0.82          |
| (1,1862) | 1:32:A:ALA:HB2   | 1:31:A:LEU:HD12 | 8        | 0.82          |
| (1,1675) | 1:88:A:VAL:HG23  | 1:92:A:ALA:HB3  | 8        | 0.82          |
| (1,1675) | 1:88:A:VAL:HG21  | 1:92:A:ALA:HB3  | 17       | 0.82          |
| (1,1534) | 1:56:A:LEU:HB2   | 1:35:A:PHE:HE2  | 1        | 0.82          |
| (1,1534) | 1:56:A:LEU:HB2   | 1:35:A:PHE:HE2  | 10       | 0.82          |
| (1,1534) | 1:56:A:LEU:HB2   | 1:35:A:PHE:HE2  | 17       | 0.82          |
| (1,1065) | 1:21:A:LEU:HD12  | 1:21:A:LEU:H    | 2        | 0.82          |
| (1,561)  | 1:116:A:GLN:HE21 | 1:120:A:ALA:H   | 3        | 0.82          |
| (1,554)  | 1:70:A:GLN:HA    | 1:70:A:GLN:HE21 | 11       | 0.82          |
| (3,146)  | 1:52:A:ILE:H     | 1:52:A:ILE:HD12 | 13       | 0.81          |
| (3,142)  | 1:59:A:ARG:H     | 1:57:A:VAL:HG12 | 4        | 0.81          |
| (3,142)  | 1:59:A:ARG:H     | 1:57:A:VAL:HG11 | 14       | 0.81          |
| (3,51)   | 1:95:A:VAL:HG23  | 1:49:A:LYS:HA   | 15       | 0.81          |
| (3,27)   | 1:71:A:LEU:HD13  | 1:71:A:LEU:H    | 3        | 0.81          |
| (1,4122) | 1:116:A:GLN:HE21 | 1:113:A:ALA:HA  | 3        | 0.81          |
| (1,4120) | 1:116:A:GLN:HE21 | 1:119:A:GLU:HB2 | 4        | 0.81          |
| (1,4045) | 1:21:A:LEU:HD12  | 1:23:A:SER:H    | 7        | 0.81          |
| (1,3951) | 1:56:A:LEU:HB2   | 1:60:A:VAL:H    | 4        | 0.81          |
| (1,3951) | 1:56:A:LEU:HB2   | 1:60:A:VAL:H    | 6        | 0.81          |
| (1,3951) | 1:56:A:LEU:HB2   | 1:60:A:VAL:H    | 9        | 0.81          |
| (1,3951) | 1:56:A:LEU:HB2   | 1:60:A:VAL:H    | 12       | 0.81          |
| (1,3951) | 1:56:A:LEU:HB2   | 1:60:A:VAL:H    | 13       | 0.81          |
| (1,3951) | 1:56:A:LEU:HB2   | 1:60:A:VAL:H    | 14       | 0.81          |
| (1,3951) | 1:56:A:LEU:HB2   | 1:60:A:VAL:H    | 15       | 0.81          |
| (1,3893) | 1:79:A:THR:HG22  | 1:81:A:SER:H    | 15       | 0.81          |
| (1,3376) | 1:41:A:ALA:HB1   | 1:40:A:SER:HB3  | 17       | 0.81          |
| (1,3249) | 1:94:A:ARG:HD2   | 1:92:A:ALA:HB1  | 4        | 0.81          |
| (1,3248) | 1:88:A:VAL:HG21  | 1:92:A:ALA:HB1  | 7        | 0.81          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3248) | 1:88:A:VAL:HG21  | 1:92:A:ALA:HB3  | 12       | 0.81          |
| (1,3088) | 1:56:A:LEU:HB2   | 1:35:A:PHE:HE2  | 3        | 0.81          |
| (1,3088) | 1:56:A:LEU:HB2   | 1:35:A:PHE:HE2  | 4        | 0.81          |
| (1,3088) | 1:56:A:LEU:HB2   | 1:35:A:PHE:HE1  | 13       | 0.81          |
| (1,3046) | 1:52:A:ILE:HG12  | 1:54:A:GLN:HE21 | 11       | 0.81          |
| (1,2956) | 1:48:A:LEU:HD13  | 1:75:A:LEU:HD13 | 15       | 0.81          |
| (1,2903) | 1:50:A:ILE:HD12  | 1:51:A:GLY:H    | 3        | 0.81          |
| (1,2902) | 1:50:A:ILE:HD11  | 1:76:A:ARG:H    | 16       | 0.81          |
| (1,2894) | 1:52:A:ILE:HD12  | 1:53:A:PHE:HB2  | 17       | 0.81          |
| (1,2673) | 1:97:A:LEU:HD12  | 1:35:A:PHE:HD2  | 9        | 0.81          |
| (1,2602) | 1:21:A:LEU:HD13  | 1:21:A:LEU:H    | 13       | 0.81          |
| (1,2363) | 1:48:A:LEU:HD13  | 1:84:A:TYR:HE1  | 12       | 0.81          |
| (1,2337) | 1:66:A:LEU:HD12  | 1:31:A:LEU:HD11 | 13       | 0.81          |
| (1,2334) | 1:60:A:VAL:HG11  | 1:63:A:GLU:HG3  | 8        | 0.81          |
| (1,2326) | 1:31:A:LEU:HD11  | 1:27:A:VAL:HG13 | 12       | 0.81          |
| (1,1137) | 1:97:A:LEU:HD13  | 1:35:A:PHE:HD2  | 4        | 0.81          |
| (1,1065) | 1:21:A:LEU:HD12  | 1:21:A:LEU:H    | 16       | 0.81          |
| (1,805)  | 1:57:A:VAL:HG11  | 1:53:A:PHE:HD1  | 15       | 0.81          |
| (1,720)  | 1:120:A:ALA:H    | 1:85:A:LEU:HD21 | 17       | 0.81          |
| (1,559)  | 1:116:A:GLN:HE21 | 1:113:A:ALA:HA  | 1        | 0.81          |
| (1,559)  | 1:116:A:GLN:HE21 | 1:113:A:ALA:HA  | 10       | 0.81          |
| (3,150)  | 1:77:A:LEU:H     | 1:79:A:THR:HG23 | 5        | 0.8           |
| (3,150)  | 1:77:A:LEU:HD22  | 1:77:A:LEU:H    | 14       | 0.8           |
| (3,142)  | 1:59:A:ARG:H     | 1:57:A:VAL:HG13 | 8        | 0.8           |
| (3,76)   | 1:116:A:GLN:HE21 | 1:85:A:LEU:HD11 | 15       | 0.8           |
| (3,65)   | 1:52:A:ILE:HG13  | 1:52:A:ILE:HG22 | 4        | 0.8           |
| (3,30)   | 1:64:A:MET:HE1   | 1:34:A:ARG:HB3  | 8        | 0.8           |
| (1,4168) | 1:48:A:LEU:H     | 1:48:A:LEU:HD13 | 4        | 0.8           |
| (1,4124) | 1:116:A:GLN:HE21 | 1:120:A:ALA:H   | 9        | 0.8           |
| (1,4120) | 1:116:A:GLN:HE21 | 1:119:A:GLU:HB2 | 8        | 0.8           |
| (1,3951) | 1:56:A:LEU:HB2   | 1:60:A:VAL:H    | 3        | 0.8           |
| (1,3951) | 1:56:A:LEU:HB2   | 1:60:A:VAL:H    | 5        | 0.8           |
| (1,3951) | 1:56:A:LEU:HB2   | 1:60:A:VAL:H    | 16       | 0.8           |
| (1,3474) | 1:32:A:ALA:HB2   | 1:31:A:LEU:HD13 | 4        | 0.8           |
| (1,3474) | 1:32:A:ALA:HB1   | 1:31:A:LEU:HD13 | 6        | 0.8           |
| (1,3474) | 1:32:A:ALA:HB1   | 1:31:A:LEU:HD13 | 7        | 0.8           |
| (1,3474) | 1:32:A:ALA:HB2   | 1:31:A:LEU:HD12 | 16       | 0.8           |
| (1,3474) | 1:32:A:ALA:HB2   | 1:31:A:LEU:HD12 | 17       | 0.8           |
| (1,3248) | 1:88:A:VAL:HG21  | 1:92:A:ALA:HB1  | 4        | 0.8           |
| (1,3060) | 1:52:A:ILE:HG22  | 1:97:A:LEU:HD21 | 11       | 0.8           |
| (1,3046) | 1:52:A:ILE:HG12  | 1:54:A:GLN:HE21 | 1        | 0.8           |
| (1,2903) | 1:50:A:ILE:HD12  | 1:51:A:GLY:H    | 4        | 0.8           |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2820) | 1:97:A:LEU:HD12  | 1:52:A:ILE:H    | 5        | 0.8           |
| (1,2820) | 1:97:A:LEU:HD13  | 1:52:A:ILE:H    | 11       | 0.8           |
| (1,2681) | 1:120:A:ALA:HB2  | 1:82:A:TRP:HD1  | 7        | 0.8           |
| (1,2617) | 1:21:A:LEU:HD23  | 1:30:A:PHE:HD1  | 16       | 0.8           |
| (1,2334) | 1:60:A:VAL:HG13  | 1:63:A:GLU:HG3  | 6        | 0.8           |
| (1,2334) | 1:60:A:VAL:HG13  | 1:63:A:GLU:HG3  | 16       | 0.8           |
| (1,2192) | 1:55:A:ASP:HB2   | 1:52:A:ILE:HD12 | 4        | 0.8           |
| (1,2192) | 1:55:A:ASP:HB2   | 1:52:A:ILE:HD12 | 9        | 0.8           |
| (1,2157) | 1:99:A:GLY:HA3   | 1:95:A:VAL:HG23 | 4        | 0.8           |
| (1,1800) | 1:75:A:LEU:HA    | 1:31:A:LEU:HD11 | 1        | 0.8           |
| (1,1675) | 1:88:A:VAL:HG23  | 1:92:A:ALA:HB2  | 13       | 0.8           |
| (1,1503) | 1:52:A:ILE:HG12  | 1:54:A:GLN:HE21 | 5        | 0.8           |
| (1,1503) | 1:52:A:ILE:HG12  | 1:54:A:GLN:HE21 | 6        | 0.8           |
| (1,1415) | 1:48:A:LEU:HD13  | 1:75:A:LEU:HD12 | 1        | 0.8           |
| (1,1137) | 1:97:A:LEU:HD13  | 1:35:A:PHE:HD2  | 3        | 0.8           |
| (1,1137) | 1:97:A:LEU:HD13  | 1:35:A:PHE:HD2  | 15       | 0.8           |
| (1,1069) | 1:48:A:LEU:HD12  | 1:52:A:ILE:HG12 | 2        | 0.8           |
| (1,805)  | 1:57:A:VAL:HG11  | 1:53:A:PHE:HD1  | 3        | 0.8           |
| (1,805)  | 1:57:A:VAL:HG11  | 1:53:A:PHE:HD1  | 13       | 0.8           |
| (3,86)   | 1:84:A:TYR:HE1   | 1:47:A:PRO:HB3  | 5        | 0.79          |
| (3,76)   | 1:116:A:GLN:HE21 | 1:85:A:LEU:HD12 | 17       | 0.79          |
| (3,30)   | 1:64:A:MET:HE3   | 1:34:A:ARG:HB3  | 10       | 0.79          |
| (3,30)   | 1:64:A:MET:HE2   | 1:34:A:ARG:HB3  | 13       | 0.79          |
| (3,27)   | 1:71:A:LEU:HD11  | 1:71:A:LEU:H    | 14       | 0.79          |
| (1,4247) | 1:54:A:GLN:HE22  | 1:57:A:VAL:HG11 | 3        | 0.79          |
| (1,4247) | 1:54:A:GLN:HE22  | 1:57:A:VAL:HG11 | 4        | 0.79          |
| (1,4247) | 1:54:A:GLN:HE22  | 1:57:A:VAL:HG11 | 9        | 0.79          |
| (1,4122) | 1:116:A:GLN:HE21 | 1:113:A:ALA:HA  | 15       | 0.79          |
| (1,4116) | 1:70:A:GLN:HA    | 1:70:A:GLN:HE21 | 9        | 0.79          |
| (1,3951) | 1:56:A:LEU:HB2   | 1:60:A:VAL:H    | 1        | 0.79          |
| (1,3951) | 1:56:A:LEU:HB2   | 1:60:A:VAL:H    | 2        | 0.79          |
| (1,3951) | 1:56:A:LEU:HB2   | 1:60:A:VAL:H    | 11       | 0.79          |
| (1,3893) | 1:79:A:THR:HG22  | 1:81:A:SER:H    | 6        | 0.79          |
| (1,3893) | 1:79:A:THR:HG21  | 1:81:A:SER:H    | 7        | 0.79          |
| (1,3893) | 1:79:A:THR:HG23  | 1:81:A:SER:H    | 10       | 0.79          |
| (1,3474) | 1:32:A:ALA:HB2   | 1:31:A:LEU:HD11 | 11       | 0.79          |
| (1,3352) | 1:79:A:THR:HG23  | 1:48:A:LEU:HD12 | 6        | 0.79          |
| (1,3248) | 1:88:A:VAL:HG23  | 1:92:A:ALA:HB3  | 6        | 0.79          |
| (1,3088) | 1:56:A:LEU:HB2   | 1:35:A:PHE:HE1  | 2        | 0.79          |
| (1,3088) | 1:56:A:LEU:HB2   | 1:35:A:PHE:HE2  | 5        | 0.79          |
| (1,3088) | 1:56:A:LEU:HB2   | 1:35:A:PHE:HE1  | 12       | 0.79          |
| (1,3046) | 1:52:A:ILE:HG12  | 1:54:A:GLN:HE21 | 3        | 0.79          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2903) | 1:50:A:ILE:HD11  | 1:51:A:GLY:H    | 8        | 0.79          |
| (1,2903) | 1:50:A:ILE:HD11  | 1:51:A:GLY:H    | 14       | 0.79          |
| (1,2902) | 1:50:A:ILE:HD12  | 1:76:A:ARG:H    | 8        | 0.79          |
| (1,2820) | 1:97:A:LEU:HD11  | 1:52:A:ILE:H    | 7        | 0.79          |
| (1,2602) | 1:21:A:LEU:HD12  | 1:21:A:LEU:H    | 6        | 0.79          |
| (1,2363) | 1:48:A:LEU:HD13  | 1:84:A:TYR:HE1  | 6        | 0.79          |
| (1,2337) | 1:66:A:LEU:HD13  | 1:31:A:LEU:HD12 | 1        | 0.79          |
| (1,2192) | 1:55:A:ASP:HB2   | 1:52:A:ILE:HD11 | 13       | 0.79          |
| (1,2157) | 1:99:A:GLY:HA3   | 1:95:A:VAL:HG21 | 5        | 0.79          |
| (1,2157) | 1:99:A:GLY:HA3   | 1:95:A:VAL:HG22 | 10       | 0.79          |
| (1,2028) | 1:97:A:LEU:HD23  | 1:97:A:LEU:H    | 16       | 0.79          |
| (1,1676) | 1:94:A:ARG:HD2   | 1:92:A:ALA:HB2  | 1        | 0.79          |
| (1,1676) | 1:94:A:ARG:HD2   | 1:92:A:ALA:HB3  | 17       | 0.79          |
| (1,1675) | 1:88:A:VAL:HG21  | 1:92:A:ALA:HB1  | 5        | 0.79          |
| (1,1503) | 1:52:A:ILE:HG12  | 1:54:A:GLN:HE21 | 4        | 0.79          |
| (1,1503) | 1:52:A:ILE:HG12  | 1:54:A:GLN:HE21 | 7        | 0.79          |
| (1,1503) | 1:52:A:ILE:HG12  | 1:54:A:GLN:HE21 | 9        | 0.79          |
| (1,1482) | 1:64:A:MET:HE1   | 1:27:A:VAL:HA   | 5        | 0.79          |
| (1,1309) | 1:97:A:LEU:HD23  | 1:97:A:LEU:H    | 16       | 0.79          |
| (1,1050) | 1:56:A:LEU:HB2   | 1:60:A:VAL:HG12 | 5        | 0.79          |
| (1,1050) | 1:56:A:LEU:HB2   | 1:60:A:VAL:HG12 | 6        | 0.79          |
| (1,1050) | 1:56:A:LEU:HB2   | 1:60:A:VAL:HG13 | 8        | 0.79          |
| (1,805)  | 1:57:A:VAL:HG11  | 1:53:A:PHE:HD2  | 9        | 0.79          |
| (1,559)  | 1:116:A:GLN:HE21 | 1:113:A:ALA:HA  | 5        | 0.79          |
| (1,559)  | 1:116:A:GLN:HE21 | 1:113:A:ALA:HA  | 7        | 0.79          |
| (1,559)  | 1:116:A:GLN:HE21 | 1:113:A:ALA:HA  | 16       | 0.79          |
| (1,559)  | 1:116:A:GLN:HE21 | 1:113:A:ALA:HA  | 17       | 0.79          |
| (1,554)  | 1:70:A:GLN:HA    | 1:70:A:GLN:HE21 | 2        | 0.79          |
| (1,554)  | 1:70:A:GLN:HA    | 1:70:A:GLN:HE21 | 6        | 0.79          |
| (1,376)  | 1:56:A:LEU:HB2   | 1:60:A:VAL:H    | 10       | 0.79          |
| (3,107)  | 1:95:A:VAL:HG23  | 1:102:A:CYS:HB3 | 13       | 0.78          |
| (3,76)   | 1:116:A:GLN:HE21 | 1:85:A:LEU:HD11 | 3        | 0.78          |
| (3,76)   | 1:116:A:GLN:HE21 | 1:85:A:LEU:HD13 | 12       | 0.78          |
| (3,70)   | 1:58:A:ASP:HA    | 1:57:A:VAL:HG12 | 6        | 0.78          |
| (3,30)   | 1:64:A:MET:HE3   | 1:34:A:ARG:HB3  | 17       | 0.78          |
| (1,4122) | 1:116:A:GLN:HE21 | 1:113:A:ALA:HA  | 11       | 0.78          |
| (1,4091) | 1:65:A:ASN:HD22  | 1:20:A:LYS:HA   | 6        | 0.78          |
| (1,3826) | 1:102:A:CYS:H    | 1:95:A:VAL:HG11 | 15       | 0.78          |
| (1,3474) | 1:32:A:ALA:HB1   | 1:31:A:LEU:HD11 | 5        | 0.78          |
| (1,3474) | 1:32:A:ALA:HB2   | 1:31:A:LEU:HD11 | 9        | 0.78          |
| (1,3474) | 1:32:A:ALA:HB3   | 1:31:A:LEU:HD11 | 15       | 0.78          |
| (1,3377) | 1:40:A:SER:HB2   | 1:41:A:ALA:HB1  | 15       | 0.78          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3249) | 1:94:A:ARG:HD2   | 1:92:A:ALA:HB3  | 15       | 0.78          |
| (1,3248) | 1:88:A:VAL:HG23  | 1:92:A:ALA:HB3  | 8        | 0.78          |
| (1,3248) | 1:88:A:VAL:HG21  | 1:92:A:ALA:HB3  | 17       | 0.78          |
| (1,3088) | 1:56:A:LEU:HB2   | 1:35:A:PHE:HE1  | 16       | 0.78          |
| (1,3046) | 1:52:A:ILE:HG12  | 1:54:A:GLN:HE21 | 13       | 0.78          |
| (1,2956) | 1:48:A:LEU:HD13  | 1:75:A:LEU:HD12 | 3        | 0.78          |
| (1,2956) | 1:48:A:LEU:HD12  | 1:75:A:LEU:HD12 | 9        | 0.78          |
| (1,2956) | 1:48:A:LEU:HD12  | 1:75:A:LEU:HD13 | 13       | 0.78          |
| (1,2820) | 1:97:A:LEU:HD12  | 1:52:A:ILE:H    | 4        | 0.78          |
| (1,2820) | 1:97:A:LEU:HD12  | 1:52:A:ILE:H    | 13       | 0.78          |
| (1,2820) | 1:97:A:LEU:HD12  | 1:52:A:ILE:H    | 14       | 0.78          |
| (1,2820) | 1:97:A:LEU:HD12  | 1:52:A:ILE:H    | 16       | 0.78          |
| (1,2602) | 1:21:A:LEU:HD12  | 1:21:A:LEU:H    | 2        | 0.78          |
| (1,2334) | 1:60:A:VAL:HG13  | 1:63:A:GLU:HG3  | 15       | 0.78          |
| (1,2028) | 1:97:A:LEU:HD21  | 1:97:A:LEU:H    | 2        | 0.78          |
| (1,1882) | 1:64:A:MET:HE3   | 1:65:A:ASN:HD22 | 11       | 0.78          |
| (1,1800) | 1:75:A:LEU:HA    | 1:31:A:LEU:HD13 | 3        | 0.78          |
| (1,1800) | 1:75:A:LEU:HA    | 1:31:A:LEU:HD13 | 14       | 0.78          |
| (1,1758) | 1:79:A:THR:HG21  | 1:48:A:LEU:HD13 | 2        | 0.78          |
| (1,1675) | 1:88:A:VAL:HG23  | 1:92:A:ALA:HB2  | 9        | 0.78          |
| (1,1675) | 1:88:A:VAL:HG23  | 1:92:A:ALA:HB2  | 11       | 0.78          |
| (1,1534) | 1:56:A:LEU:HB2   | 1:35:A:PHE:HE2  | 14       | 0.78          |
| (1,1309) | 1:97:A:LEU:HD21  | 1:97:A:LEU:H    | 2        | 0.78          |
| (1,1137) | 1:97:A:LEU:HD12  | 1:35:A:PHE:HD1  | 8        | 0.78          |
| (1,1050) | 1:56:A:LEU:HB2   | 1:60:A:VAL:HG11 | 3        | 0.78          |
| (1,1050) | 1:56:A:LEU:HB2   | 1:60:A:VAL:HG12 | 16       | 0.78          |
| (1,805)  | 1:57:A:VAL:HG11  | 1:53:A:PHE:HD1  | 4        | 0.78          |
| (1,805)  | 1:57:A:VAL:HG12  | 1:53:A:PHE:HD2  | 8        | 0.78          |
| (1,561)  | 1:116:A:GLN:HE21 | 1:120:A:ALA:H   | 15       | 0.78          |
| (1,556)  | 1:71:A:LEU:H     | 1:70:A:GLN:HE21 | 4        | 0.78          |
| (1,554)  | 1:70:A:GLN:HA    | 1:70:A:GLN:HE21 | 4        | 0.78          |
| (1,554)  | 1:70:A:GLN:HA    | 1:70:A:GLN:HE21 | 7        | 0.78          |
| (1,376)  | 1:56:A:LEU:HB2   | 1:60:A:VAL:H    | 7        | 0.78          |
| (1,376)  | 1:56:A:LEU:HB2   | 1:60:A:VAL:H    | 8        | 0.78          |
| (1,376)  | 1:56:A:LEU:HB2   | 1:60:A:VAL:H    | 17       | 0.78          |
| (3,142)  | 1:59:A:ARG:H     | 1:57:A:VAL:HG12 | 6        | 0.77          |
| (3,117)  | 1:48:A:LEU:HD21  | 1:39:A:PHE:HD2  | 5        | 0.77          |
| (3,86)   | 1:84:A:TYR:HE1   | 1:47:A:PRO:HB3  | 10       | 0.77          |
| (3,27)   | 1:71:A:LEU:HD12  | 1:71:A:LEU:H    | 10       | 0.77          |
| (3,27)   | 1:71:A:LEU:HD12  | 1:71:A:LEU:H    | 13       | 0.77          |
| (3,20)   | 1:88:A:VAL:HG12  | 1:93:A:THR:HG21 | 3        | 0.77          |
| (1,4122) | 1:116:A:GLN:HE21 | 1:113:A:ALA:HA  | 4        | 0.77          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3893) | 1:79:A:THR:HG22  | 1:81:A:SER:H    | 17       | 0.77          |
| (1,3826) | 1:102:A:CYS:H    | 1:95:A:VAL:HG11 | 13       | 0.77          |
| (1,3509) | 1:64:A:MET:HE2   | 1:65:A:ASN:HD22 | 5        | 0.77          |
| (1,3397) | 1:75:A:LEU:HA    | 1:31:A:LEU:HD11 | 10       | 0.77          |
| (1,3088) | 1:56:A:LEU:HB2   | 1:35:A:PHE:HE2  | 1        | 0.77          |
| (1,2902) | 1:50:A:ILE:HD12  | 1:76:A:ARG:H    | 2        | 0.77          |
| (1,2902) | 1:50:A:ILE:HD11  | 1:76:A:ARG:H    | 6        | 0.77          |
| (1,2894) | 1:52:A:ILE:HD11  | 1:53:A:PHE:HB2  | 12       | 0.77          |
| (1,2820) | 1:97:A:LEU:HD12  | 1:52:A:ILE:H    | 3        | 0.77          |
| (1,2820) | 1:97:A:LEU:HD11  | 1:52:A:ILE:H    | 8        | 0.77          |
| (1,2820) | 1:97:A:LEU:HD11  | 1:52:A:ILE:H    | 9        | 0.77          |
| (1,2820) | 1:97:A:LEU:HD12  | 1:52:A:ILE:H    | 15       | 0.77          |
| (1,2681) | 1:120:A:ALA:HB3  | 1:82:A:TRP:HD1  | 15       | 0.77          |
| (1,2602) | 1:21:A:LEU:HD12  | 1:21:A:LEU:H    | 16       | 0.77          |
| (1,2423) | 1:64:A:MET:HA    | 1:64:A:MET:HE3  | 11       | 0.77          |
| (1,2384) | 1:57:A:VAL:HG11  | 1:53:A:PHE:HD1  | 13       | 0.77          |
| (1,2384) | 1:57:A:VAL:HG11  | 1:53:A:PHE:HD1  | 15       | 0.77          |
| (1,2363) | 1:48:A:LEU:HD11  | 1:84:A:TYR:HE2  | 1        | 0.77          |
| (1,2348) | 1:30:A:PHE:HD2   | 1:21:A:LEU:HD13 | 9        | 0.77          |
| (1,2337) | 1:66:A:LEU:HD11  | 1:31:A:LEU:HD11 | 4        | 0.77          |
| (1,2334) | 1:60:A:VAL:HG13  | 1:63:A:GLU:HG3  | 2        | 0.77          |
| (1,2334) | 1:60:A:VAL:HG11  | 1:63:A:GLU:HG3  | 12       | 0.77          |
| (1,2334) | 1:60:A:VAL:HG11  | 1:63:A:GLU:HG3  | 17       | 0.77          |
| (1,2326) | 1:31:A:LEU:HD12  | 1:27:A:VAL:HG11 | 11       | 0.77          |
| (1,2192) | 1:55:A:ASP:HB2   | 1:52:A:ILE:HD13 | 11       | 0.77          |
| (1,2028) | 1:97:A:LEU:HD21  | 1:97:A:LEU:H    | 14       | 0.77          |
| (1,1800) | 1:75:A:LEU:HA    | 1:31:A:LEU:HD11 | 2        | 0.77          |
| (1,1800) | 1:75:A:LEU:HA    | 1:31:A:LEU:HD12 | 8        | 0.77          |
| (1,1800) | 1:75:A:LEU:HA    | 1:31:A:LEU:HD13 | 13       | 0.77          |
| (1,1675) | 1:88:A:VAL:HG23  | 1:92:A:ALA:HB1  | 2        | 0.77          |
| (1,1482) | 1:64:A:MET:HE2   | 1:27:A:VAL:HA   | 1        | 0.77          |
| (1,1309) | 1:97:A:LEU:HD21  | 1:97:A:LEU:H    | 14       | 0.77          |
| (1,1050) | 1:56:A:LEU:HB2   | 1:60:A:VAL:HG12 | 14       | 0.77          |
| (1,805)  | 1:57:A:VAL:HG11  | 1:53:A:PHE:HD2  | 1        | 0.77          |
| (1,559)  | 1:116:A:GLN:HE21 | 1:113:A:ALA:HA  | 2        | 0.77          |
| (1,376)  | 1:56:A:LEU:HB2   | 1:60:A:VAL:H    | 6        | 0.77          |
| (1,376)  | 1:56:A:LEU:HB2   | 1:60:A:VAL:H    | 12       | 0.77          |
| (1,376)  | 1:56:A:LEU:HB2   | 1:60:A:VAL:H    | 14       | 0.77          |
| (1,376)  | 1:56:A:LEU:HB2   | 1:60:A:VAL:H    | 15       | 0.77          |
| (3,119)  | 1:98:A:ASP:HB3   | 1:99:A:GLY:HA2  | 1        | 0.76          |
| (3,113)  | 1:61:A:ALA:HB1   | 1:60:A:VAL:HB   | 17       | 0.76          |
| (3,107)  | 1:95:A:VAL:HG22  | 1:102:A:CYS:HB3 | 5        | 0.76          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (3,98)   | 1:64:A:MET:HE2   | 1:63:A:GLU:HG3  | 13       | 0.76          |
| (3,86)   | 1:84:A:TYR:HE2   | 1:47:A:PRO:HB3  | 3        | 0.76          |
| (3,76)   | 1:116:A:GLN:HE21 | 1:85:A:LEU:HD13 | 9        | 0.76          |
| (3,55)   | 1:97:A:LEU:HD23  | 1:75:A:LEU:HD11 | 7        | 0.76          |
| (3,27)   | 1:71:A:LEU:HD11  | 1:71:A:LEU:H    | 6        | 0.76          |
| (1,4168) | 1:48:A:LEU:H     | 1:48:A:LEU:HD11 | 15       | 0.76          |
| (1,4118) | 1:71:A:LEU:H     | 1:70:A:GLN:HE21 | 15       | 0.76          |
| (1,4116) | 1:70:A:GLN:HA    | 1:70:A:GLN:HE21 | 8        | 0.76          |
| (1,4045) | 1:21:A:LEU:HD13  | 1:23:A:SER:H    | 4        | 0.76          |
| (1,3474) | 1:32:A:ALA:HB2   | 1:31:A:LEU:HD12 | 8        | 0.76          |
| (1,3248) | 1:88:A:VAL:HG23  | 1:92:A:ALA:HB2  | 13       | 0.76          |
| (1,3088) | 1:56:A:LEU:HB2   | 1:35:A:PHE:HE2  | 10       | 0.76          |
| (1,3088) | 1:56:A:LEU:HB2   | 1:35:A:PHE:HE2  | 17       | 0.76          |
| (1,2903) | 1:50:A:ILE:HD12  | 1:51:A:GLY:H    | 17       | 0.76          |
| (1,2894) | 1:52:A:ILE:HD11  | 1:53:A:PHE:HB2  | 10       | 0.76          |
| (1,2820) | 1:97:A:LEU:HD11  | 1:52:A:ILE:H    | 2        | 0.76          |
| (1,2673) | 1:97:A:LEU:HD13  | 1:35:A:PHE:HD2  | 3        | 0.76          |
| (1,2673) | 1:97:A:LEU:HD13  | 1:35:A:PHE:HD2  | 4        | 0.76          |
| (1,2580) | 1:56:A:LEU:HB2   | 1:60:A:VAL:HG12 | 5        | 0.76          |
| (1,2580) | 1:56:A:LEU:HB2   | 1:60:A:VAL:HG12 | 6        | 0.76          |
| (1,2384) | 1:57:A:VAL:HG11  | 1:53:A:PHE:HD1  | 3        | 0.76          |
| (1,2363) | 1:48:A:LEU:HD13  | 1:84:A:TYR:HE1  | 8        | 0.76          |
| (1,2337) | 1:66:A:LEU:HD13  | 1:31:A:LEU:HD12 | 9        | 0.76          |
| (1,2337) | 1:66:A:LEU:HD12  | 1:31:A:LEU:HD11 | 14       | 0.76          |
| (1,2192) | 1:55:A:ASP:HB2   | 1:52:A:ILE:HD12 | 2        | 0.76          |
| (1,2192) | 1:55:A:ASP:HB2   | 1:52:A:ILE:HD13 | 3        | 0.76          |
| (1,2192) | 1:55:A:ASP:HB2   | 1:52:A:ILE:HD13 | 7        | 0.76          |
| (1,2188) | 1:124:A:VAL:HG11 | 1:124:A:VAL:H   | 2        | 0.76          |
| (1,2157) | 1:99:A:GLY:HA3   | 1:95:A:VAL:HG22 | 13       | 0.76          |
| (1,2028) | 1:97:A:LEU:HD23  | 1:97:A:LEU:H    | 1        | 0.76          |
| (1,1800) | 1:75:A:LEU:HA    | 1:31:A:LEU:HD13 | 7        | 0.76          |
| (1,1676) | 1:94:A:ARG:HD2   | 1:92:A:ALA:HB1  | 3        | 0.76          |
| (1,1676) | 1:94:A:ARG:HD2   | 1:92:A:ALA:HB1  | 7        | 0.76          |
| (1,1676) | 1:94:A:ARG:HD2   | 1:92:A:ALA:HB2  | 13       | 0.76          |
| (1,1502) | 1:52:A:ILE:HG13  | 1:54:A:GLN:HE21 | 10       | 0.76          |
| (1,1309) | 1:97:A:LEU:HD23  | 1:97:A:LEU:H    | 1        | 0.76          |
| (1,1137) | 1:97:A:LEU:HD11  | 1:35:A:PHE:HD2  | 11       | 0.76          |
| (1,1125) | 1:97:A:LEU:HD13  | 1:60:A:VAL:HG12 | 3        | 0.76          |
| (1,1065) | 1:21:A:LEU:HD11  | 1:21:A:LEU:H    | 12       | 0.76          |
| (1,1050) | 1:56:A:LEU:HB2   | 1:60:A:VAL:HG12 | 15       | 0.76          |
| (1,805)  | 1:57:A:VAL:HG11  | 1:53:A:PHE:HD1  | 6        | 0.76          |
| (1,576)  | 1:50:A:ILE:HD13  | 1:50:A:ILE:H    | 4        | 0.76          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,576)  | 1:50:A:ILE:HD13  | 1:50:A:ILE:H    | 17       | 0.76          |
| (1,559)  | 1:116:A:GLN:HE21 | 1:113:A:ALA:HA  | 3        | 0.76          |
| (1,488)  | 1:21:A:LEU:HD12  | 1:23:A:SER:H    | 7        | 0.76          |
| (1,376)  | 1:56:A:LEU:HB2   | 1:60:A:VAL:H    | 3        | 0.76          |
| (1,376)  | 1:56:A:LEU:HB2   | 1:60:A:VAL:H    | 4        | 0.76          |
| (1,376)  | 1:56:A:LEU:HB2   | 1:60:A:VAL:H    | 5        | 0.76          |
| (1,376)  | 1:56:A:LEU:HB2   | 1:60:A:VAL:H    | 9        | 0.76          |
| (1,376)  | 1:56:A:LEU:HB2   | 1:60:A:VAL:H    | 13       | 0.76          |
| (1,376)  | 1:56:A:LEU:HB2   | 1:60:A:VAL:H    | 16       | 0.76          |
| (3,65)   | 1:52:A:ILE:HG13  | 1:52:A:ILE:HG21 | 16       | 0.75          |
| (3,62)   | 1:52:A:ILE:HG21  | 1:56:A:LEU:H    | 14       | 0.75          |
| (3,55)   | 1:57:A:VAL:HG11  | 1:75:A:LEU:HD11 | 17       | 0.75          |
| (3,30)   | 1:64:A:MET:HE2   | 1:34:A:ARG:HB3  | 3        | 0.75          |
| (3,30)   | 1:64:A:MET:HE3   | 1:34:A:ARG:HB3  | 4        | 0.75          |
| (3,30)   | 1:64:A:MET:HE2   | 1:34:A:ARG:HB3  | 9        | 0.75          |
| (3,30)   | 1:64:A:MET:HE2   | 1:34:A:ARG:HB3  | 11       | 0.75          |
| (3,30)   | 1:64:A:MET:HE1   | 1:34:A:ARG:HB3  | 14       | 0.75          |
| (3,27)   | 1:71:A:LEU:HD11  | 1:71:A:LEU:H    | 15       | 0.75          |
| (3,27)   | 1:71:A:LEU:HD12  | 1:71:A:LEU:H    | 16       | 0.75          |
| (3,21)   | 1:31:A:LEU:H     | 1:21:A:LEU:HD12 | 17       | 0.75          |
| (1,4229) | 1:122:A:ALA:HB3  | 1:124:A:VAL:H   | 2        | 0.75          |
| (1,4168) | 1:48:A:LEU:H     | 1:48:A:LEU:HD13 | 16       | 0.75          |
| (1,4120) | 1:116:A:GLN:HE21 | 1:119:A:GLU:HB2 | 1        | 0.75          |
| (1,4116) | 1:70:A:GLN:HA    | 1:70:A:GLN:HE21 | 1        | 0.75          |
| (1,4084) | 1:20:A:LYS:HB3   | 1:22:A:ASN:HD22 | 6        | 0.75          |
| (1,3893) | 1:79:A:THR:HG22  | 1:81:A:SER:H    | 8        | 0.75          |
| (1,3377) | 1:40:A:SER:HB2   | 1:41:A:ALA:HB2  | 11       | 0.75          |
| (1,3248) | 1:88:A:VAL:HG21  | 1:92:A:ALA:HB1  | 5        | 0.75          |
| (1,3046) | 1:52:A:ILE:HG12  | 1:54:A:GLN:HE21 | 6        | 0.75          |
| (1,2956) | 1:48:A:LEU:HD13  | 1:75:A:LEU:HD12 | 1        | 0.75          |
| (1,2903) | 1:50:A:ILE:HD12  | 1:51:A:GLY:H    | 5        | 0.75          |
| (1,2832) | 1:97:A:LEU:HD23  | 1:97:A:LEU:H    | 16       | 0.75          |
| (1,2673) | 1:97:A:LEU:HD13  | 1:35:A:PHE:HD2  | 15       | 0.75          |
| (1,2608) | 1:48:A:LEU:HD12  | 1:52:A:ILE:HG12 | 2        | 0.75          |
| (1,2580) | 1:56:A:LEU:HB2   | 1:60:A:VAL:HG11 | 3        | 0.75          |
| (1,2580) | 1:56:A:LEU:HB2   | 1:60:A:VAL:HG13 | 8        | 0.75          |
| (1,2384) | 1:57:A:VAL:HG11  | 1:53:A:PHE:HD2  | 9        | 0.75          |
| (1,2338) | 1:61:A:ALA:HB2   | 1:66:A:LEU:HD11 | 6        | 0.75          |
| (1,2338) | 1:61:A:ALA:HB1   | 1:66:A:LEU:HD13 | 13       | 0.75          |
| (1,2338) | 1:61:A:ALA:HB2   | 1:66:A:LEU:HD13 | 17       | 0.75          |
| (1,2337) | 1:66:A:LEU:HD11  | 1:31:A:LEU:HD11 | 3        | 0.75          |
| (1,2337) | 1:66:A:LEU:HD11  | 1:31:A:LEU:HD12 | 10       | 0.75          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2337) | 1:66:A:LEU:HD12  | 1:31:A:LEU:HD13 | 17       | 0.75          |
| (1,2326) | 1:31:A:LEU:HD11  | 1:27:A:VAL:HG11 | 7        | 0.75          |
| (1,2192) | 1:55:A:ASP:HB2   | 1:52:A:ILE:HD12 | 1        | 0.75          |
| (1,2188) | 1:124:A:VAL:HG13 | 1:124:A:VAL:H   | 3        | 0.75          |
| (1,2188) | 1:124:A:VAL:HG13 | 1:124:A:VAL:H   | 5        | 0.75          |
| (1,2188) | 1:124:A:VAL:HG11 | 1:124:A:VAL:H   | 10       | 0.75          |
| (1,2188) | 1:124:A:VAL:HG13 | 1:124:A:VAL:H   | 12       | 0.75          |
| (1,2157) | 1:99:A:GLY:HA3   | 1:95:A:VAL:HG21 | 7        | 0.75          |
| (1,1676) | 1:94:A:ARG:HD2   | 1:92:A:ALA:HB1  | 2        | 0.75          |
| (1,1676) | 1:94:A:ARG:HD2   | 1:92:A:ALA:HB3  | 10       | 0.75          |
| (1,1482) | 1:64:A:MET:HE3   | 1:27:A:VAL:HA   | 15       | 0.75          |
| (1,1125) | 1:97:A:LEU:HD12  | 1:60:A:VAL:HG11 | 9        | 0.75          |
| (1,1050) | 1:56:A:LEU:HB2   | 1:60:A:VAL:HG12 | 2        | 0.75          |
| (1,1050) | 1:56:A:LEU:HB2   | 1:60:A:VAL:HG13 | 4        | 0.75          |
| (1,1050) | 1:56:A:LEU:HB2   | 1:60:A:VAL:HG13 | 9        | 0.75          |
| (1,1050) | 1:56:A:LEU:HB2   | 1:60:A:VAL:HG13 | 17       | 0.75          |
| (1,815)  | 1:50:A:ILE:HD12  | 1:50:A:ILE:HA   | 3        | 0.75          |
| (1,815)  | 1:50:A:ILE:HD11  | 1:50:A:ILE:HA   | 5        | 0.75          |
| (1,805)  | 1:57:A:VAL:HG11  | 1:53:A:PHE:HD1  | 2        | 0.75          |
| (1,805)  | 1:57:A:VAL:HG12  | 1:53:A:PHE:HD2  | 5        | 0.75          |
| (1,559)  | 1:116:A:GLN:HE21 | 1:113:A:ALA:HA  | 15       | 0.75          |
| (1,376)  | 1:56:A:LEU:HB2   | 1:60:A:VAL:H    | 1        | 0.75          |
| (1,376)  | 1:56:A:LEU:HB2   | 1:60:A:VAL:H    | 2        | 0.75          |
| (1,376)  | 1:56:A:LEU:HB2   | 1:60:A:VAL:H    | 11       | 0.75          |
| (3,150)  | 1:77:A:LEU:H     | 1:79:A:THR:HG21 | 1        | 0.74          |
| (3,120)  | 1:49:A:LYS:HB2   | 1:52:A:ILE:HD12 | 14       | 0.74          |
| (3,113)  | 1:61:A:ALA:HB1   | 1:60:A:VAL:HB   | 10       | 0.74          |
| (3,65)   | 1:52:A:ILE:HG13  | 1:52:A:ILE:HG22 | 15       | 0.74          |
| (3,59)   | 1:117:A:LEU:HA   | 1:85:A:LEU:HD21 | 2        | 0.74          |
| (3,59)   | 1:117:A:LEU:HA   | 1:85:A:LEU:HD22 | 11       | 0.74          |
| (3,55)   | 1:97:A:LEU:HD23  | 1:75:A:LEU:HD11 | 10       | 0.74          |
| (3,27)   | 1:71:A:LEU:HD11  | 1:71:A:LEU:H    | 1        | 0.74          |
| (3,27)   | 1:71:A:LEU:HD13  | 1:71:A:LEU:H    | 2        | 0.74          |
| (3,27)   | 1:71:A:LEU:HD13  | 1:71:A:LEU:H    | 7        | 0.74          |
| (3,27)   | 1:71:A:LEU:HD12  | 1:71:A:LEU:H    | 12       | 0.74          |
| (3,21)   | 1:22:A:ASN:H     | 1:21:A:LEU:HD13 | 3        | 0.74          |
| (3,21)   | 1:31:A:LEU:H     | 1:21:A:LEU:HD12 | 16       | 0.74          |
| (3,20)   | 1:88:A:VAL:HG13  | 1:93:A:THR:HG22 | 1        | 0.74          |
| (1,4247) | 1:54:A:GLN:HE22  | 1:57:A:VAL:HG12 | 11       | 0.74          |
| (1,4229) | 1:122:A:ALA:HB3  | 1:124:A:VAL:H   | 17       | 0.74          |
| (1,4168) | 1:48:A:LEU:H     | 1:48:A:LEU:HD11 | 9        | 0.74          |
| (1,4118) | 1:71:A:LEU:H     | 1:70:A:GLN:HE21 | 11       | 0.74          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,4080) | 1:54:A:GLN:HE22  | 1:57:A:VAL:HG22 | 7        | 0.74          |
| (1,3826) | 1:102:A:CYS:H    | 1:95:A:VAL:HG13 | 10       | 0.74          |
| (1,3397) | 1:75:A:LEU:HA    | 1:31:A:LEU:HD11 | 1        | 0.74          |
| (1,3302) | 1:83:A:ARG:HB2   | 1:86:A:TYR:HD1  | 17       | 0.74          |
| (1,3249) | 1:94:A:ARG:HD2   | 1:92:A:ALA:HB2  | 1        | 0.74          |
| (1,3249) | 1:94:A:ARG:HD2   | 1:92:A:ALA:HB3  | 17       | 0.74          |
| (1,3248) | 1:88:A:VAL:HG23  | 1:92:A:ALA:HB2  | 9        | 0.74          |
| (1,3248) | 1:88:A:VAL:HG23  | 1:92:A:ALA:HB2  | 11       | 0.74          |
| (1,3046) | 1:52:A:ILE:HG12  | 1:54:A:GLN:HE21 | 4        | 0.74          |
| (1,3046) | 1:52:A:ILE:HG12  | 1:54:A:GLN:HE21 | 5        | 0.74          |
| (1,3046) | 1:52:A:ILE:HG12  | 1:54:A:GLN:HE21 | 7        | 0.74          |
| (1,3046) | 1:52:A:ILE:HG12  | 1:54:A:GLN:HE21 | 9        | 0.74          |
| (1,2832) | 1:97:A:LEU:HD21  | 1:97:A:LEU:H    | 2        | 0.74          |
| (1,2820) | 1:97:A:LEU:HD12  | 1:52:A:ILE:H    | 1        | 0.74          |
| (1,2580) | 1:56:A:LEU:HB2   | 1:60:A:VAL:HG12 | 14       | 0.74          |
| (1,2580) | 1:56:A:LEU:HB2   | 1:60:A:VAL:HG12 | 16       | 0.74          |
| (1,2384) | 1:57:A:VAL:HG11  | 1:53:A:PHE:HD2  | 1        | 0.74          |
| (1,2384) | 1:57:A:VAL:HG11  | 1:53:A:PHE:HD1  | 4        | 0.74          |
| (1,2384) | 1:57:A:VAL:HG12  | 1:53:A:PHE:HD2  | 8        | 0.74          |
| (1,2363) | 1:48:A:LEU:HD11  | 1:84:A:TYR:HE2  | 3        | 0.74          |
| (1,2363) | 1:48:A:LEU:HD13  | 1:84:A:TYR:HE1  | 13       | 0.74          |
| (1,2326) | 1:31:A:LEU:HD12  | 1:27:A:VAL:HG11 | 10       | 0.74          |
| (1,2326) | 1:31:A:LEU:HD13  | 1:27:A:VAL:HG12 | 17       | 0.74          |
| (1,2188) | 1:124:A:VAL:HG12 | 1:124:A:VAL:H   | 6        | 0.74          |
| (1,2188) | 1:124:A:VAL:HG13 | 1:124:A:VAL:H   | 7        | 0.74          |
| (1,2188) | 1:124:A:VAL:HG12 | 1:124:A:VAL:H   | 8        | 0.74          |
| (1,2188) | 1:124:A:VAL:HG13 | 1:124:A:VAL:H   | 9        | 0.74          |
| (1,2188) | 1:124:A:VAL:HG11 | 1:124:A:VAL:H   | 17       | 0.74          |
| (1,2026) | 1:57:A:VAL:HG11  | 1:53:A:PHE:HD1  | 13       | 0.74          |
| (1,2026) | 1:57:A:VAL:HG11  | 1:53:A:PHE:HD1  | 15       | 0.74          |
| (1,1990) | 1:92:A:ALA:HB2   | 1:91:A:GLY:H    | 2        | 0.74          |
| (1,1882) | 1:64:A:MET:HE1   | 1:65:A:ASN:HD22 | 15       | 0.74          |
| (1,1800) | 1:75:A:LEU:HA    | 1:31:A:LEU:HD11 | 5        | 0.74          |
| (1,1676) | 1:94:A:ARG:HD2   | 1:92:A:ALA:HB2  | 9        | 0.74          |
| (1,1676) | 1:94:A:ARG:HD2   | 1:92:A:ALA:HB1  | 14       | 0.74          |
| (1,1502) | 1:52:A:ILE:HG13  | 1:54:A:GLN:HE21 | 12       | 0.74          |
| (1,1125) | 1:97:A:LEU:HD12  | 1:60:A:VAL:HG11 | 8        | 0.74          |
| (1,1069) | 1:48:A:LEU:HD13  | 1:52:A:ILE:HG12 | 4        | 0.74          |
| (1,1050) | 1:56:A:LEU:HB2   | 1:60:A:VAL:HG11 | 10       | 0.74          |
| (1,1050) | 1:56:A:LEU:HB2   | 1:60:A:VAL:HG13 | 13       | 0.74          |
| (1,815)  | 1:50:A:ILE:HD13  | 1:50:A:ILE:HA   | 1        | 0.74          |
| (1,805)  | 1:57:A:VAL:HG12  | 1:53:A:PHE:HD1  | 11       | 0.74          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,561)  | 1:116:A:GLN:HE21 | 1:120:A:ALA:H   | 9        | 0.74          |
| (1,554)  | 1:70:A:GLN:HA    | 1:70:A:GLN:HE21 | 9        | 0.74          |
| (1,222)  | 1:102:A:CYS:H    | 1:95:A:VAL:HG11 | 15       | 0.74          |
| (3,123)  | 1:50:A:ILE:HD12  | 1:79:A:THR:HA   | 11       | 0.73          |
| (3,113)  | 1:61:A:ALA:HB1   | 1:60:A:VAL:HB   | 12       | 0.73          |
| (3,107)  | 1:95:A:VAL:HG22  | 1:102:A:CYS:HB3 | 7        | 0.73          |
| (3,98)   | 1:64:A:MET:HE3   | 1:63:A:GLU:HG3  | 5        | 0.73          |
| (3,76)   | 1:116:A:GLN:HE21 | 1:85:A:LEU:HD13 | 4        | 0.73          |
| (3,55)   | 1:97:A:LEU:HD21  | 1:75:A:LEU:HD13 | 8        | 0.73          |
| (3,55)   | 1:97:A:LEU:HD23  | 1:75:A:LEU:HD12 | 14       | 0.73          |
| (3,27)   | 1:71:A:LEU:HD13  | 1:71:A:LEU:H    | 8        | 0.73          |
| (3,21)   | 1:31:A:LEU:H     | 1:21:A:LEU:HD11 | 14       | 0.73          |
| (1,4247) | 1:54:A:GLN:HE22  | 1:57:A:VAL:HG11 | 1        | 0.73          |
| (1,4247) | 1:54:A:GLN:HE22  | 1:57:A:VAL:HG11 | 2        | 0.73          |
| (1,4229) | 1:122:A:ALA:HB2  | 1:124:A:VAL:H   | 3        | 0.73          |
| (1,4229) | 1:122:A:ALA:HB3  | 1:124:A:VAL:H   | 5        | 0.73          |
| (1,4229) | 1:122:A:ALA:HB3  | 1:124:A:VAL:H   | 14       | 0.73          |
| (1,4168) | 1:48:A:LEU:H     | 1:48:A:LEU:HD12 | 2        | 0.73          |
| (1,4168) | 1:48:A:LEU:H     | 1:48:A:LEU:HD12 | 3        | 0.73          |
| (1,4122) | 1:116:A:GLN:HE21 | 1:113:A:ALA:HA  | 13       | 0.73          |
| (1,4118) | 1:71:A:LEU:H     | 1:70:A:GLN:HE21 | 7        | 0.73          |
| (1,4080) | 1:54:A:GLN:HE22  | 1:57:A:VAL:HG23 | 5        | 0.73          |
| (1,4080) | 1:54:A:GLN:HE22  | 1:57:A:VAL:HG22 | 10       | 0.73          |
| (1,4080) | 1:54:A:GLN:HE22  | 1:57:A:VAL:HG22 | 13       | 0.73          |
| (1,3892) | 1:45:A:ALA:HB2   | 1:81:A:SER:H    | 11       | 0.73          |
| (1,3397) | 1:75:A:LEU:HA    | 1:31:A:LEU:HD13 | 14       | 0.73          |
| (1,3377) | 1:40:A:SER:HB2   | 1:41:A:ALA:HB2  | 2        | 0.73          |
| (1,3377) | 1:40:A:SER:HB2   | 1:41:A:ALA:HB1  | 14       | 0.73          |
| (1,3352) | 1:79:A:THR:HG21  | 1:48:A:LEU:HD13 | 2        | 0.73          |
| (1,3248) | 1:88:A:VAL:HG23  | 1:92:A:ALA:HB1  | 2        | 0.73          |
| (1,3023) | 1:64:A:MET:HE1   | 1:27:A:VAL:HA   | 5        | 0.73          |
| (1,2902) | 1:50:A:ILE:HD13  | 1:76:A:ARG:H    | 9        | 0.73          |
| (1,2832) | 1:97:A:LEU:HD21  | 1:97:A:LEU:H    | 14       | 0.73          |
| (1,2820) | 1:97:A:LEU:HD13  | 1:52:A:ILE:H    | 10       | 0.73          |
| (1,2820) | 1:97:A:LEU:HD13  | 1:52:A:ILE:H    | 17       | 0.73          |
| (1,2673) | 1:97:A:LEU:HD12  | 1:35:A:PHE:HD1  | 8        | 0.73          |
| (1,2363) | 1:48:A:LEU:HD13  | 1:84:A:TYR:HE2  | 16       | 0.73          |
| (1,2337) | 1:66:A:LEU:HD13  | 1:31:A:LEU:HD13 | 8        | 0.73          |
| (1,2326) | 1:31:A:LEU:HD13  | 1:27:A:VAL:HG13 | 16       | 0.73          |
| (1,2192) | 1:55:A:ASP:HB2   | 1:52:A:ILE:HD13 | 16       | 0.73          |
| (1,2188) | 1:124:A:VAL:HG12 | 1:124:A:VAL:H   | 1        | 0.73          |
| (1,2188) | 1:124:A:VAL:HG12 | 1:124:A:VAL:H   | 4        | 0.73          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2188) | 1:124:A:VAL:HG13 | 1:124:A:VAL:H   | 13       | 0.73          |
| (1,2188) | 1:124:A:VAL:HG11 | 1:124:A:VAL:H   | 14       | 0.73          |
| (1,2188) | 1:124:A:VAL:HG11 | 1:124:A:VAL:H   | 15       | 0.73          |
| (1,2188) | 1:124:A:VAL:HG11 | 1:124:A:VAL:H   | 16       | 0.73          |
| (1,2142) | 1:21:A:LEU:HD11  | 1:30:A:PHE:HA   | 11       | 0.73          |
| (1,2026) | 1:57:A:VAL:HG11  | 1:53:A:PHE:HD1  | 3        | 0.73          |
| (1,1990) | 1:92:A:ALA:HB1   | 1:91:A:GLY:H    | 9        | 0.73          |
| (1,1800) | 1:75:A:LEU:HA    | 1:31:A:LEU:HD11 | 11       | 0.73          |
| (1,1676) | 1:94:A:ARG:HD2   | 1:92:A:ALA:HB3  | 8        | 0.73          |
| (1,1675) | 1:88:A:VAL:HG23  | 1:92:A:ALA:HB1  | 15       | 0.73          |
| (1,1503) | 1:52:A:ILE:HG12  | 1:54:A:GLN:HE21 | 2        | 0.73          |
| (1,1502) | 1:52:A:ILE:HG13  | 1:54:A:GLN:HE21 | 8        | 0.73          |
| (1,1158) | 1:120:A:ALA:HB2  | 1:82:A:TRP:HD1  | 14       | 0.73          |
| (1,805)  | 1:57:A:VAL:HG13  | 1:53:A:PHE:HD1  | 7        | 0.73          |
| (1,805)  | 1:57:A:VAL:HG12  | 1:53:A:PHE:HD1  | 10       | 0.73          |
| (1,559)  | 1:116:A:GLN:HE21 | 1:113:A:ALA:HA  | 11       | 0.73          |
| (3,146)  | 1:52:A:ILE:H     | 1:52:A:ILE:HD12 | 6        | 0.72          |
| (3,113)  | 1:61:A:ALA:HB3   | 1:60:A:VAL:HB   | 5        | 0.72          |
| (3,107)  | 1:95:A:VAL:HG22  | 1:102:A:CYS:HB3 | 16       | 0.72          |
| (3,86)   | 1:84:A:TYR:HE1   | 1:47:A:PRO:HB3  | 6        | 0.72          |
| (3,86)   | 1:84:A:TYR:HE1   | 1:47:A:PRO:HB3  | 11       | 0.72          |
| (3,65)   | 1:52:A:ILE:HG13  | 1:52:A:ILE:HG22 | 8        | 0.72          |
| (3,65)   | 1:52:A:ILE:HG13  | 1:52:A:ILE:HG22 | 13       | 0.72          |
| (3,52)   | 1:95:A:VAL:HG23  | 1:37:A:HIS:HB2  | 5        | 0.72          |
| (3,27)   | 1:71:A:LEU:HD12  | 1:71:A:LEU:H    | 4        | 0.72          |
| (3,27)   | 1:71:A:LEU:HD13  | 1:71:A:LEU:H    | 17       | 0.72          |
| (3,11)   | 1:93:A:THR:HB    | 1:104:A:GLU:HG2 | 7        | 0.72          |
| (1,4229) | 1:122:A:ALA:HB1  | 1:124:A:VAL:H   | 8        | 0.72          |
| (1,4229) | 1:122:A:ALA:HB2  | 1:124:A:VAL:H   | 11       | 0.72          |
| (1,4229) | 1:122:A:ALA:HB1  | 1:124:A:VAL:H   | 12       | 0.72          |
| (1,4229) | 1:122:A:ALA:HB3  | 1:124:A:VAL:H   | 15       | 0.72          |
| (1,4168) | 1:48:A:LEU:H     | 1:48:A:LEU:HD13 | 13       | 0.72          |
| (1,4080) | 1:54:A:GLN:HE22  | 1:57:A:VAL:HG21 | 12       | 0.72          |
| (1,3826) | 1:102:A:CYS:H    | 1:95:A:VAL:HG11 | 7        | 0.72          |
| (1,3509) | 1:64:A:MET:HE3   | 1:65:A:ASN:HD22 | 11       | 0.72          |
| (1,3397) | 1:75:A:LEU:HA    | 1:31:A:LEU:HD11 | 2        | 0.72          |
| (1,3397) | 1:75:A:LEU:HA    | 1:31:A:LEU:HD13 | 3        | 0.72          |
| (1,3376) | 1:41:A:ALA:HB3   | 1:40:A:SER:HB3  | 7        | 0.72          |
| (1,3376) | 1:41:A:ALA:HB1   | 1:40:A:SER:HB3  | 13       | 0.72          |
| (1,3088) | 1:56:A:LEU:HB2   | 1:35:A:PHE:HE2  | 14       | 0.72          |
| (1,2903) | 1:50:A:ILE:HD11  | 1:51:A:GLY:H    | 1        | 0.72          |
| (1,2902) | 1:50:A:ILE:HD11  | 1:76:A:ARG:H    | 4        | 0.72          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2902) | 1:50:A:ILE:HD13  | 1:76:A:ARG:H    | 15       | 0.72          |
| (1,2894) | 1:52:A:ILE:HD11  | 1:53:A:PHE:HB2  | 14       | 0.72          |
| (1,2832) | 1:97:A:LEU:HD23  | 1:97:A:LEU:H    | 1        | 0.72          |
| (1,2820) | 1:97:A:LEU:HD11  | 1:52:A:ILE:H    | 12       | 0.72          |
| (1,2664) | 1:97:A:LEU:HD13  | 1:60:A:VAL:HG12 | 3        | 0.72          |
| (1,2602) | 1:21:A:LEU:HD11  | 1:21:A:LEU:H    | 12       | 0.72          |
| (1,2580) | 1:56:A:LEU:HB2   | 1:60:A:VAL:HG12 | 2        | 0.72          |
| (1,2580) | 1:56:A:LEU:HB2   | 1:60:A:VAL:HG13 | 9        | 0.72          |
| (1,2580) | 1:56:A:LEU:HB2   | 1:60:A:VAL:HG12 | 15       | 0.72          |
| (1,2580) | 1:56:A:LEU:HB2   | 1:60:A:VAL:HG13 | 17       | 0.72          |
| (1,2384) | 1:57:A:VAL:HG12  | 1:53:A:PHE:HD2  | 5        | 0.72          |
| (1,2384) | 1:57:A:VAL:HG11  | 1:53:A:PHE:HD1  | 6        | 0.72          |
| (1,2363) | 1:48:A:LEU:HD13  | 1:84:A:TYR:HE2  | 7        | 0.72          |
| (1,2363) | 1:48:A:LEU:HD13  | 1:84:A:TYR:HE2  | 15       | 0.72          |
| (1,2337) | 1:66:A:LEU:HD13  | 1:31:A:LEU:HD11 | 7        | 0.72          |
| (1,2337) | 1:66:A:LEU:HD11  | 1:31:A:LEU:HD11 | 12       | 0.72          |
| (1,2334) | 1:60:A:VAL:HG12  | 1:63:A:GLU:HG3  | 10       | 0.72          |
| (1,2157) | 1:99:A:GLY:HA3   | 1:95:A:VAL:HG21 | 16       | 0.72          |
| (1,2028) | 1:97:A:LEU:HD21  | 1:97:A:LEU:H    | 5        | 0.72          |
| (1,2026) | 1:57:A:VAL:HG11  | 1:53:A:PHE:HD2  | 9        | 0.72          |
| (1,1990) | 1:92:A:ALA:HB1   | 1:91:A:GLY:H    | 17       | 0.72          |
| (1,1882) | 1:64:A:MET:HE3   | 1:65:A:ASN:HD22 | 1        | 0.72          |
| (1,1800) | 1:75:A:LEU:HA    | 1:31:A:LEU:HD12 | 16       | 0.72          |
| (1,1800) | 1:75:A:LEU:HA    | 1:31:A:LEU:HD12 | 17       | 0.72          |
| (1,1676) | 1:94:A:ARG:HD2   | 1:92:A:ALA:HB3  | 12       | 0.72          |
| (1,1676) | 1:94:A:ARG:HD2   | 1:92:A:ALA:HB2  | 16       | 0.72          |
| (1,1503) | 1:52:A:ILE:HG12  | 1:54:A:GLN:HE21 | 14       | 0.72          |
| (1,1482) | 1:64:A:MET:HE1   | 1:27:A:VAL:HA   | 2        | 0.72          |
| (1,1309) | 1:97:A:LEU:HD21  | 1:97:A:LEU:H    | 5        | 0.72          |
| (1,1125) | 1:97:A:LEU:HD11  | 1:60:A:VAL:HG13 | 6        | 0.72          |
| (1,1050) | 1:56:A:LEU:HB2   | 1:60:A:VAL:HG11 | 7        | 0.72          |
| (1,1050) | 1:56:A:LEU:HB2   | 1:60:A:VAL:HG11 | 11       | 0.72          |
| (1,805)  | 1:57:A:VAL:HG13  | 1:53:A:PHE:HD2  | 14       | 0.72          |
| (1,576)  | 1:50:A:ILE:HD11  | 1:50:A:ILE:H    | 2        | 0.72          |
| (1,559)  | 1:116:A:GLN:HE21 | 1:113:A:ALA:HA  | 4        | 0.72          |
| (1,222)  | 1:102:A:CYS:H    | 1:95:A:VAL:HG11 | 13       | 0.72          |
| (3,153)  | 1:110:A:VAL:HG21 | 1:114:A:ARG:H   | 11       | 0.71          |
| (3,150)  | 1:77:A:LEU:H     | 1:79:A:THR:HG21 | 7        | 0.71          |
| (3,120)  | 1:49:A:LYS:HB2   | 1:52:A:ILE:HD12 | 5        | 0.71          |
| (3,107)  | 1:95:A:VAL:HG23  | 1:102:A:CYS:HB3 | 2        | 0.71          |
| (3,76)   | 1:116:A:GLN:HE21 | 1:85:A:LEU:HD12 | 13       | 0.71          |
| (3,59)   | 1:117:A:LEU:HA   | 1:85:A:LEU:HD22 | 9        | 0.71          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (3,30)   | 1:64:A:MET:HE3   | 1:34:A:ARG:HB3  | 2        | 0.71          |
| (3,27)   | 1:71:A:LEU:HD12  | 1:71:A:LEU:H    | 9        | 0.71          |
| (3,21)   | 1:22:A:ASN:H     | 1:21:A:LEU:HD12 | 6        | 0.71          |
| (1,4229) | 1:122:A:ALA:HB1  | 1:124:A:VAL:H   | 4        | 0.71          |
| (1,4229) | 1:122:A:ALA:HB1  | 1:124:A:VAL:H   | 9        | 0.71          |
| (1,4168) | 1:48:A:LEU:H     | 1:48:A:LEU:HD12 | 10       | 0.71          |
| (1,4124) | 1:116:A:GLN:HE21 | 1:120:A:ALA:H   | 14       | 0.71          |
| (1,4080) | 1:54:A:GLN:HE22  | 1:57:A:VAL:HG21 | 14       | 0.71          |
| (1,3987) | 1:50:A:ILE:HG21  | 1:50:A:ILE:H    | 2        | 0.71          |
| (1,3987) | 1:50:A:ILE:HG22  | 1:50:A:ILE:H    | 17       | 0.71          |
| (1,3397) | 1:75:A:LEU:HA    | 1:31:A:LEU:HD12 | 8        | 0.71          |
| (1,3397) | 1:75:A:LEU:HA    | 1:31:A:LEU:HD13 | 13       | 0.71          |
| (1,3249) | 1:94:A:ARG:HD2   | 1:92:A:ALA:HB1  | 3        | 0.71          |
| (1,3249) | 1:94:A:ARG:HD2   | 1:92:A:ALA:HB1  | 7        | 0.71          |
| (1,3249) | 1:94:A:ARG:HD2   | 1:92:A:ALA:HB2  | 13       | 0.71          |
| (1,3023) | 1:64:A:MET:HE2   | 1:27:A:VAL:HA   | 1        | 0.71          |
| (1,2902) | 1:50:A:ILE:HD11  | 1:76:A:ARG:H    | 17       | 0.71          |
| (1,2894) | 1:52:A:ILE:HD11  | 1:53:A:PHE:HB2  | 7        | 0.71          |
| (1,2673) | 1:97:A:LEU:HD11  | 1:35:A:PHE:HD2  | 11       | 0.71          |
| (1,2580) | 1:56:A:LEU:HB2   | 1:60:A:VAL:HG13 | 4        | 0.71          |
| (1,2580) | 1:56:A:LEU:HB2   | 1:60:A:VAL:HG13 | 13       | 0.71          |
| (1,2397) | 1:50:A:ILE:HD11  | 1:50:A:ILE:HA   | 5        | 0.71          |
| (1,2384) | 1:57:A:VAL:HG11  | 1:53:A:PHE:HD1  | 2        | 0.71          |
| (1,2363) | 1:48:A:LEU:HD13  | 1:84:A:TYR:HE1  | 14       | 0.71          |
| (1,2338) | 1:61:A:ALA:HB3   | 1:66:A:LEU:HD13 | 14       | 0.71          |
| (1,2337) | 1:66:A:LEU:HD12  | 1:31:A:LEU:HD12 | 15       | 0.71          |
| (1,2326) | 1:31:A:LEU:HD12  | 1:27:A:VAL:HG11 | 2        | 0.71          |
| (1,2206) | 1:57:A:VAL:HG21  | 1:57:A:VAL:HA   | 7        | 0.71          |
| (1,2206) | 1:57:A:VAL:HG22  | 1:57:A:VAL:HA   | 10       | 0.71          |
| (1,2206) | 1:57:A:VAL:HG21  | 1:57:A:VAL:HA   | 17       | 0.71          |
| (1,2188) | 1:124:A:VAL:HG11 | 1:124:A:VAL:H   | 11       | 0.71          |
| (1,2142) | 1:21:A:LEU:HD12  | 1:30:A:PHE:HA   | 16       | 0.71          |
| (1,2026) | 1:57:A:VAL:HG11  | 1:53:A:PHE:HD2  | 1        | 0.71          |
| (1,2026) | 1:57:A:VAL:HG11  | 1:53:A:PHE:HD1  | 4        | 0.71          |
| (1,2026) | 1:57:A:VAL:HG12  | 1:53:A:PHE:HD2  | 8        | 0.71          |
| (1,1800) | 1:75:A:LEU:HA    | 1:31:A:LEU:HD13 | 12       | 0.71          |
| (1,1758) | 1:79:A:THR:HG21  | 1:48:A:LEU:HD11 | 4        | 0.71          |
| (1,1502) | 1:52:A:ILE:HG13  | 1:54:A:GLN:HE21 | 1        | 0.71          |
| (1,1502) | 1:52:A:ILE:HG13  | 1:54:A:GLN:HE21 | 11       | 0.71          |
| (1,1158) | 1:120:A:ALA:HB2  | 1:82:A:TRP:HD1  | 6        | 0.71          |
| (1,1157) | 1:117:A:LEU:HD12 | 1:82:A:TRP:HD1  | 8        | 0.71          |
| (1,1137) | 1:97:A:LEU:HD13  | 1:35:A:PHE:HD1  | 13       | 0.71          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1069) | 1:48:A:LEU:HD13  | 1:52:A:ILE:HG12 | 17       | 0.71          |
| (1,815)  | 1:50:A:ILE:HD13  | 1:50:A:ILE:HA   | 7        | 0.71          |
| (1,805)  | 1:57:A:VAL:HG11  | 1:53:A:PHE:HD2  | 16       | 0.71          |
| (1,556)  | 1:71:A:LEU:H     | 1:70:A:GLN:HE21 | 15       | 0.71          |
| (1,554)  | 1:70:A:GLN:HA    | 1:70:A:GLN:HE21 | 8        | 0.71          |
| (1,488)  | 1:21:A:LEU:HD13  | 1:23:A:SER:H    | 4        | 0.71          |
| (3,146)  | 1:52:A:ILE:H     | 1:52:A:ILE:HD11 | 7        | 0.7           |
| (3,146)  | 1:52:A:ILE:H     | 1:52:A:ILE:HD12 | 14       | 0.7           |
| (3,116)  | 1:95:A:VAL:H     | 1:48:A:LEU:HD12 | 3        | 0.7           |
| (3,62)   | 1:52:A:ILE:HG23  | 1:56:A:LEU:H    | 1        | 0.7           |
| (3,59)   | 1:117:A:LEU:HA   | 1:85:A:LEU:HD21 | 3        | 0.7           |
| (3,59)   | 1:117:A:LEU:HA   | 1:85:A:LEU:HD21 | 15       | 0.7           |
| (3,55)   | 1:57:A:VAL:HG11  | 1:75:A:LEU:HD13 | 2        | 0.7           |
| (3,55)   | 1:97:A:LEU:HD23  | 1:75:A:LEU:HD11 | 5        | 0.7           |
| (3,55)   | 1:97:A:LEU:HD22  | 1:75:A:LEU:HD13 | 16       | 0.7           |
| (3,51)   | 1:95:A:VAL:HG21  | 1:49:A:LYS:HA   | 4        | 0.7           |
| (3,27)   | 1:71:A:LEU:HD13  | 1:71:A:LEU:H    | 5        | 0.7           |
| (3,11)   | 1:93:A:THR:HB    | 1:104:A:GLU:HG2 | 10       | 0.7           |
| (3,11)   | 1:93:A:THR:HB    | 1:104:A:GLU:HG2 | 17       | 0.7           |
| (1,4229) | 1:122:A:ALA:HB2  | 1:124:A:VAL:H   | 1        | 0.7           |
| (1,4229) | 1:122:A:ALA:HB3  | 1:124:A:VAL:H   | 6        | 0.7           |
| (1,4229) | 1:122:A:ALA:HB2  | 1:124:A:VAL:H   | 7        | 0.7           |
| (1,4229) | 1:122:A:ALA:HB3  | 1:124:A:VAL:H   | 10       | 0.7           |
| (1,4132) | 1:60:A:VAL:HG13  | 1:34:A:ARG:HE   | 1        | 0.7           |
| (1,4122) | 1:116:A:GLN:HE21 | 1:113:A:ALA:HA  | 6        | 0.7           |
| (1,4091) | 1:65:A:ASN:HD22  | 1:20:A:LYS:HA   | 17       | 0.7           |
| (1,4082) | 1:22:A:ASN:HD21  | 1:22:A:ASN:HB3  | 7        | 0.7           |
| (1,4080) | 1:54:A:GLN:HE22  | 1:57:A:VAL:HG21 | 8        | 0.7           |
| (1,4080) | 1:54:A:GLN:HE22  | 1:57:A:VAL:HG22 | 17       | 0.7           |
| (1,3987) | 1:50:A:ILE:HG22  | 1:50:A:ILE:H    | 4        | 0.7           |
| (1,3870) | 1:85:A:LEU:HD21  | 1:87:A:GLY:H    | 3        | 0.7           |
| (1,3845) | 1:95:A:VAL:HG11  | 1:96:A:ASP:H    | 11       | 0.7           |
| (1,3397) | 1:75:A:LEU:HA    | 1:31:A:LEU:HD13 | 7        | 0.7           |
| (1,3377) | 1:40:A:SER:HB2   | 1:41:A:ALA:HB3  | 5        | 0.7           |
| (1,3377) | 1:40:A:SER:HB2   | 1:41:A:ALA:HB2  | 9        | 0.7           |
| (1,3376) | 1:41:A:ALA:HB1   | 1:40:A:SER:HB3  | 8        | 0.7           |
| (1,3249) | 1:94:A:ARG:HD2   | 1:92:A:ALA:HB1  | 2        | 0.7           |
| (1,3249) | 1:94:A:ARG:HD2   | 1:92:A:ALA:HB3  | 10       | 0.7           |
| (1,3045) | 1:52:A:ILE:HG13  | 1:54:A:GLN:HE21 | 10       | 0.7           |
| (1,3023) | 1:64:A:MET:HE3   | 1:27:A:VAL:HA   | 15       | 0.7           |
| (1,2926) | 1:21:A:LEU:HB2   | 1:21:A:LEU:HD22 | 1        | 0.7           |
| (1,2894) | 1:52:A:ILE:HD11  | 1:53:A:PHE:HB2  | 15       | 0.7           |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2664) | 1:97:A:LEU:HD12 | 1:60:A:VAL:HG11  | 8        | 0.7           |
| (1,2664) | 1:97:A:LEU:HD12 | 1:60:A:VAL:HG11  | 9        | 0.7           |
| (1,2582) | 1:60:A:VAL:HG12 | 1:57:A:VAL:HG13  | 5        | 0.7           |
| (1,2580) | 1:56:A:LEU:HB2  | 1:60:A:VAL:HG11  | 10       | 0.7           |
| (1,2397) | 1:50:A:ILE:HD13 | 1:50:A:ILE:HA    | 1        | 0.7           |
| (1,2397) | 1:50:A:ILE:HD12 | 1:50:A:ILE:HA    | 3        | 0.7           |
| (1,2384) | 1:57:A:VAL:HG12 | 1:53:A:PHE:HD1   | 11       | 0.7           |
| (1,2363) | 1:48:A:LEU:HD11 | 1:84:A:TYR:HE1   | 10       | 0.7           |
| (1,2338) | 1:61:A:ALA:HB3  | 1:66:A:LEU:HD11  | 9        | 0.7           |
| (1,2334) | 1:60:A:VAL:HG11 | 1:63:A:GLU:HG3   | 13       | 0.7           |
| (1,2308) | 1:82:A:TRP:HB2  | 1:117:A:LEU:HD12 | 7        | 0.7           |
| (1,2206) | 1:57:A:VAL:HG22 | 1:57:A:VAL:HA    | 13       | 0.7           |
| (1,2094) | 1:95:A:VAL:HG21 | 1:97:A:LEU:HD23  | 16       | 0.7           |
| (1,1676) | 1:94:A:ARG:HD2  | 1:92:A:ALA:HB3   | 6        | 0.7           |
| (1,1502) | 1:52:A:ILE:HG13 | 1:54:A:GLN:HE21  | 17       | 0.7           |
| (1,1482) | 1:64:A:MET:HE2  | 1:27:A:VAL:HA    | 8        | 0.7           |
| (1,1137) | 1:97:A:LEU:HD13 | 1:35:A:PHE:HD2   | 1        | 0.7           |
| (1,1125) | 1:97:A:LEU:HD13 | 1:60:A:VAL:HG13  | 15       | 0.7           |
| (1,1050) | 1:56:A:LEU:HB2  | 1:60:A:VAL:HG13  | 12       | 0.7           |
| (1,815)  | 1:50:A:ILE:HD13 | 1:50:A:ILE:HA    | 14       | 0.7           |
| (1,805)  | 1:57:A:VAL:HG12 | 1:53:A:PHE:HD1   | 12       | 0.7           |
| (1,554)  | 1:70:A:GLN:HA   | 1:70:A:GLN:HE21  | 1        | 0.7           |
| (1,524)  | 1:20:A:LYS:HB3  | 1:22:A:ASN:HD22  | 6        | 0.7           |
| (1,522)  | 1:54:A:GLN:HE22 | 1:57:A:VAL:HG22  | 7        | 0.7           |
| (1,222)  | 1:102:A:CYS:H   | 1:95:A:VAL:HG13  | 10       | 0.7           |
| (3,150)  | 1:77:A:LEU:H    | 1:79:A:THR:HG22  | 8        | 0.69          |
| (3,113)  | 1:61:A:ALA:HB2  | 1:60:A:VAL:HB    | 2        | 0.69          |
| (3,113)  | 1:61:A:ALA:HB3  | 1:60:A:VAL:HB    | 13       | 0.69          |
| (3,98)   | 1:64:A:MET:HE3  | 1:63:A:GLU:HG3   | 2        | 0.69          |
| (3,98)   | 1:64:A:MET:HE2  | 1:63:A:GLU:HG3   | 6        | 0.69          |
| (3,86)   | 1:84:A:TYR:HE2  | 1:47:A:PRO:HB3   | 16       | 0.69          |
| (3,59)   | 1:117:A:LEU:HA  | 1:85:A:LEU:HD23  | 12       | 0.69          |
| (3,55)   | 1:97:A:LEU:HD21 | 1:75:A:LEU:HD13  | 4        | 0.69          |
| (3,40)   | 1:55:A:ASP:H    | 1:52:A:ILE:HD12  | 8        | 0.69          |
| (3,40)   | 1:55:A:ASP:H    | 1:52:A:ILE:HD11  | 10       | 0.69          |
| (3,27)   | 1:71:A:LEU:HD11 | 1:71:A:LEU:H     | 11       | 0.69          |
| (3,21)   | 1:31:A:LEU:H    | 1:21:A:LEU:HD12  | 1        | 0.69          |
| (3,21)   | 1:31:A:LEU:H    | 1:21:A:LEU:HD13  | 2        | 0.69          |
| (3,21)   | 1:22:A:ASN:H    | 1:21:A:LEU:HD13  | 4        | 0.69          |
| (3,11)   | 1:93:A:THR:HB   | 1:104:A:GLU:HG2  | 2        | 0.69          |
| (3,11)   | 1:93:A:THR:HB   | 1:104:A:GLU:HG2  | 3        | 0.69          |
| (3,11)   | 1:93:A:THR:HB   | 1:104:A:GLU:HG2  | 8        | 0.69          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (3,8)    | 1:57:A:VAL:HB    | 1:54:A:GLN:HA    | 2        | 0.69          |
| (1,4229) | 1:122:A:ALA:HB2  | 1:124:A:VAL:H    | 13       | 0.69          |
| (1,4168) | 1:48:A:LEU:H     | 1:48:A:LEU:HD11  | 7        | 0.69          |
| (1,4168) | 1:48:A:LEU:H     | 1:48:A:LEU:HD12  | 17       | 0.69          |
| (1,4080) | 1:54:A:GLN:HE22  | 1:57:A:VAL:HG21  | 15       | 0.69          |
| (1,3892) | 1:45:A:ALA:HB1   | 1:81:A:SER:H     | 2        | 0.69          |
| (1,3870) | 1:85:A:LEU:HD23  | 1:87:A:GLY:H     | 9        | 0.69          |
| (1,3826) | 1:102:A:CYS:H    | 1:95:A:VAL:HG12  | 8        | 0.69          |
| (1,3377) | 1:40:A:SER:HB2   | 1:41:A:ALA:HB3   | 12       | 0.69          |
| (1,3249) | 1:94:A:ARG:HD2   | 1:92:A:ALA:HB2   | 9        | 0.69          |
| (1,3249) | 1:94:A:ARG:HD2   | 1:92:A:ALA:HB1   | 14       | 0.69          |
| (1,3248) | 1:88:A:VAL:HG23  | 1:92:A:ALA:HB1   | 15       | 0.69          |
| (1,2894) | 1:52:A:ILE:HD11  | 1:53:A:PHE:HB2   | 5        | 0.69          |
| (1,2864) | 1:78:A:TYR:HE1   | 1:78:A:TYR:HB3   | 11       | 0.69          |
| (1,2610) | 1:105:A:LEU:HD12 | 1:105:A:LEU:HA   | 6        | 0.69          |
| (1,2610) | 1:105:A:LEU:HD12 | 1:105:A:LEU:HA   | 12       | 0.69          |
| (1,2608) | 1:48:A:LEU:HD13  | 1:52:A:ILE:HG12  | 4        | 0.69          |
| (1,2600) | 1:105:A:LEU:HA   | 1:105:A:LEU:HD23 | 11       | 0.69          |
| (1,2582) | 1:60:A:VAL:HG11  | 1:57:A:VAL:HG12  | 3        | 0.69          |
| (1,2580) | 1:56:A:LEU:HB2   | 1:60:A:VAL:HG11  | 7        | 0.69          |
| (1,2580) | 1:56:A:LEU:HB2   | 1:60:A:VAL:HG11  | 11       | 0.69          |
| (1,2384) | 1:57:A:VAL:HG13  | 1:53:A:PHE:HD1   | 7        | 0.69          |
| (1,2384) | 1:57:A:VAL:HG12  | 1:53:A:PHE:HD1   | 10       | 0.69          |
| (1,2363) | 1:48:A:LEU:HD11  | 1:84:A:TYR:HE1   | 5        | 0.69          |
| (1,2338) | 1:61:A:ALA:HB2   | 1:66:A:LEU:HD12  | 10       | 0.69          |
| (1,2338) | 1:61:A:ALA:HB1   | 1:66:A:LEU:HD13  | 16       | 0.69          |
| (1,2334) | 1:60:A:VAL:HG12  | 1:63:A:GLU:HG3   | 7        | 0.69          |
| (1,2324) | 1:97:A:LEU:HD21  | 1:39:A:PHE:H     | 7        | 0.69          |
| (1,2308) | 1:82:A:TRP:HB2   | 1:117:A:LEU:HD13 | 17       | 0.69          |
| (1,2305) | 1:45:A:ALA:HB2   | 1:44:A:GLU:HA    | 11       | 0.69          |
| (1,2190) | 1:61:A:ALA:HB2   | 1:62:A:GLY:HA2   | 11       | 0.69          |
| (1,2142) | 1:21:A:LEU:HD12  | 1:30:A:PHE:HA    | 17       | 0.69          |
| (1,2026) | 1:57:A:VAL:HG12  | 1:53:A:PHE:HD2   | 5        | 0.69          |
| (1,2026) | 1:57:A:VAL:HG11  | 1:53:A:PHE:HD1   | 6        | 0.69          |
| (1,1990) | 1:92:A:ALA:HB2   | 1:91:A:GLY:H     | 12       | 0.69          |
| (1,1851) | 1:35:A:PHE:HE2   | 1:38:A:CYS:HB2   | 4        | 0.69          |
| (1,1361) | 1:41:A:ALA:HA    | 1:32:A:ALA:HB2   | 11       | 0.69          |
| (1,1342) | 1:48:A:LEU:HD13  | 1:84:A:TYR:HE1   | 12       | 0.69          |
| (1,1125) | 1:97:A:LEU:HD13  | 1:60:A:VAL:HG11  | 4        | 0.69          |
| (1,522)  | 1:54:A:GLN:HE22  | 1:57:A:VAL:HG23  | 5        | 0.69          |
| (1,522)  | 1:54:A:GLN:HE22  | 1:57:A:VAL:HG22  | 10       | 0.69          |
| (1,522)  | 1:54:A:GLN:HE22  | 1:57:A:VAL:HG22  | 13       | 0.69          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (3,113)  | 1:61:A:ALA:HB1   | 1:60:A:VAL:HB    | 1        | 0.68          |
| (3,113)  | 1:61:A:ALA:HB3   | 1:60:A:VAL:HB    | 3        | 0.68          |
| (3,113)  | 1:61:A:ALA:HB1   | 1:60:A:VAL:HB    | 8        | 0.68          |
| (3,86)   | 1:84:A:TYR:HE2   | 1:47:A:PRO:HB3   | 15       | 0.68          |
| (3,62)   | 1:52:A:ILE:HG23  | 1:56:A:LEU:H     | 4        | 0.68          |
| (3,62)   | 1:52:A:ILE:HG21  | 1:56:A:LEU:H     | 9        | 0.68          |
| (3,40)   | 1:55:A:ASP:H     | 1:52:A:ILE:HD11  | 14       | 0.68          |
| (3,11)   | 1:93:A:THR:HB    | 1:104:A:GLU:HG2  | 13       | 0.68          |
| (1,4229) | 1:122:A:ALA:HB2  | 1:124:A:VAL:H    | 16       | 0.68          |
| (1,4124) | 1:116:A:GLN:HE21 | 1:120:A:ALA:H    | 8        | 0.68          |
| (1,4124) | 1:116:A:GLN:HE21 | 1:120:A:ALA:H    | 13       | 0.68          |
| (1,4120) | 1:116:A:GLN:HE21 | 1:119:A:GLU:HB2  | 5        | 0.68          |
| (1,4084) | 1:20:A:LYS:HB3   | 1:22:A:ASN:HD22  | 14       | 0.68          |
| (1,3987) | 1:50:A:ILE:HG22  | 1:50:A:ILE:H     | 8        | 0.68          |
| (1,3870) | 1:85:A:LEU:HD23  | 1:87:A:GLY:H     | 12       | 0.68          |
| (1,3541) | 1:64:A:MET:HB2   | 1:21:A:LEU:HD21  | 10       | 0.68          |
| (1,3509) | 1:64:A:MET:HE1   | 1:65:A:ASN:HD22  | 15       | 0.68          |
| (1,3397) | 1:75:A:LEU:HA    | 1:31:A:LEU:HD11  | 5        | 0.68          |
| (1,3397) | 1:75:A:LEU:HA    | 1:31:A:LEU:HD11  | 11       | 0.68          |
| (1,3377) | 1:40:A:SER:HB2   | 1:41:A:ALA:HB3   | 3        | 0.68          |
| (1,3377) | 1:40:A:SER:HB2   | 1:41:A:ALA:HB2   | 10       | 0.68          |
| (1,3376) | 1:41:A:ALA:HB1   | 1:40:A:SER:HB3   | 16       | 0.68          |
| (1,3249) | 1:94:A:ARG:HD2   | 1:92:A:ALA:HB3   | 8        | 0.68          |
| (1,3060) | 1:52:A:ILE:HG22  | 1:97:A:LEU:HD23  | 7        | 0.68          |
| (1,3046) | 1:52:A:ILE:HG12  | 1:54:A:GLN:HE21  | 2        | 0.68          |
| (1,3045) | 1:52:A:ILE:HG13  | 1:54:A:GLN:HE21  | 12       | 0.68          |
| (1,2864) | 1:78:A:TYR:HE2   | 1:78:A:TYR:HB3   | 2        | 0.68          |
| (1,2864) | 1:78:A:TYR:HE2   | 1:78:A:TYR:HB3   | 4        | 0.68          |
| (1,2832) | 1:97:A:LEU:HD21  | 1:97:A:LEU:H     | 5        | 0.68          |
| (1,2600) | 1:105:A:LEU:HA   | 1:105:A:LEU:HD23 | 2        | 0.68          |
| (1,2384) | 1:57:A:VAL:HG13  | 1:53:A:PHE:HD2   | 14       | 0.68          |
| (1,2384) | 1:57:A:VAL:HG11  | 1:53:A:PHE:HD2   | 16       | 0.68          |
| (1,2363) | 1:48:A:LEU:HD13  | 1:84:A:TYR:HE1   | 9        | 0.68          |
| (1,2338) | 1:61:A:ALA:HB2   | 1:66:A:LEU:HD12  | 12       | 0.68          |
| (1,2337) | 1:66:A:LEU:HD11  | 1:31:A:LEU:HD12  | 2        | 0.68          |
| (1,2337) | 1:66:A:LEU:HD11  | 1:31:A:LEU:HD12  | 5        | 0.68          |
| (1,2334) | 1:60:A:VAL:HG11  | 1:63:A:GLU:HG3   | 9        | 0.68          |
| (1,2324) | 1:97:A:LEU:HD21  | 1:39:A:PHE:H     | 14       | 0.68          |
| (1,2206) | 1:57:A:VAL:HG22  | 1:57:A:VAL:HA    | 3        | 0.68          |
| (1,2206) | 1:57:A:VAL:HG22  | 1:57:A:VAL:HA    | 5        | 0.68          |
| (1,2206) | 1:57:A:VAL:HG23  | 1:57:A:VAL:HA    | 8        | 0.68          |
| (1,2206) | 1:57:A:VAL:HG23  | 1:57:A:VAL:HA    | 12       | 0.68          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2142) | 1:21:A:LEU:HD13  | 1:30:A:PHE:HA   | 12       | 0.68          |
| (1,2026) | 1:57:A:VAL:HG11  | 1:53:A:PHE:HD1  | 2        | 0.68          |
| (1,1990) | 1:92:A:ALA:HB2   | 1:91:A:GLY:H    | 4        | 0.68          |
| (1,1800) | 1:75:A:LEU:HA    | 1:31:A:LEU:HD13 | 6        | 0.68          |
| (1,1800) | 1:75:A:LEU:HA    | 1:31:A:LEU:HD11 | 15       | 0.68          |
| (1,1502) | 1:52:A:ILE:HG13  | 1:54:A:GLN:HE21 | 3        | 0.68          |
| (1,1482) | 1:64:A:MET:HE3   | 1:27:A:VAL:HA   | 13       | 0.68          |
| (1,1125) | 1:97:A:LEU:HD13  | 1:60:A:VAL:HG12 | 1        | 0.68          |
| (1,559)  | 1:116:A:GLN:HE21 | 1:113:A:ALA:HA  | 13       | 0.68          |
| (1,556)  | 1:71:A:LEU:H     | 1:70:A:GLN:HE21 | 7        | 0.68          |
| (1,556)  | 1:71:A:LEU:H     | 1:70:A:GLN:HE21 | 11       | 0.68          |
| (1,522)  | 1:54:A:GLN:HE22  | 1:57:A:VAL:HG21 | 12       | 0.68          |
| (1,303)  | 1:45:A:ALA:HB2   | 1:81:A:SER:H    | 11       | 0.68          |
| (3,153)  | 1:110:A:VAL:HG23 | 1:114:A:ARG:H   | 5        | 0.67          |
| (3,116)  | 1:95:A:VAL:H     | 1:48:A:LEU:HD12 | 1        | 0.67          |
| (3,113)  | 1:61:A:ALA:HB3   | 1:60:A:VAL:HB   | 14       | 0.67          |
| (3,105)  | 1:64:A:MET:H     | 1:66:A:LEU:HD23 | 9        | 0.67          |
| (3,76)   | 1:116:A:GLN:HE21 | 1:85:A:LEU:HD13 | 1        | 0.67          |
| (3,76)   | 1:116:A:GLN:HE21 | 1:85:A:LEU:HD12 | 8        | 0.67          |
| (3,62)   | 1:52:A:ILE:HG21  | 1:56:A:LEU:H    | 3        | 0.67          |
| (3,59)   | 1:117:A:LEU:HA   | 1:85:A:LEU:HD21 | 7        | 0.67          |
| (3,55)   | 1:97:A:LEU:HD23  | 1:75:A:LEU:HD12 | 6        | 0.67          |
| (1,4124) | 1:116:A:GLN:HE21 | 1:120:A:ALA:H   | 6        | 0.67          |
| (1,4122) | 1:116:A:GLN:HE21 | 1:113:A:ALA:HA  | 8        | 0.67          |
| (1,4091) | 1:65:A:ASN:HD22  | 1:20:A:LYS:HA   | 3        | 0.67          |
| (1,4082) | 1:22:A:ASN:HD21  | 1:22:A:ASN:HB3  | 13       | 0.67          |
| (1,4082) | 1:22:A:ASN:HD21  | 1:22:A:ASN:HB3  | 17       | 0.67          |
| (1,4080) | 1:54:A:GLN:HE22  | 1:57:A:VAL:HG21 | 6        | 0.67          |
| (1,4045) | 1:21:A:LEU:HD12  | 1:23:A:SER:H    | 9        | 0.67          |
| (1,3870) | 1:85:A:LEU:HD21  | 1:87:A:GLY:H    | 7        | 0.67          |
| (1,3826) | 1:102:A:CYS:H    | 1:95:A:VAL:HG13 | 9        | 0.67          |
| (1,3826) | 1:102:A:CYS:H    | 1:95:A:VAL:HG13 | 14       | 0.67          |
| (1,3826) | 1:102:A:CYS:H    | 1:95:A:VAL:HG12 | 17       | 0.67          |
| (1,3397) | 1:75:A:LEU:HA    | 1:31:A:LEU:HD12 | 16       | 0.67          |
| (1,3397) | 1:75:A:LEU:HA    | 1:31:A:LEU:HD12 | 17       | 0.67          |
| (1,3281) | 1:93:A:THR:HG23  | 1:104:A:GLU:HG2 | 8        | 0.67          |
| (1,3249) | 1:94:A:ARG:HD2   | 1:92:A:ALA:HB3  | 12       | 0.67          |
| (1,3249) | 1:94:A:ARG:HD2   | 1:92:A:ALA:HB2  | 16       | 0.67          |
| (1,3046) | 1:52:A:ILE:HG12  | 1:54:A:GLN:HE21 | 14       | 0.67          |
| (1,3045) | 1:52:A:ILE:HG13  | 1:54:A:GLN:HE21 | 8        | 0.67          |
| (1,2894) | 1:52:A:ILE:HD11  | 1:53:A:PHE:HB2  | 6        | 0.67          |
| (1,2681) | 1:120:A:ALA:HB2  | 1:82:A:TRP:HD1  | 14       | 0.67          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2669) | 1:75:A:LEU:HD21  | 1:78:A:TYR:HE2  | 1        | 0.67          |
| (1,2669) | 1:75:A:LEU:HD22  | 1:78:A:TYR:HE1  | 11       | 0.67          |
| (1,2664) | 1:97:A:LEU:HD11  | 1:60:A:VAL:HG13 | 6        | 0.67          |
| (1,2610) | 1:105:A:LEU:HD12 | 1:105:A:LEU:HA  | 2        | 0.67          |
| (1,2610) | 1:105:A:LEU:HD11 | 1:105:A:LEU:HA  | 15       | 0.67          |
| (1,2610) | 1:105:A:LEU:HD11 | 1:105:A:LEU:HA  | 16       | 0.67          |
| (1,2610) | 1:105:A:LEU:HD13 | 1:105:A:LEU:HA  | 17       | 0.67          |
| (1,2608) | 1:48:A:LEU:HD13  | 1:52:A:ILE:HG12 | 17       | 0.67          |
| (1,2580) | 1:56:A:LEU:HB2   | 1:60:A:VAL:HG13 | 12       | 0.67          |
| (1,2397) | 1:50:A:ILE:HD13  | 1:50:A:ILE:HA   | 7        | 0.67          |
| (1,2337) | 1:66:A:LEU:HD12  | 1:31:A:LEU:HD13 | 16       | 0.67          |
| (1,2334) | 1:60:A:VAL:HG11  | 1:63:A:GLU:HG3  | 4        | 0.67          |
| (1,2324) | 1:97:A:LEU:HD22  | 1:39:A:PHE:H    | 13       | 0.67          |
| (1,2206) | 1:57:A:VAL:HG21  | 1:57:A:VAL:HA   | 1        | 0.67          |
| (1,2206) | 1:57:A:VAL:HG22  | 1:57:A:VAL:HA   | 4        | 0.67          |
| (1,2206) | 1:57:A:VAL:HG23  | 1:57:A:VAL:HA   | 6        | 0.67          |
| (1,2206) | 1:57:A:VAL:HG23  | 1:57:A:VAL:HA   | 15       | 0.67          |
| (1,2206) | 1:57:A:VAL:HG23  | 1:57:A:VAL:HA   | 16       | 0.67          |
| (1,2192) | 1:55:A:ASP:HB2   | 1:52:A:ILE:HD12 | 8        | 0.67          |
| (1,2190) | 1:61:A:ALA:HB1   | 1:62:A:GLY:HA2  | 5        | 0.67          |
| (1,2178) | 1:48:A:LEU:HB2   | 1:52:A:ILE:HG21 | 5        | 0.67          |
| (1,2142) | 1:21:A:LEU:HD13  | 1:30:A:PHE:HA   | 10       | 0.67          |
| (1,2026) | 1:57:A:VAL:HG12  | 1:53:A:PHE:HD1  | 11       | 0.67          |
| (1,1990) | 1:92:A:ALA:HB3   | 1:91:A:GLY:H    | 7        | 0.67          |
| (1,1882) | 1:64:A:MET:HE1   | 1:65:A:ASN:HD22 | 6        | 0.67          |
| (1,1800) | 1:75:A:LEU:HA    | 1:31:A:LEU:HD13 | 4        | 0.67          |
| (1,1361) | 1:41:A:ALA:HA    | 1:32:A:ALA:HB1  | 6        | 0.67          |
| (1,1356) | 1:61:A:ALA:HB1   | 1:57:A:VAL:HG12 | 1        | 0.67          |
| (1,1342) | 1:48:A:LEU:HD13  | 1:84:A:TYR:HE1  | 6        | 0.67          |
| (1,1137) | 1:97:A:LEU:HD13  | 1:35:A:PHE:HD2  | 5        | 0.67          |
| (1,1065) | 1:21:A:LEU:HD12  | 1:21:A:LEU:H    | 8        | 0.67          |
| (1,1050) | 1:56:A:LEU:HB2   | 1:60:A:VAL:HG11 | 1        | 0.67          |
| (1,815)  | 1:50:A:ILE:HD11  | 1:50:A:ILE:HA   | 10       | 0.67          |
| (1,522)  | 1:54:A:GLN:HE22  | 1:57:A:VAL:HG21 | 14       | 0.67          |
| (1,423)  | 1:50:A:ILE:HG21  | 1:50:A:ILE:H    | 2        | 0.67          |
| (1,423)  | 1:50:A:ILE:HG22  | 1:50:A:ILE:H    | 17       | 0.67          |
| (1,222)  | 1:102:A:CYS:H    | 1:95:A:VAL:HG11 | 7        | 0.67          |
| (3,153)  | 1:110:A:VAL:HG21 | 1:114:A:ARG:H   | 15       | 0.66          |
| (3,150)  | 1:77:A:LEU:H     | 1:79:A:THR:HG22 | 2        | 0.66          |
| (3,146)  | 1:52:A:ILE:H     | 1:52:A:ILE:HD12 | 5        | 0.66          |
| (3,136)  | 1:82:A:TRP:HD1   | 1:82:A:TRP:H    | 6        | 0.66          |
| (3,113)  | 1:61:A:ALA:HB1   | 1:60:A:VAL:HB   | 11       | 0.66          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (3,76)   | 1:116:A:GLN:HE21 | 1:85:A:LEU:HD13  | 10       | 0.66          |
| (3,76)   | 1:116:A:GLN:HE21 | 1:85:A:LEU:HD11  | 16       | 0.66          |
| (3,59)   | 1:117:A:LEU:HA   | 1:85:A:LEU:HD21  | 17       | 0.66          |
| (3,40)   | 1:55:A:ASP:H     | 1:52:A:ILE:HD11  | 17       | 0.66          |
| (3,21)   | 1:31:A:LEU:H     | 1:21:A:LEU:HD13  | 5        | 0.66          |
| (3,11)   | 1:93:A:THR:HB    | 1:104:A:GLU:HG2  | 4        | 0.66          |
| (3,8)    | 1:57:A:VAL:HB    | 1:54:A:GLN:HA    | 4        | 0.66          |
| (1,4168) | 1:48:A:LEU:H     | 1:48:A:LEU:HD11  | 14       | 0.66          |
| (1,4124) | 1:116:A:GLN:HE21 | 1:120:A:ALA:H    | 4        | 0.66          |
| (1,4084) | 1:20:A:LYS:HB3   | 1:22:A:ASN:HD22  | 16       | 0.66          |
| (1,4082) | 1:22:A:ASN:HD21  | 1:22:A:ASN:HB3   | 4        | 0.66          |
| (1,4080) | 1:54:A:GLN:HE22  | 1:57:A:VAL:HG21  | 16       | 0.66          |
| (1,3870) | 1:85:A:LEU:HD23  | 1:87:A:GLY:H     | 11       | 0.66          |
| (1,3826) | 1:102:A:CYS:H    | 1:95:A:VAL:HG12  | 6        | 0.66          |
| (1,3826) | 1:102:A:CYS:H    | 1:95:A:VAL:HG13  | 12       | 0.66          |
| (1,3509) | 1:64:A:MET:HE3   | 1:65:A:ASN:HD22  | 1        | 0.66          |
| (1,3377) | 1:40:A:SER:HB2   | 1:41:A:ALA:HB1   | 4        | 0.66          |
| (1,3377) | 1:40:A:SER:HB2   | 1:41:A:ALA:HB2   | 6        | 0.66          |
| (1,3376) | 1:41:A:ALA:HB1   | 1:40:A:SER:HB3   | 1        | 0.66          |
| (1,3362) | 1:56:A:LEU:HD21  | 1:56:A:LEU:HA    | 8        | 0.66          |
| (1,3352) | 1:79:A:THR:HG21  | 1:48:A:LEU:HD11  | 4        | 0.66          |
| (1,3302) | 1:83:A:ARG:HB2   | 1:86:A:TYR:HD2   | 4        | 0.66          |
| (1,3281) | 1:93:A:THR:HG23  | 1:104:A:GLU:HG2  | 2        | 0.66          |
| (1,3281) | 1:93:A:THR:HG21  | 1:104:A:GLU:HG2  | 10       | 0.66          |
| (1,3281) | 1:93:A:THR:HG23  | 1:104:A:GLU:HG2  | 13       | 0.66          |
| (1,3281) | 1:93:A:THR:HG21  | 1:104:A:GLU:HG2  | 17       | 0.66          |
| (1,3045) | 1:52:A:ILE:HG13  | 1:54:A:GLN:HE21  | 1        | 0.66          |
| (1,3023) | 1:64:A:MET:HE1   | 1:27:A:VAL:HA    | 2        | 0.66          |
| (1,2926) | 1:21:A:LEU:HB2   | 1:21:A:LEU:HD22  | 15       | 0.66          |
| (1,2926) | 1:21:A:LEU:HB2   | 1:21:A:LEU:HD21  | 16       | 0.66          |
| (1,2894) | 1:52:A:ILE:HD13  | 1:53:A:PHE:HB2   | 4        | 0.66          |
| (1,2845) | 1:22:A:ASN:H     | 1:27:A:VAL:HG11  | 6        | 0.66          |
| (1,2680) | 1:117:A:LEU:HD12 | 1:82:A:TRP:HD1   | 8        | 0.66          |
| (1,2673) | 1:97:A:LEU:HD13  | 1:35:A:PHE:HD1   | 13       | 0.66          |
| (1,2664) | 1:97:A:LEU:HD13  | 1:60:A:VAL:HG13  | 15       | 0.66          |
| (1,2610) | 1:105:A:LEU:HD12 | 1:105:A:LEU:HA   | 1        | 0.66          |
| (1,2610) | 1:105:A:LEU:HD13 | 1:105:A:LEU:HA   | 3        | 0.66          |
| (1,2610) | 1:105:A:LEU:HD12 | 1:105:A:LEU:HA   | 7        | 0.66          |
| (1,2610) | 1:105:A:LEU:HD11 | 1:105:A:LEU:HA   | 9        | 0.66          |
| (1,2610) | 1:105:A:LEU:HD11 | 1:105:A:LEU:HA   | 14       | 0.66          |
| (1,2600) | 1:105:A:LEU:HA   | 1:105:A:LEU:HD22 | 5        | 0.66          |
| (1,2582) | 1:60:A:VAL:HG11  | 1:57:A:VAL:HG13  | 11       | 0.66          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2397) | 1:50:A:ILE:HD13  | 1:50:A:ILE:HA    | 14       | 0.66          |
| (1,2384) | 1:57:A:VAL:HG12  | 1:53:A:PHE:HD1   | 12       | 0.66          |
| (1,2338) | 1:61:A:ALA:HB3   | 1:66:A:LEU:HD12  | 2        | 0.66          |
| (1,2338) | 1:61:A:ALA:HB1   | 1:66:A:LEU:HD11  | 7        | 0.66          |
| (1,2338) | 1:61:A:ALA:HB2   | 1:66:A:LEU:HD11  | 8        | 0.66          |
| (1,2337) | 1:66:A:LEU:HD12  | 1:31:A:LEU:HD12  | 11       | 0.66          |
| (1,2324) | 1:97:A:LEU:HD21  | 1:39:A:PHE:H     | 2        | 0.66          |
| (1,2324) | 1:97:A:LEU:HD21  | 1:39:A:PHE:H     | 12       | 0.66          |
| (1,2206) | 1:57:A:VAL:HG23  | 1:57:A:VAL:HA    | 2        | 0.66          |
| (1,2206) | 1:57:A:VAL:HG22  | 1:57:A:VAL:HA    | 9        | 0.66          |
| (1,2206) | 1:57:A:VAL:HG22  | 1:57:A:VAL:HA    | 11       | 0.66          |
| (1,2206) | 1:57:A:VAL:HG23  | 1:57:A:VAL:HA    | 14       | 0.66          |
| (1,2178) | 1:48:A:LEU:HB2   | 1:52:A:ILE:HG23  | 14       | 0.66          |
| (1,2142) | 1:21:A:LEU:HD11  | 1:30:A:PHE:HA    | 14       | 0.66          |
| (1,2094) | 1:95:A:VAL:HG21  | 1:97:A:LEU:HD21  | 7        | 0.66          |
| (1,2026) | 1:57:A:VAL:HG13  | 1:53:A:PHE:HD1   | 7        | 0.66          |
| (1,2026) | 1:57:A:VAL:HG12  | 1:53:A:PHE:HD1   | 10       | 0.66          |
| (1,1990) | 1:92:A:ALA:HB3   | 1:91:A:GLY:H     | 3        | 0.66          |
| (1,1851) | 1:35:A:PHE:HE2   | 1:38:A:CYS:HB2   | 9        | 0.66          |
| (1,1800) | 1:75:A:LEU:HA    | 1:31:A:LEU:HD11  | 9        | 0.66          |
| (1,1635) | 1:121:A:LYS:HB2  | 1:117:A:LEU:HD11 | 1        | 0.66          |
| (1,1482) | 1:64:A:MET:HE3   | 1:27:A:VAL:HA    | 6        | 0.66          |
| (1,1420) | 1:97:A:LEU:HD23  | 1:56:A:LEU:HD23  | 2        | 0.66          |
| (1,1420) | 1:97:A:LEU:HD23  | 1:56:A:LEU:HD21  | 12       | 0.66          |
| (1,1420) | 1:97:A:LEU:HD23  | 1:56:A:LEU:HD22  | 15       | 0.66          |
| (1,1361) | 1:41:A:ALA:HA    | 1:32:A:ALA:HB3   | 2        | 0.66          |
| (1,1343) | 1:78:A:TYR:HE1   | 1:48:A:LEU:HD11  | 3        | 0.66          |
| (1,1301) | 1:97:A:LEU:HD13  | 1:97:A:LEU:HA    | 8        | 0.66          |
| (1,815)  | 1:50:A:ILE:HD13  | 1:50:A:ILE:HA    | 13       | 0.66          |
| (1,576)  | 1:50:A:ILE:HD12  | 1:50:A:ILE:H     | 8        | 0.66          |
| (1,561)  | 1:116:A:GLN:HE21 | 1:120:A:ALA:H    | 14       | 0.66          |
| (1,522)  | 1:54:A:GLN:HE22  | 1:57:A:VAL:HG21  | 8        | 0.66          |
| (1,522)  | 1:54:A:GLN:HE22  | 1:57:A:VAL:HG22  | 17       | 0.66          |
| (1,423)  | 1:50:A:ILE:HG22  | 1:50:A:ILE:H     | 4        | 0.66          |
| (1,241)  | 1:95:A:VAL:HG11  | 1:96:A:ASP:H     | 11       | 0.66          |
| (3,153)  | 1:110:A:VAL:HG23 | 1:114:A:ARG:H    | 1        | 0.65          |
| (3,153)  | 1:110:A:VAL:HG23 | 1:114:A:ARG:H    | 4        | 0.65          |
| (3,113)  | 1:61:A:ALA:HB1   | 1:60:A:VAL:HB    | 6        | 0.65          |
| (3,105)  | 1:64:A:MET:H     | 1:66:A:LEU:HD21  | 14       | 0.65          |
| (3,102)  | 1:65:A:ASN:HB2   | 1:64:A:MET:HG2   | 3        | 0.65          |
| (3,102)  | 1:65:A:ASN:HB2   | 1:64:A:MET:HG2   | 14       | 0.65          |
| (3,98)   | 1:64:A:MET:HE1   | 1:63:A:GLU:HG3   | 8        | 0.65          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (3,76)   | 1:116:A:GLN:HE21 | 1:85:A:LEU:HD12  | 5        | 0.65          |
| (3,76)   | 1:116:A:GLN:HE21 | 1:85:A:LEU:HD11  | 14       | 0.65          |
| (3,65)   | 1:52:A:ILE:HG13  | 1:52:A:ILE:HG22  | 12       | 0.65          |
| (3,62)   | 1:52:A:ILE:HG21  | 1:56:A:LEU:H     | 2        | 0.65          |
| (3,55)   | 1:97:A:LEU:HD21  | 1:75:A:LEU:HD13  | 13       | 0.65          |
| (3,55)   | 1:97:A:LEU:HD23  | 1:75:A:LEU:HD13  | 15       | 0.65          |
| (3,21)   | 1:22:A:ASN:H     | 1:21:A:LEU:HD12  | 11       | 0.65          |
| (3,21)   | 1:31:A:LEU:H     | 1:21:A:LEU:HD13  | 15       | 0.65          |
| (3,11)   | 1:93:A:THR:HB    | 1:104:A:GLU:HG2  | 12       | 0.65          |
| (3,8)    | 1:57:A:VAL:HB    | 1:54:A:GLN:HA    | 1        | 0.65          |
| (3,8)    | 1:57:A:VAL:HB    | 1:54:A:GLN:HA    | 16       | 0.65          |
| (1,4168) | 1:48:A:LEU:H     | 1:48:A:LEU:HD13  | 8        | 0.65          |
| (1,4124) | 1:116:A:GLN:HE21 | 1:120:A:ALA:H    | 16       | 0.65          |
| (1,4116) | 1:70:A:GLN:HA    | 1:70:A:GLN:HE21  | 14       | 0.65          |
| (1,4084) | 1:20:A:LYS:HB3   | 1:22:A:ASN:HD22  | 4        | 0.65          |
| (1,3826) | 1:102:A:CYS:H    | 1:95:A:VAL:HG12  | 2        | 0.65          |
| (1,3826) | 1:102:A:CYS:H    | 1:95:A:VAL:HG12  | 3        | 0.65          |
| (1,3541) | 1:64:A:MET:HB2   | 1:21:A:LEU:HD23  | 12       | 0.65          |
| (1,3397) | 1:75:A:LEU:HA    | 1:31:A:LEU:HD13  | 12       | 0.65          |
| (1,3377) | 1:40:A:SER:HB2   | 1:41:A:ALA:HB2   | 1        | 0.65          |
| (1,3362) | 1:56:A:LEU:HD21  | 1:56:A:LEU:HA    | 12       | 0.65          |
| (1,3281) | 1:93:A:THR:HG23  | 1:104:A:GLU:HG2  | 7        | 0.65          |
| (1,3249) | 1:94:A:ARG:HD2   | 1:92:A:ALA:HB3   | 6        | 0.65          |
| (1,3060) | 1:52:A:ILE:HG22  | 1:97:A:LEU:HD23  | 17       | 0.65          |
| (1,3045) | 1:52:A:ILE:HG13  | 1:54:A:GLN:HE21  | 11       | 0.65          |
| (1,3045) | 1:52:A:ILE:HG13  | 1:54:A:GLN:HE21  | 17       | 0.65          |
| (1,2954) | 1:71:A:LEU:HB2   | 1:75:A:LEU:HD12  | 17       | 0.65          |
| (1,2926) | 1:21:A:LEU:HB2   | 1:21:A:LEU:HD22  | 8        | 0.65          |
| (1,2902) | 1:50:A:ILE:HD12  | 1:76:A:ARG:H     | 11       | 0.65          |
| (1,2894) | 1:52:A:ILE:HD13  | 1:53:A:PHE:HB2   | 8        | 0.65          |
| (1,2681) | 1:120:A:ALA:HB2  | 1:82:A:TRP:HD1   | 6        | 0.65          |
| (1,2673) | 1:97:A:LEU:HD13  | 1:35:A:PHE:HD2   | 1        | 0.65          |
| (1,2610) | 1:105:A:LEU:HD13 | 1:105:A:LEU:HA   | 4        | 0.65          |
| (1,2610) | 1:105:A:LEU:HD11 | 1:105:A:LEU:HA   | 8        | 0.65          |
| (1,2600) | 1:105:A:LEU:HA   | 1:105:A:LEU:HD22 | 13       | 0.65          |
| (1,2400) | 1:28:A:ILE:HB    | 1:28:A:ILE:HD13  | 6        | 0.65          |
| (1,2400) | 1:28:A:ILE:HB    | 1:28:A:ILE:HD11  | 8        | 0.65          |
| (1,2338) | 1:61:A:ALA:HB2   | 1:66:A:LEU:HD11  | 1        | 0.65          |
| (1,2338) | 1:61:A:ALA:HB3   | 1:66:A:LEU:HD12  | 4        | 0.65          |
| (1,2324) | 1:97:A:LEU:HD21  | 1:39:A:PHE:H     | 5        | 0.65          |
| (1,2324) | 1:97:A:LEU:HD22  | 1:39:A:PHE:H     | 9        | 0.65          |
| (1,2324) | 1:97:A:LEU:HD21  | 1:39:A:PHE:H     | 10       | 0.65          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2324) | 1:97:A:LEU:HD23  | 1:39:A:PHE:H     | 16       | 0.65          |
| (1,2324) | 1:97:A:LEU:HD21  | 1:39:A:PHE:H     | 17       | 0.65          |
| (1,2190) | 1:61:A:ALA:HB1   | 1:62:A:GLY:HA2   | 3        | 0.65          |
| (1,2179) | 1:52:A:ILE:HG22  | 1:48:A:LEU:HB3   | 14       | 0.65          |
| (1,2142) | 1:21:A:LEU:HD12  | 1:30:A:PHE:HA    | 3        | 0.65          |
| (1,2026) | 1:57:A:VAL:HG13  | 1:53:A:PHE:HD2   | 14       | 0.65          |
| (1,2026) | 1:57:A:VAL:HG11  | 1:53:A:PHE:HD2   | 16       | 0.65          |
| (1,1839) | 1:95:A:VAL:HA    | 1:93:A:THR:HG22  | 13       | 0.65          |
| (1,1751) | 1:32:A:ALA:HB3   | 1:41:A:ALA:H     | 17       | 0.65          |
| (1,1682) | 1:41:A:ALA:HB2   | 1:33:A:GLU:H     | 8        | 0.65          |
| (1,1635) | 1:121:A:LYS:HB2  | 1:117:A:LEU:HD13 | 14       | 0.65          |
| (1,1601) | 1:75:A:LEU:HD21  | 1:31:A:LEU:HD12  | 6        | 0.65          |
| (1,1361) | 1:41:A:ALA:HA    | 1:32:A:ALA:HB2   | 10       | 0.65          |
| (1,1361) | 1:41:A:ALA:HA    | 1:32:A:ALA:HB1   | 16       | 0.65          |
| (1,1360) | 1:32:A:ALA:HB3   | 1:31:A:LEU:H     | 2        | 0.65          |
| (1,1342) | 1:48:A:LEU:HD11  | 1:84:A:TYR:HE2   | 1        | 0.65          |
| (1,1301) | 1:97:A:LEU:HD13  | 1:97:A:LEU:HA    | 12       | 0.65          |
| (1,1157) | 1:117:A:LEU:HD12 | 1:82:A:TRP:HD1   | 4        | 0.65          |
| (1,1157) | 1:117:A:LEU:HD12 | 1:82:A:TRP:HD1   | 13       | 0.65          |
| (1,1125) | 1:97:A:LEU:HD13  | 1:60:A:VAL:HG13  | 5        | 0.65          |
| (1,815)  | 1:50:A:ILE:HD12  | 1:50:A:ILE:HA    | 6        | 0.65          |
| (1,815)  | 1:50:A:ILE:HD11  | 1:50:A:ILE:HA    | 9        | 0.65          |
| (1,815)  | 1:50:A:ILE:HD13  | 1:50:A:ILE:HA    | 11       | 0.65          |
| (1,805)  | 1:57:A:VAL:HG13  | 1:53:A:PHE:HD1   | 17       | 0.65          |
| (1,559)  | 1:116:A:GLN:HE21 | 1:113:A:ALA:HA   | 6        | 0.65          |
| (1,522)  | 1:54:A:GLN:HE22  | 1:57:A:VAL:HG21  | 15       | 0.65          |
| (1,275)  | 1:85:A:LEU:HD21  | 1:87:A:GLY:H     | 3        | 0.65          |
| (1,275)  | 1:85:A:LEU:HD23  | 1:87:A:GLY:H     | 9        | 0.65          |
| (3,153)  | 1:110:A:VAL:HG21 | 1:114:A:ARG:H    | 2        | 0.64          |
| (3,153)  | 1:110:A:VAL:HG23 | 1:114:A:ARG:H    | 3        | 0.64          |
| (3,153)  | 1:110:A:VAL:HG21 | 1:114:A:ARG:H    | 13       | 0.64          |
| (3,153)  | 1:110:A:VAL:HG23 | 1:114:A:ARG:H    | 16       | 0.64          |
| (3,117)  | 1:48:A:LEU:HD23  | 1:39:A:PHE:HD1   | 9        | 0.64          |
| (3,113)  | 1:61:A:ALA:HB1   | 1:60:A:VAL:HB    | 15       | 0.64          |
| (3,86)   | 1:84:A:TYR:HE1   | 1:47:A:PRO:HB3   | 9        | 0.64          |
| (3,78)   | 1:77:A:LEU:HD23  | 1:77:A:LEU:H     | 4        | 0.64          |
| (3,55)   | 1:97:A:LEU:HD22  | 1:75:A:LEU:HD12  | 1        | 0.64          |
| (3,55)   | 1:97:A:LEU:HD23  | 1:75:A:LEU:HD11  | 12       | 0.64          |
| (3,51)   | 1:95:A:VAL:HG22  | 1:49:A:LYS:HA    | 14       | 0.64          |
| (3,40)   | 1:55:A:ASP:H     | 1:52:A:ILE:HD13  | 15       | 0.64          |
| (3,18)   | 1:58:A:ASP:HB3   | 1:60:A:VAL:HG13  | 16       | 0.64          |
| (3,11)   | 1:93:A:THR:HB    | 1:104:A:GLU:HG2  | 9        | 0.64          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (3,11)   | 1:93:A:THR:HB    | 1:104:A:GLU:HG2  | 15       | 0.64          |
| (3,11)   | 1:93:A:THR:HB    | 1:104:A:GLU:HG2  | 16       | 0.64          |
| (3,8)    | 1:57:A:VAL:HB    | 1:54:A:GLN:HA    | 9        | 0.64          |
| (3,8)    | 1:57:A:VAL:HB    | 1:54:A:GLN:HA    | 13       | 0.64          |
| (1,4283) | 1:120:A:ALA:H    | 1:85:A:LEU:HD23  | 5        | 0.64          |
| (1,4124) | 1:116:A:GLN:HE21 | 1:120:A:ALA:H    | 1        | 0.64          |
| (1,4124) | 1:116:A:GLN:HE21 | 1:120:A:ALA:H    | 5        | 0.64          |
| (1,4122) | 1:116:A:GLN:HE21 | 1:113:A:ALA:HA   | 9        | 0.64          |
| (1,3947) | 1:71:A:LEU:HD12  | 1:61:A:ALA:H     | 12       | 0.64          |
| (1,3870) | 1:85:A:LEU:HD21  | 1:87:A:GLY:H     | 6        | 0.64          |
| (1,3870) | 1:85:A:LEU:HD22  | 1:87:A:GLY:H     | 17       | 0.64          |
| (1,3826) | 1:102:A:CYS:H    | 1:95:A:VAL:HG12  | 5        | 0.64          |
| (1,3362) | 1:56:A:LEU:HD23  | 1:56:A:LEU:HA    | 10       | 0.64          |
| (1,3362) | 1:56:A:LEU:HD21  | 1:56:A:LEU:HA    | 15       | 0.64          |
| (1,3302) | 1:83:A:ARG:HB2   | 1:86:A:TYR:HD2   | 1        | 0.64          |
| (1,3281) | 1:93:A:THR:HG22  | 1:104:A:GLU:HG2  | 4        | 0.64          |
| (1,3281) | 1:93:A:THR:HG23  | 1:104:A:GLU:HG2  | 12       | 0.64          |
| (1,3023) | 1:64:A:MET:HE2   | 1:27:A:VAL:HA    | 8        | 0.64          |
| (1,2926) | 1:21:A:LEU:HB2   | 1:21:A:LEU:HD21  | 12       | 0.64          |
| (1,2886) | 1:41:A:ALA:HA    | 1:32:A:ALA:HB2   | 11       | 0.64          |
| (1,2664) | 1:97:A:LEU:HD13  | 1:60:A:VAL:HG12  | 1        | 0.64          |
| (1,2664) | 1:97:A:LEU:HD13  | 1:60:A:VAL:HG11  | 4        | 0.64          |
| (1,2610) | 1:105:A:LEU:HD12 | 1:105:A:LEU:HA   | 5        | 0.64          |
| (1,2610) | 1:105:A:LEU:HD11 | 1:105:A:LEU:HA   | 13       | 0.64          |
| (1,2600) | 1:105:A:LEU:HA   | 1:105:A:LEU:HD22 | 3        | 0.64          |
| (1,2600) | 1:105:A:LEU:HA   | 1:105:A:LEU:HD22 | 7        | 0.64          |
| (1,2600) | 1:105:A:LEU:HA   | 1:105:A:LEU:HD23 | 10       | 0.64          |
| (1,2585) | 1:92:A:ALA:HA    | 1:93:A:THR:HG22  | 7        | 0.64          |
| (1,2582) | 1:60:A:VAL:HG13  | 1:57:A:VAL:HG13  | 8        | 0.64          |
| (1,2580) | 1:56:A:LEU:HB2   | 1:60:A:VAL:HG11  | 1        | 0.64          |
| (1,2400) | 1:28:A:ILE:HB    | 1:28:A:ILE:HD12  | 12       | 0.64          |
| (1,2400) | 1:28:A:ILE:HB    | 1:28:A:ILE:HD11  | 17       | 0.64          |
| (1,2324) | 1:97:A:LEU:HD21  | 1:39:A:PHE:H     | 15       | 0.64          |
| (1,2308) | 1:82:A:TRP:HB2   | 1:117:A:LEU:HD11 | 3        | 0.64          |
| (1,2308) | 1:82:A:TRP:HB2   | 1:117:A:LEU:HD11 | 12       | 0.64          |
| (1,2308) | 1:82:A:TRP:HB2   | 1:117:A:LEU:HD12 | 15       | 0.64          |
| (1,2192) | 1:55:A:ASP:HB2   | 1:52:A:ILE:HD11  | 10       | 0.64          |
| (1,2192) | 1:55:A:ASP:HB2   | 1:52:A:ILE:HD13  | 15       | 0.64          |
| (1,2179) | 1:52:A:ILE:HG23  | 1:48:A:LEU:HB3   | 5        | 0.64          |
| (1,2178) | 1:48:A:LEU:HB2   | 1:52:A:ILE:HG22  | 6        | 0.64          |
| (1,1990) | 1:92:A:ALA:HB2   | 1:91:A:GLY:H     | 8        | 0.64          |
| (1,1990) | 1:92:A:ALA:HB1   | 1:91:A:GLY:H     | 13       | 0.64          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1990) | 1:92:A:ALA:HB1   | 1:91:A:GLY:H    | 16       | 0.64          |
| (1,1839) | 1:95:A:VAL:HA    | 1:93:A:THR:HG22 | 15       | 0.64          |
| (1,1502) | 1:52:A:ILE:HG13  | 1:54:A:GLN:HE21 | 4        | 0.64          |
| (1,1502) | 1:52:A:ILE:HG13  | 1:54:A:GLN:HE21 | 9        | 0.64          |
| (1,1502) | 1:52:A:ILE:HG13  | 1:54:A:GLN:HE21 | 15       | 0.64          |
| (1,1450) | 1:54:A:GLN:HE22  | 1:54:A:GLN:HG2  | 3        | 0.64          |
| (1,1420) | 1:97:A:LEU:HD23  | 1:56:A:LEU:HD22 | 14       | 0.64          |
| (1,1361) | 1:41:A:ALA:HA    | 1:32:A:ALA:HB1  | 4        | 0.64          |
| (1,1361) | 1:41:A:ALA:HA    | 1:32:A:ALA:HB3  | 5        | 0.64          |
| (1,1361) | 1:41:A:ALA:HA    | 1:32:A:ALA:HB3  | 7        | 0.64          |
| (1,1361) | 1:41:A:ALA:HA    | 1:32:A:ALA:HB1  | 8        | 0.64          |
| (1,1360) | 1:32:A:ALA:HB2   | 1:31:A:LEU:H    | 12       | 0.64          |
| (1,1342) | 1:48:A:LEU:HD13  | 1:84:A:TYR:HE1  | 8        | 0.64          |
| (1,1308) | 1:97:A:LEU:HD23  | 1:35:A:PHE:HD2  | 11       | 0.64          |
| (1,1301) | 1:97:A:LEU:HD12  | 1:97:A:LEU:HA   | 6        | 0.64          |
| (1,1301) | 1:97:A:LEU:HD12  | 1:97:A:LEU:HA   | 10       | 0.64          |
| (1,570)  | 1:60:A:VAL:HG13  | 1:34:A:ARG:HE   | 1        | 0.64          |
| (1,423)  | 1:50:A:ILE:HG22  | 1:50:A:ILE:H    | 8        | 0.64          |
| (1,303)  | 1:45:A:ALA:HB1   | 1:81:A:SER:H    | 2        | 0.64          |
| (1,275)  | 1:85:A:LEU:HD23  | 1:87:A:GLY:H    | 12       | 0.64          |
| (1,222)  | 1:102:A:CYS:H    | 1:95:A:VAL:HG12 | 8        | 0.64          |
| (3,153)  | 1:110:A:VAL:HG23 | 1:114:A:ARG:H   | 17       | 0.63          |
| (3,136)  | 1:82:A:TRP:HD1   | 1:82:A:TRP:H    | 14       | 0.63          |
| (3,136)  | 1:81:A:SER:H     | 1:82:A:TRP:H    | 17       | 0.63          |
| (3,126)  | 1:21:A:LEU:HD22  | 1:22:A:ASN:H    | 1        | 0.63          |
| (3,113)  | 1:61:A:ALA:HB2   | 1:60:A:VAL:HB   | 4        | 0.63          |
| (3,78)   | 1:77:A:LEU:HD21  | 1:77:A:LEU:H    | 8        | 0.63          |
| (3,62)   | 1:52:A:ILE:HG22  | 1:56:A:LEU:H    | 11       | 0.63          |
| (3,55)   | 1:97:A:LEU:HD23  | 1:75:A:LEU:HD12 | 3        | 0.63          |
| (3,52)   | 1:95:A:VAL:HG23  | 1:37:A:HIS:HB2  | 9        | 0.63          |
| (3,40)   | 1:55:A:ASP:H     | 1:52:A:ILE:HD11 | 5        | 0.63          |
| (3,40)   | 1:55:A:ASP:H     | 1:52:A:ILE:HD13 | 12       | 0.63          |
| (3,21)   | 1:31:A:LEU:H     | 1:21:A:LEU:HD13 | 10       | 0.63          |
| (3,11)   | 1:93:A:THR:HB    | 1:104:A:GLU:HG2 | 1        | 0.63          |
| (3,8)    | 1:57:A:VAL:HB    | 1:54:A:GLN:HA   | 3        | 0.63          |
| (3,8)    | 1:57:A:VAL:HB    | 1:54:A:GLN:HA   | 14       | 0.63          |
| (1,4259) | 1:57:A:VAL:HG12  | 1:56:A:LEU:H    | 11       | 0.63          |
| (1,4168) | 1:48:A:LEU:H     | 1:48:A:LEU:HD12 | 5        | 0.63          |
| (1,4164) | 1:32:A:ALA:HB3   | 1:41:A:ALA:H    | 17       | 0.63          |
| (1,4120) | 1:116:A:GLN:HE21 | 1:119:A:GLU:HB2 | 16       | 0.63          |
| (1,3870) | 1:85:A:LEU:HD22  | 1:87:A:GLY:H    | 1        | 0.63          |
| (1,3826) | 1:102:A:CYS:H    | 1:95:A:VAL:HG13 | 16       | 0.63          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3799) | 1:105:A:LEU:HD12 | 1:111:A:GLU:H    | 14       | 0.63          |
| (1,3742) | 1:28:A:ILE:H     | 1:29:A:ALA:HB1   | 6        | 0.63          |
| (1,3484) | 1:32:A:ALA:H     | 1:31:A:LEU:HD11  | 1        | 0.63          |
| (1,3484) | 1:32:A:ALA:H     | 1:31:A:LEU:HD13  | 7        | 0.63          |
| (1,3397) | 1:75:A:LEU:HA    | 1:31:A:LEU:HD11  | 15       | 0.63          |
| (1,3376) | 1:41:A:ALA:HB3   | 1:40:A:SER:HB3   | 4        | 0.63          |
| (1,3376) | 1:41:A:ALA:HB1   | 1:40:A:SER:HB3   | 10       | 0.63          |
| (1,3362) | 1:56:A:LEU:HD21  | 1:56:A:LEU:HA    | 16       | 0.63          |
| (1,3362) | 1:56:A:LEU:HD23  | 1:56:A:LEU:HA    | 17       | 0.63          |
| (1,3060) | 1:52:A:ILE:HG21  | 1:97:A:LEU:HD23  | 5        | 0.63          |
| (1,3045) | 1:52:A:ILE:HG13  | 1:54:A:GLN:HE21  | 3        | 0.63          |
| (1,3023) | 1:64:A:MET:HE3   | 1:27:A:VAL:HA    | 13       | 0.63          |
| (1,2962) | 1:97:A:LEU:HD23  | 1:56:A:LEU:HD23  | 2        | 0.63          |
| (1,2962) | 1:97:A:LEU:HD23  | 1:56:A:LEU:HD21  | 12       | 0.63          |
| (1,2954) | 1:71:A:LEU:HB2   | 1:75:A:LEU:HD12  | 16       | 0.63          |
| (1,2926) | 1:21:A:LEU:HB2   | 1:21:A:LEU:HD22  | 2        | 0.63          |
| (1,2894) | 1:52:A:ILE:HD11  | 1:53:A:PHE:HB2   | 16       | 0.63          |
| (1,2886) | 1:41:A:ALA:HA    | 1:32:A:ALA:HB1   | 6        | 0.63          |
| (1,2880) | 1:61:A:ALA:HB1   | 1:57:A:VAL:HG12  | 1        | 0.63          |
| (1,2864) | 1:78:A:TYR:HE1   | 1:78:A:TYR:HB3   | 7        | 0.63          |
| (1,2845) | 1:22:A:ASN:H     | 1:27:A:VAL:HG12  | 2        | 0.63          |
| (1,2845) | 1:22:A:ASN:H     | 1:27:A:VAL:HG11  | 12       | 0.63          |
| (1,2610) | 1:105:A:LEU:HD12 | 1:105:A:LEU:HA   | 10       | 0.63          |
| (1,2602) | 1:21:A:LEU:HD12  | 1:21:A:LEU:H     | 8        | 0.63          |
| (1,2600) | 1:105:A:LEU:HA   | 1:105:A:LEU:HD23 | 8        | 0.63          |
| (1,2600) | 1:105:A:LEU:HA   | 1:105:A:LEU:HD23 | 9        | 0.63          |
| (1,2582) | 1:60:A:VAL:HG11  | 1:57:A:VAL:HG11  | 7        | 0.63          |
| (1,2582) | 1:60:A:VAL:HG11  | 1:57:A:VAL:HG13  | 10       | 0.63          |
| (1,2572) | 1:125:A:GLN:H    | 1:124:A:VAL:HG22 | 10       | 0.63          |
| (1,2400) | 1:28:A:ILE:HB    | 1:28:A:ILE:HD11  | 5        | 0.63          |
| (1,2400) | 1:28:A:ILE:HB    | 1:28:A:ILE:HD12  | 9        | 0.63          |
| (1,2400) | 1:28:A:ILE:HB    | 1:28:A:ILE:HD11  | 13       | 0.63          |
| (1,2400) | 1:28:A:ILE:HB    | 1:28:A:ILE:HD11  | 14       | 0.63          |
| (1,2398) | 1:50:A:ILE:HD11  | 1:50:A:ILE:H     | 11       | 0.63          |
| (1,2398) | 1:50:A:ILE:HD13  | 1:50:A:ILE:H     | 12       | 0.63          |
| (1,2398) | 1:50:A:ILE:HD12  | 1:50:A:ILE:H     | 15       | 0.63          |
| (1,2397) | 1:50:A:ILE:HD11  | 1:50:A:ILE:HA    | 10       | 0.63          |
| (1,2324) | 1:97:A:LEU:HD22  | 1:39:A:PHE:H     | 4        | 0.63          |
| (1,2028) | 1:97:A:LEU:HD21  | 1:97:A:LEU:H     | 7        | 0.63          |
| (1,2026) | 1:57:A:VAL:HG12  | 1:53:A:PHE:HD1   | 12       | 0.63          |
| (1,1839) | 1:95:A:VAL:HA    | 1:93:A:THR:HG23  | 6        | 0.63          |
| (1,1839) | 1:95:A:VAL:HA    | 1:93:A:THR:HG23  | 10       | 0.63          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1751) | 1:32:A:ALA:HB1   | 1:41:A:ALA:H     | 12       | 0.63          |
| (1,1635) | 1:121:A:LYS:HB2  | 1:117:A:LEU:HD12 | 6        | 0.63          |
| (1,1450) | 1:54:A:GLN:HE22  | 1:54:A:GLN:HG2   | 9        | 0.63          |
| (1,1450) | 1:54:A:GLN:HE22  | 1:54:A:GLN:HG2   | 11       | 0.63          |
| (1,1420) | 1:97:A:LEU:HD23  | 1:56:A:LEU:HD23  | 5        | 0.63          |
| (1,1369) | 1:39:A:PHE:HZ    | 1:28:A:ILE:HD11  | 6        | 0.63          |
| (1,1356) | 1:61:A:ALA:HB2   | 1:57:A:VAL:HG12  | 2        | 0.63          |
| (1,1356) | 1:61:A:ALA:HB3   | 1:57:A:VAL:HG13  | 13       | 0.63          |
| (1,1309) | 1:97:A:LEU:HD21  | 1:97:A:LEU:H     | 7        | 0.63          |
| (1,1308) | 1:97:A:LEU:HD23  | 1:35:A:PHE:HD2   | 9        | 0.63          |
| (1,1157) | 1:117:A:LEU:HD12 | 1:82:A:TRP:HD1   | 10       | 0.63          |
| (1,1137) | 1:97:A:LEU:HD11  | 1:35:A:PHE:HD2   | 10       | 0.63          |
| (1,1125) | 1:97:A:LEU:HD11  | 1:60:A:VAL:HG12  | 10       | 0.63          |
| (1,561)  | 1:116:A:GLN:HE21 | 1:120:A:ALA:H    | 13       | 0.63          |
| (1,524)  | 1:20:A:LYS:HB3   | 1:22:A:ASN:HD22  | 14       | 0.63          |
| (1,522)  | 1:54:A:GLN:HE22  | 1:57:A:VAL:HG21  | 6        | 0.63          |
| (1,222)  | 1:102:A:CYS:H    | 1:95:A:VAL:HG13  | 14       | 0.63          |
| (1,222)  | 1:102:A:CYS:H    | 1:95:A:VAL:HG12  | 17       | 0.63          |
| (3,153)  | 1:110:A:VAL:HG22 | 1:114:A:ARG:H    | 8        | 0.62          |
| (3,153)  | 1:110:A:VAL:HG21 | 1:114:A:ARG:H    | 10       | 0.62          |
| (3,146)  | 1:52:A:ILE:H     | 1:52:A:ILE:HD12  | 10       | 0.62          |
| (3,136)  | 1:81:A:SER:H     | 1:82:A:TRP:H     | 12       | 0.62          |
| (3,113)  | 1:61:A:ALA:HB3   | 1:60:A:VAL:HB    | 16       | 0.62          |
| (3,98)   | 1:64:A:MET:HE2   | 1:63:A:GLU:HG3   | 15       | 0.62          |
| (3,78)   | 1:77:A:LEU:HD21  | 1:77:A:LEU:H     | 9        | 0.62          |
| (3,76)   | 1:116:A:GLN:HE21 | 1:85:A:LEU:HD11  | 6        | 0.62          |
| (3,55)   | 1:97:A:LEU:HD21  | 1:75:A:LEU:HD12  | 9        | 0.62          |
| (3,40)   | 1:55:A:ASP:H     | 1:52:A:ILE:HD11  | 6        | 0.62          |
| (3,40)   | 1:55:A:ASP:H     | 1:52:A:ILE:HD13  | 7        | 0.62          |
| (3,40)   | 1:55:A:ASP:H     | 1:52:A:ILE:HD11  | 13       | 0.62          |
| (3,36)   | 1:48:A:LEU:HD21  | 1:49:A:LYS:HB2   | 4        | 0.62          |
| (3,21)   | 1:31:A:LEU:H     | 1:21:A:LEU:HD11  | 8        | 0.62          |
| (3,21)   | 1:22:A:ASN:H     | 1:21:A:LEU:HD12  | 9        | 0.62          |
| (3,8)    | 1:57:A:VAL:HB    | 1:54:A:GLN:HA    | 6        | 0.62          |
| (3,8)    | 1:57:A:VAL:HB    | 1:54:A:GLN:HA    | 7        | 0.62          |
| (3,8)    | 1:57:A:VAL:HB    | 1:54:A:GLN:HA    | 15       | 0.62          |
| (3,8)    | 1:57:A:VAL:HB    | 1:54:A:GLN:HA    | 17       | 0.62          |
| (1,4283) | 1:120:A:ALA:H    | 1:85:A:LEU:HD23  | 6        | 0.62          |
| (1,4283) | 1:120:A:ALA:H    | 1:85:A:LEU:HD21  | 14       | 0.62          |
| (1,4259) | 1:57:A:VAL:HG11  | 1:56:A:LEU:H     | 1        | 0.62          |
| (1,4168) | 1:48:A:LEU:H     | 1:48:A:LEU:HD13  | 12       | 0.62          |
| (1,4122) | 1:116:A:GLN:HE21 | 1:113:A:ALA:HA   | 12       | 0.62          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3957) | 1:58:A:ASP:H     | 1:57:A:VAL:HG13  | 11       | 0.62          |
| (1,3947) | 1:71:A:LEU:HD13  | 1:61:A:ALA:H     | 8        | 0.62          |
| (1,3947) | 1:71:A:LEU:HD12  | 1:61:A:ALA:H     | 10       | 0.62          |
| (1,3845) | 1:95:A:VAL:HG13  | 1:96:A:ASP:H     | 3        | 0.62          |
| (1,3826) | 1:102:A:CYS:H    | 1:95:A:VAL:HG12  | 1        | 0.62          |
| (1,3799) | 1:105:A:LEU:HD13 | 1:111:A:GLU:H    | 2        | 0.62          |
| (1,3799) | 1:105:A:LEU:HD13 | 1:111:A:GLU:H    | 6        | 0.62          |
| (1,3509) | 1:64:A:MET:HE1   | 1:65:A:ASN:HD22  | 6        | 0.62          |
| (1,3484) | 1:32:A:ALA:H     | 1:31:A:LEU:HD11  | 10       | 0.62          |
| (1,3484) | 1:32:A:ALA:H     | 1:31:A:LEU:HD13  | 14       | 0.62          |
| (1,3463) | 1:35:A:PHE:HE2   | 1:38:A:CYS:HB2   | 4        | 0.62          |
| (1,3397) | 1:75:A:LEU:HA    | 1:31:A:LEU:HD13  | 6        | 0.62          |
| (1,3376) | 1:41:A:ALA:HB2   | 1:40:A:SER:HB3   | 3        | 0.62          |
| (1,3376) | 1:41:A:ALA:HB2   | 1:40:A:SER:HB3   | 5        | 0.62          |
| (1,3362) | 1:56:A:LEU:HD21  | 1:56:A:LEU:HA    | 3        | 0.62          |
| (1,3362) | 1:56:A:LEU:HD23  | 1:56:A:LEU:HA    | 6        | 0.62          |
| (1,3362) | 1:56:A:LEU:HD22  | 1:56:A:LEU:HA    | 14       | 0.62          |
| (1,3281) | 1:93:A:THR:HG21  | 1:104:A:GLU:HG2  | 3        | 0.62          |
| (1,3281) | 1:93:A:THR:HG22  | 1:104:A:GLU:HG2  | 16       | 0.62          |
| (1,2962) | 1:97:A:LEU:HD23  | 1:56:A:LEU:HD22  | 15       | 0.62          |
| (1,2926) | 1:21:A:LEU:HB2   | 1:21:A:LEU:HD23  | 11       | 0.62          |
| (1,2903) | 1:50:A:ILE:HD11  | 1:51:A:GLY:H     | 2        | 0.62          |
| (1,2894) | 1:52:A:ILE:HD12  | 1:53:A:PHE:HB2   | 13       | 0.62          |
| (1,2886) | 1:41:A:ALA:HA    | 1:32:A:ALA:HB3   | 2        | 0.62          |
| (1,2865) | 1:78:A:TYR:HE1   | 1:48:A:LEU:HD11  | 3        | 0.62          |
| (1,2864) | 1:78:A:TYR:HE2   | 1:78:A:TYR:HB3   | 1        | 0.62          |
| (1,2864) | 1:78:A:TYR:HE1   | 1:78:A:TYR:HB3   | 16       | 0.62          |
| (1,2673) | 1:97:A:LEU:HD13  | 1:35:A:PHE:HD2   | 5        | 0.62          |
| (1,2669) | 1:75:A:LEU:HD21  | 1:78:A:TYR:HE1   | 2        | 0.62          |
| (1,2669) | 1:75:A:LEU:HD21  | 1:78:A:TYR:HE1   | 3        | 0.62          |
| (1,2610) | 1:105:A:LEU:HD13 | 1:105:A:LEU:HA   | 11       | 0.62          |
| (1,2600) | 1:105:A:LEU:HA   | 1:105:A:LEU:HD23 | 6        | 0.62          |
| (1,2600) | 1:105:A:LEU:HA   | 1:105:A:LEU:HD22 | 14       | 0.62          |
| (1,2600) | 1:105:A:LEU:HA   | 1:105:A:LEU:HD23 | 17       | 0.62          |
| (1,2582) | 1:60:A:VAL:HG13  | 1:57:A:VAL:HG13  | 12       | 0.62          |
| (1,2582) | 1:60:A:VAL:HG12  | 1:57:A:VAL:HG12  | 15       | 0.62          |
| (1,2400) | 1:28:A:ILE:HB    | 1:28:A:ILE:HD12  | 2        | 0.62          |
| (1,2400) | 1:28:A:ILE:HB    | 1:28:A:ILE:HD12  | 15       | 0.62          |
| (1,2398) | 1:50:A:ILE:HD13  | 1:50:A:ILE:H     | 6        | 0.62          |
| (1,2397) | 1:50:A:ILE:HD13  | 1:50:A:ILE:HA    | 13       | 0.62          |
| (1,2348) | 1:30:A:PHE:HD2   | 1:21:A:LEU:HD11  | 4        | 0.62          |
| (1,2338) | 1:61:A:ALA:HB2   | 1:66:A:LEU:HD13  | 15       | 0.62          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2308) | 1:82:A:TRP:HB2   | 1:117:A:LEU:HD11 | 2        | 0.62          |
| (1,2192) | 1:55:A:ASP:HB2   | 1:52:A:ILE:HD11  | 17       | 0.62          |
| (1,1998) | 1:116:A:GLN:HG3  | 1:116:A:GLN:HE21 | 2        | 0.62          |
| (1,1998) | 1:116:A:GLN:HG3  | 1:116:A:GLN:HE21 | 7        | 0.62          |
| (1,1998) | 1:116:A:GLN:HG3  | 1:116:A:GLN:HE21 | 17       | 0.62          |
| (1,1839) | 1:95:A:VAL:HA    | 1:93:A:THR:HG22  | 3        | 0.62          |
| (1,1839) | 1:95:A:VAL:HA    | 1:93:A:THR:HG23  | 17       | 0.62          |
| (1,1751) | 1:32:A:ALA:HB1   | 1:41:A:ALA:H     | 10       | 0.62          |
| (1,1635) | 1:121:A:LYS:HB2  | 1:117:A:LEU:HD13 | 5        | 0.62          |
| (1,1601) | 1:75:A:LEU:HD22  | 1:31:A:LEU:HD13  | 11       | 0.62          |
| (1,1601) | 1:75:A:LEU:HD22  | 1:31:A:LEU:HD12  | 12       | 0.62          |
| (1,1450) | 1:54:A:GLN:HE22  | 1:54:A:GLN:HG2   | 4        | 0.62          |
| (1,1420) | 1:97:A:LEU:HD22  | 1:56:A:LEU:HD23  | 1        | 0.62          |
| (1,1420) | 1:97:A:LEU:HD21  | 1:56:A:LEU:HD21  | 4        | 0.62          |
| (1,1420) | 1:97:A:LEU:HD23  | 1:56:A:LEU:HD23  | 7        | 0.62          |
| (1,1420) | 1:97:A:LEU:HD21  | 1:56:A:LEU:HD21  | 8        | 0.62          |
| (1,1369) | 1:39:A:PHE:HZ    | 1:28:A:ILE:HD13  | 12       | 0.62          |
| (1,1361) | 1:41:A:ALA:HA    | 1:32:A:ALA:HB3   | 3        | 0.62          |
| (1,1361) | 1:41:A:ALA:HA    | 1:32:A:ALA:HB1   | 13       | 0.62          |
| (1,1360) | 1:32:A:ALA:HB1   | 1:31:A:LEU:H     | 17       | 0.62          |
| (1,1356) | 1:61:A:ALA:HB2   | 1:57:A:VAL:HG13  | 4        | 0.62          |
| (1,1356) | 1:61:A:ALA:HB1   | 1:57:A:VAL:HG12  | 15       | 0.62          |
| (1,1356) | 1:61:A:ALA:HB3   | 1:57:A:VAL:HG13  | 16       | 0.62          |
| (1,1343) | 1:78:A:TYR:HE2   | 1:48:A:LEU:HD13  | 6        | 0.62          |
| (1,1342) | 1:48:A:LEU:HD11  | 1:84:A:TYR:HE2   | 3        | 0.62          |
| (1,1342) | 1:48:A:LEU:HD13  | 1:84:A:TYR:HE1   | 13       | 0.62          |
| (1,1334) | 1:81:A:SER:HB3   | 1:84:A:TYR:HD1   | 5        | 0.62          |
| (1,1334) | 1:81:A:SER:HB3   | 1:84:A:TYR:HD2   | 11       | 0.62          |
| (1,1158) | 1:120:A:ALA:HB2  | 1:82:A:TRP:HD1   | 5        | 0.62          |
| (1,1157) | 1:117:A:LEU:HD11 | 1:82:A:TRP:HD1   | 1        | 0.62          |
| (1,1125) | 1:97:A:LEU:HD13  | 1:60:A:VAL:HG11  | 13       | 0.62          |
| (1,561)  | 1:116:A:GLN:HE21 | 1:120:A:ALA:H    | 6        | 0.62          |
| (1,561)  | 1:116:A:GLN:HE21 | 1:120:A:ALA:H    | 8        | 0.62          |
| (1,559)  | 1:116:A:GLN:HE21 | 1:113:A:ALA:HA   | 8        | 0.62          |
| (1,522)  | 1:54:A:GLN:HE22  | 1:57:A:VAL:HG21  | 16       | 0.62          |
| (1,488)  | 1:21:A:LEU:HD12  | 1:23:A:SER:H     | 9        | 0.62          |
| (1,275)  | 1:85:A:LEU:HD21  | 1:87:A:GLY:H     | 7        | 0.62          |
| (1,275)  | 1:85:A:LEU:HD23  | 1:87:A:GLY:H     | 11       | 0.62          |
| (1,222)  | 1:102:A:CYS:H    | 1:95:A:VAL:HG12  | 6        | 0.62          |
| (1,222)  | 1:102:A:CYS:H    | 1:95:A:VAL:HG13  | 9        | 0.62          |
| (1,222)  | 1:102:A:CYS:H    | 1:95:A:VAL:HG13  | 12       | 0.62          |
| (3,153)  | 1:110:A:VAL:HG22 | 1:114:A:ARG:H    | 6        | 0.61          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (3,153)  | 1:110:A:VAL:HG23 | 1:114:A:ARG:H    | 9        | 0.61          |
| (3,153)  | 1:110:A:VAL:HG21 | 1:114:A:ARG:H    | 14       | 0.61          |
| (3,113)  | 1:61:A:ALA:HB3   | 1:60:A:VAL:HB    | 9        | 0.61          |
| (3,105)  | 1:64:A:MET:H     | 1:66:A:LEU:HD22  | 4        | 0.61          |
| (3,105)  | 1:64:A:MET:H     | 1:66:A:LEU:HD22  | 7        | 0.61          |
| (3,99)   | 1:72:A:ARG:HG3   | 1:75:A:LEU:HD11  | 9        | 0.61          |
| (3,97)   | 1:31:A:LEU:HD21  | 1:30:A:PHE:HB3   | 4        | 0.61          |
| (3,97)   | 1:31:A:LEU:HD23  | 1:30:A:PHE:HB3   | 7        | 0.61          |
| (3,78)   | 1:77:A:LEU:HD23  | 1:77:A:LEU:H     | 6        | 0.61          |
| (3,78)   | 1:77:A:LEU:HD21  | 1:77:A:LEU:H     | 11       | 0.61          |
| (3,78)   | 1:77:A:LEU:HD21  | 1:77:A:LEU:H     | 12       | 0.61          |
| (3,65)   | 1:52:A:ILE:HG13  | 1:52:A:ILE:HG22  | 10       | 0.61          |
| (3,36)   | 1:50:A:ILE:HG21  | 1:49:A:LYS:HB2   | 12       | 0.61          |
| (3,11)   | 1:93:A:THR:HB    | 1:104:A:GLU:HG2  | 5        | 0.61          |
| (3,11)   | 1:93:A:THR:HB    | 1:104:A:GLU:HG2  | 11       | 0.61          |
| (3,8)    | 1:57:A:VAL:HB    | 1:54:A:GLN:HA    | 11       | 0.61          |
| (1,4283) | 1:120:A:ALA:H    | 1:85:A:LEU:HD22  | 13       | 0.61          |
| (1,3947) | 1:71:A:LEU:HD11  | 1:61:A:ALA:H     | 1        | 0.61          |
| (1,3947) | 1:71:A:LEU:HD13  | 1:61:A:ALA:H     | 2        | 0.61          |
| (1,3947) | 1:71:A:LEU:HD12  | 1:61:A:ALA:H     | 13       | 0.61          |
| (1,3947) | 1:71:A:LEU:HD11  | 1:61:A:ALA:H     | 14       | 0.61          |
| (1,3947) | 1:71:A:LEU:HD12  | 1:61:A:ALA:H     | 16       | 0.61          |
| (1,3947) | 1:71:A:LEU:HD13  | 1:61:A:ALA:H     | 17       | 0.61          |
| (1,3870) | 1:85:A:LEU:HD22  | 1:87:A:GLY:H     | 2        | 0.61          |
| (1,3870) | 1:85:A:LEU:HD23  | 1:87:A:GLY:H     | 4        | 0.61          |
| (1,3870) | 1:85:A:LEU:HD21  | 1:87:A:GLY:H     | 5        | 0.61          |
| (1,3822) | 1:93:A:THR:HG21  | 1:103:A:GLY:H    | 2        | 0.61          |
| (1,3822) | 1:93:A:THR:HG23  | 1:103:A:GLY:H    | 4        | 0.61          |
| (1,3799) | 1:105:A:LEU:HD13 | 1:111:A:GLU:H    | 5        | 0.61          |
| (1,3799) | 1:105:A:LEU:HD13 | 1:111:A:GLU:H    | 12       | 0.61          |
| (1,3799) | 1:105:A:LEU:HD12 | 1:111:A:GLU:H    | 13       | 0.61          |
| (1,3627) | 1:100:A:ASN:H    | 1:100:A:ASN:HD21 | 16       | 0.61          |
| (1,3484) | 1:32:A:ALA:H     | 1:31:A:LEU:HD13  | 3        | 0.61          |
| (1,3484) | 1:32:A:ALA:H     | 1:31:A:LEU:HD11  | 11       | 0.61          |
| (1,3484) | 1:32:A:ALA:H     | 1:31:A:LEU:HD13  | 12       | 0.61          |
| (1,3484) | 1:32:A:ALA:H     | 1:31:A:LEU:HD13  | 13       | 0.61          |
| (1,3397) | 1:75:A:LEU:HA    | 1:31:A:LEU:HD13  | 4        | 0.61          |
| (1,3397) | 1:75:A:LEU:HA    | 1:31:A:LEU:HD11  | 9        | 0.61          |
| (1,3281) | 1:93:A:THR:HG22  | 1:104:A:GLU:HG2  | 14       | 0.61          |
| (1,3204) | 1:121:A:LYS:HB2  | 1:117:A:LEU:HD11 | 1        | 0.61          |
| (1,3171) | 1:75:A:LEU:HD21  | 1:31:A:LEU:HD12  | 6        | 0.61          |
| (1,3060) | 1:52:A:ILE:HG23  | 1:97:A:LEU:HD23  | 6        | 0.61          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3060) | 1:52:A:ILE:HG23 | 1:97:A:LEU:HD23  | 14       | 0.61          |
| (1,3023) | 1:64:A:MET:HE3  | 1:27:A:VAL:HA    | 6        | 0.61          |
| (1,2991) | 1:54:A:GLN:HE22 | 1:54:A:GLN:HG2   | 3        | 0.61          |
| (1,2902) | 1:50:A:ILE:HD13 | 1:76:A:ARG:H     | 10       | 0.61          |
| (1,2864) | 1:78:A:TYR:HE2  | 1:78:A:TYR:HB3   | 8        | 0.61          |
| (1,2864) | 1:78:A:TYR:HE1  | 1:78:A:TYR:HB3   | 17       | 0.61          |
| (1,2831) | 1:97:A:LEU:HD23 | 1:35:A:PHE:HD2   | 11       | 0.61          |
| (1,2817) | 1:97:A:LEU:HD13 | 1:97:A:LEU:HA    | 8        | 0.61          |
| (1,2669) | 1:75:A:LEU:HD21 | 1:78:A:TYR:HE2   | 5        | 0.61          |
| (1,2600) | 1:105:A:LEU:HA  | 1:105:A:LEU:HD21 | 1        | 0.61          |
| (1,2582) | 1:60:A:VAL:HG12 | 1:57:A:VAL:HG11  | 14       | 0.61          |
| (1,2458) | 1:21:A:LEU:HA   | 1:21:A:LEU:HD11  | 8        | 0.61          |
| (1,2400) | 1:28:A:ILE:HB   | 1:28:A:ILE:HD13  | 4        | 0.61          |
| (1,2400) | 1:28:A:ILE:HB   | 1:28:A:ILE:HD12  | 7        | 0.61          |
| (1,2400) | 1:28:A:ILE:HB   | 1:28:A:ILE:HD12  | 10       | 0.61          |
| (1,2397) | 1:50:A:ILE:HD12 | 1:50:A:ILE:HA    | 6        | 0.61          |
| (1,2397) | 1:50:A:ILE:HD11 | 1:50:A:ILE:HA    | 9        | 0.61          |
| (1,2397) | 1:50:A:ILE:HD13 | 1:50:A:ILE:HA    | 11       | 0.61          |
| (1,2384) | 1:57:A:VAL:HG13 | 1:53:A:PHE:HD1   | 17       | 0.61          |
| (1,2334) | 1:60:A:VAL:HG12 | 1:63:A:GLU:HG3   | 1        | 0.61          |
| (1,2324) | 1:97:A:LEU:HD21 | 1:39:A:PHE:H     | 6        | 0.61          |
| (1,2172) | 1:34:A:ARG:HD3  | 1:60:A:VAL:HG11  | 16       | 0.61          |
| (1,2142) | 1:21:A:LEU:HD13 | 1:30:A:PHE:HA    | 2        | 0.61          |
| (1,1998) | 1:116:A:GLN:HG3 | 1:116:A:GLN:HE21 | 3        | 0.61          |
| (1,1998) | 1:116:A:GLN:HG3 | 1:116:A:GLN:HE21 | 11       | 0.61          |
| (1,1998) | 1:116:A:GLN:HG3 | 1:116:A:GLN:HE21 | 12       | 0.61          |
| (1,1998) | 1:116:A:GLN:HG3 | 1:116:A:GLN:HE21 | 15       | 0.61          |
| (1,1851) | 1:35:A:PHE:HE2  | 1:38:A:CYS:HB2   | 15       | 0.61          |
| (1,1682) | 1:41:A:ALA:HB1  | 1:33:A:GLU:H     | 4        | 0.61          |
| (1,1635) | 1:121:A:LYS:HB2 | 1:117:A:LEU:HD12 | 13       | 0.61          |
| (1,1601) | 1:75:A:LEU:HD21 | 1:31:A:LEU:HD13  | 9        | 0.61          |
| (1,1601) | 1:75:A:LEU:HD22 | 1:31:A:LEU:HD13  | 15       | 0.61          |
| (1,1601) | 1:75:A:LEU:HD22 | 1:31:A:LEU:HD11  | 16       | 0.61          |
| (1,1480) | 1:64:A:MET:HE1  | 1:63:A:GLU:H     | 1        | 0.61          |
| (1,1480) | 1:64:A:MET:HE1  | 1:63:A:GLU:H     | 7        | 0.61          |
| (1,1450) | 1:54:A:GLN:HE22 | 1:54:A:GLN:HG2   | 1        | 0.61          |
| (1,1420) | 1:97:A:LEU:HD21 | 1:56:A:LEU:HD23  | 13       | 0.61          |
| (1,1360) | 1:32:A:ALA:HB2  | 1:31:A:LEU:H     | 14       | 0.61          |
| (1,1342) | 1:48:A:LEU:HD13 | 1:84:A:TYR:HE2   | 15       | 0.61          |
| (1,1342) | 1:48:A:LEU:HD13 | 1:84:A:TYR:HE2   | 16       | 0.61          |
| (1,1336) | 1:85:A:LEU:HD23 | 1:84:A:TYR:HD2   | 4        | 0.61          |
| (1,1301) | 1:97:A:LEU:HD11 | 1:97:A:LEU:HA    | 15       | 0.61          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1137) | 1:97:A:LEU:HD11  | 1:35:A:PHE:HD2  | 17       | 0.61          |
| (1,1069) | 1:48:A:LEU:HD12  | 1:52:A:ILE:HG12 | 12       | 0.61          |
| (1,815)  | 1:50:A:ILE:HD11  | 1:50:A:ILE:HA   | 15       | 0.61          |
| (1,561)  | 1:116:A:GLN:HE21 | 1:120:A:ALA:H   | 4        | 0.61          |
| (1,524)  | 1:20:A:LYS:HB3   | 1:22:A:ASN:HD22 | 16       | 0.61          |
| (3,136)  | 1:82:A:TRP:HD1   | 1:82:A:TRP:H    | 1        | 0.6           |
| (3,136)  | 1:82:A:TRP:HD1   | 1:82:A:TRP:H    | 13       | 0.6           |
| (3,136)  | 1:81:A:SER:H     | 1:82:A:TRP:H    | 15       | 0.6           |
| (3,113)  | 1:61:A:ALA:HB1   | 1:60:A:VAL:HB   | 7        | 0.6           |
| (3,105)  | 1:64:A:MET:H     | 1:66:A:LEU:HD23 | 8        | 0.6           |
| (3,98)   | 1:64:A:MET:HE1   | 1:63:A:GLU:HG3  | 1        | 0.6           |
| (3,78)   | 1:77:A:LEU:HD23  | 1:77:A:LEU:H    | 2        | 0.6           |
| (3,78)   | 1:77:A:LEU:HD22  | 1:77:A:LEU:H    | 17       | 0.6           |
| (3,65)   | 1:49:A:LYS:HB2   | 1:52:A:ILE:HG22 | 3        | 0.6           |
| (3,51)   | 1:95:A:VAL:HG22  | 1:49:A:LYS:HA   | 5        | 0.6           |
| (3,18)   | 1:58:A:ASP:HB3   | 1:60:A:VAL:HG13 | 14       | 0.6           |
| (3,11)   | 1:93:A:THR:HB    | 1:104:A:GLU:HG2 | 14       | 0.6           |
| (3,8)    | 1:57:A:VAL:HB    | 1:54:A:GLN:HA   | 5        | 0.6           |
| (3,8)    | 1:57:A:VAL:HB    | 1:54:A:GLN:HA   | 8        | 0.6           |
| (3,8)    | 1:57:A:VAL:HB    | 1:54:A:GLN:HA   | 10       | 0.6           |
| (3,8)    | 1:57:A:VAL:HB    | 1:54:A:GLN:HA   | 12       | 0.6           |
| (1,4259) | 1:57:A:VAL:HG11  | 1:56:A:LEU:H    | 2        | 0.6           |
| (1,4259) | 1:57:A:VAL:HG12  | 1:56:A:LEU:H    | 13       | 0.6           |
| (1,4171) | 1:48:A:LEU:HD22  | 1:49:A:LYS:H    | 8        | 0.6           |
| (1,4168) | 1:48:A:LEU:H     | 1:48:A:LEU:HD11 | 6        | 0.6           |
| (1,4164) | 1:32:A:ALA:HB1   | 1:41:A:ALA:H    | 12       | 0.6           |
| (1,4082) | 1:22:A:ASN:HD21  | 1:22:A:ASN:HB3  | 9        | 0.6           |
| (1,4028) | 1:31:A:LEU:HD23  | 1:32:A:ALA:H    | 12       | 0.6           |
| (1,3957) | 1:58:A:ASP:H     | 1:57:A:VAL:HG12 | 2        | 0.6           |
| (1,3947) | 1:71:A:LEU:HD13  | 1:61:A:ALA:H    | 3        | 0.6           |
| (1,3947) | 1:71:A:LEU:HD13  | 1:61:A:ALA:H    | 5        | 0.6           |
| (1,3947) | 1:71:A:LEU:HD11  | 1:61:A:ALA:H    | 15       | 0.6           |
| (1,3861) | 1:110:A:VAL:HG23 | 1:91:A:GLY:H    | 15       | 0.6           |
| (1,3845) | 1:95:A:VAL:HG13  | 1:96:A:ASP:H    | 1        | 0.6           |
| (1,3826) | 1:102:A:CYS:H    | 1:95:A:VAL:HG13 | 11       | 0.6           |
| (1,3799) | 1:105:A:LEU:HD13 | 1:111:A:GLU:H   | 1        | 0.6           |
| (1,3799) | 1:105:A:LEU:HD11 | 1:111:A:GLU:H   | 3        | 0.6           |
| (1,3799) | 1:105:A:LEU:HD11 | 1:111:A:GLU:H   | 11       | 0.6           |
| (1,3799) | 1:105:A:LEU:HD12 | 1:111:A:GLU:H   | 15       | 0.6           |
| (1,3799) | 1:105:A:LEU:HD12 | 1:111:A:GLU:H   | 16       | 0.6           |
| (1,3782) | 1:120:A:ALA:HB3  | 1:119:A:GLU:H   | 12       | 0.6           |
| (1,3742) | 1:28:A:ILE:H     | 1:29:A:ALA:HB2  | 14       | 0.6           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3541) | 1:64:A:MET:HB2   | 1:21:A:LEU:HD21  | 2        | 0.6           |
| (1,3484) | 1:32:A:ALA:H     | 1:31:A:LEU:HD11  | 2        | 0.6           |
| (1,3376) | 1:41:A:ALA:HB1   | 1:40:A:SER:HB3   | 6        | 0.6           |
| (1,3362) | 1:56:A:LEU:HD22  | 1:56:A:LEU:HA    | 1        | 0.6           |
| (1,3362) | 1:56:A:LEU:HD22  | 1:56:A:LEU:HA    | 2        | 0.6           |
| (1,3362) | 1:56:A:LEU:HD23  | 1:56:A:LEU:HA    | 4        | 0.6           |
| (1,3362) | 1:56:A:LEU:HD22  | 1:56:A:LEU:HA    | 5        | 0.6           |
| (1,3362) | 1:56:A:LEU:HD23  | 1:56:A:LEU:HA    | 7        | 0.6           |
| (1,3362) | 1:56:A:LEU:HD23  | 1:56:A:LEU:HA    | 11       | 0.6           |
| (1,3362) | 1:56:A:LEU:HD22  | 1:56:A:LEU:HA    | 13       | 0.6           |
| (1,3281) | 1:93:A:THR:HG21  | 1:104:A:GLU:HG2  | 6        | 0.6           |
| (1,3281) | 1:93:A:THR:HG23  | 1:104:A:GLU:HG2  | 9        | 0.6           |
| (1,3256) | 1:41:A:ALA:HB2   | 1:33:A:GLU:H     | 8        | 0.6           |
| (1,2991) | 1:54:A:GLN:HE22  | 1:54:A:GLN:HG2   | 9        | 0.6           |
| (1,2991) | 1:54:A:GLN:HE22  | 1:54:A:GLN:HG2   | 11       | 0.6           |
| (1,2962) | 1:97:A:LEU:HD23  | 1:56:A:LEU:HD22  | 14       | 0.6           |
| (1,2954) | 1:71:A:LEU:HB2   | 1:75:A:LEU:HD11  | 6        | 0.6           |
| (1,2954) | 1:71:A:LEU:HB2   | 1:75:A:LEU:HD13  | 10       | 0.6           |
| (1,2886) | 1:41:A:ALA:HA    | 1:32:A:ALA:HB1   | 4        | 0.6           |
| (1,2886) | 1:41:A:ALA:HA    | 1:32:A:ALA:HB3   | 5        | 0.6           |
| (1,2886) | 1:41:A:ALA:HA    | 1:32:A:ALA:HB2   | 10       | 0.6           |
| (1,2886) | 1:41:A:ALA:HA    | 1:32:A:ALA:HB1   | 16       | 0.6           |
| (1,2885) | 1:32:A:ALA:HB3   | 1:31:A:LEU:H     | 2        | 0.6           |
| (1,2831) | 1:97:A:LEU:HD23  | 1:35:A:PHE:HD2   | 9        | 0.6           |
| (1,2817) | 1:97:A:LEU:HD12  | 1:97:A:LEU:HA    | 10       | 0.6           |
| (1,2817) | 1:97:A:LEU:HD13  | 1:97:A:LEU:HA    | 12       | 0.6           |
| (1,2680) | 1:117:A:LEU:HD12 | 1:82:A:TRP:HD1   | 4        | 0.6           |
| (1,2680) | 1:117:A:LEU:HD12 | 1:82:A:TRP:HD1   | 13       | 0.6           |
| (1,2669) | 1:75:A:LEU:HD21  | 1:78:A:TYR:HE1   | 7        | 0.6           |
| (1,2664) | 1:97:A:LEU:HD13  | 1:60:A:VAL:HG13  | 5        | 0.6           |
| (1,2600) | 1:105:A:LEU:HA   | 1:105:A:LEU:HD21 | 15       | 0.6           |
| (1,2585) | 1:92:A:ALA:HA    | 1:93:A:THR:HG21  | 1        | 0.6           |
| (1,2585) | 1:92:A:ALA:HA    | 1:93:A:THR:HG23  | 13       | 0.6           |
| (1,2582) | 1:60:A:VAL:HG13  | 1:57:A:VAL:HG12  | 4        | 0.6           |
| (1,2582) | 1:60:A:VAL:HG13  | 1:57:A:VAL:HG12  | 9        | 0.6           |
| (1,2582) | 1:60:A:VAL:HG12  | 1:57:A:VAL:HG12  | 16       | 0.6           |
| (1,2582) | 1:60:A:VAL:HG13  | 1:57:A:VAL:HG11  | 17       | 0.6           |
| (1,2572) | 1:125:A:GLN:H    | 1:124:A:VAL:HG21 | 16       | 0.6           |
| (1,2458) | 1:21:A:LEU:HA    | 1:21:A:LEU:HD13  | 12       | 0.6           |
| (1,2423) | 1:64:A:MET:HA    | 1:64:A:MET:HE1   | 16       | 0.6           |
| (1,2400) | 1:28:A:ILE:HB    | 1:28:A:ILE:HD13  | 3        | 0.6           |
| (1,2400) | 1:28:A:ILE:HB    | 1:28:A:ILE:HD13  | 16       | 0.6           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2398) | 1:50:A:ILE:HD12  | 1:50:A:ILE:H     | 9        | 0.6           |
| (1,2398) | 1:50:A:ILE:HD13  | 1:50:A:ILE:H     | 16       | 0.6           |
| (1,2324) | 1:97:A:LEU:HD22  | 1:39:A:PHE:H     | 11       | 0.6           |
| (1,2308) | 1:82:A:TRP:HB2   | 1:117:A:LEU:HD11 | 9        | 0.6           |
| (1,2308) | 1:82:A:TRP:HB2   | 1:117:A:LEU:HD12 | 11       | 0.6           |
| (1,2305) | 1:45:A:ALA:HB2   | 1:44:A:GLU:HA    | 7        | 0.6           |
| (1,2192) | 1:55:A:ASP:HB2   | 1:52:A:ILE:HD13  | 12       | 0.6           |
| (1,1998) | 1:116:A:GLN:HG3  | 1:116:A:GLN:HE21 | 1        | 0.6           |
| (1,1851) | 1:35:A:PHE:HE2   | 1:38:A:CYS:HB2   | 5        | 0.6           |
| (1,1839) | 1:95:A:VAL:HA    | 1:93:A:THR:HG22  | 7        | 0.6           |
| (1,1751) | 1:32:A:ALA:HB1   | 1:41:A:ALA:H     | 14       | 0.6           |
| (1,1601) | 1:75:A:LEU:HD21  | 1:31:A:LEU:HD12  | 3        | 0.6           |
| (1,1601) | 1:75:A:LEU:HD23  | 1:31:A:LEU:HD12  | 4        | 0.6           |
| (1,1601) | 1:75:A:LEU:HD22  | 1:31:A:LEU:HD11  | 8        | 0.6           |
| (1,1601) | 1:75:A:LEU:HD23  | 1:31:A:LEU:HD12  | 13       | 0.6           |
| (1,1601) | 1:75:A:LEU:HD21  | 1:31:A:LEU:HD12  | 14       | 0.6           |
| (1,1482) | 1:64:A:MET:HE1   | 1:27:A:VAL:HA    | 10       | 0.6           |
| (1,1482) | 1:64:A:MET:HE1   | 1:27:A:VAL:HA    | 12       | 0.6           |
| (1,1482) | 1:64:A:MET:HE1   | 1:27:A:VAL:HA    | 17       | 0.6           |
| (1,1420) | 1:97:A:LEU:HD23  | 1:56:A:LEU:HD23  | 6        | 0.6           |
| (1,1369) | 1:39:A:PHE:HZ    | 1:28:A:ILE:HD13  | 7        | 0.6           |
| (1,1369) | 1:39:A:PHE:HZ    | 1:28:A:ILE:HD12  | 8        | 0.6           |
| (1,1360) | 1:32:A:ALA:HB3   | 1:31:A:LEU:H     | 10       | 0.6           |
| (1,1356) | 1:61:A:ALA:HB3   | 1:57:A:VAL:HG13  | 9        | 0.6           |
| (1,1343) | 1:78:A:TYR:HE1   | 1:48:A:LEU:HD11  | 10       | 0.6           |
| (1,1342) | 1:48:A:LEU:HD13  | 1:84:A:TYR:HE2   | 7        | 0.6           |
| (1,1336) | 1:85:A:LEU:HD22  | 1:84:A:TYR:HD1   | 1        | 0.6           |
| (1,1334) | 1:81:A:SER:HB3   | 1:84:A:TYR:HD1   | 8        | 0.6           |
| (1,1158) | 1:120:A:ALA:HB2  | 1:82:A:TRP:HD1   | 16       | 0.6           |
| (1,1069) | 1:48:A:LEU:HD13  | 1:52:A:ILE:HG12  | 15       | 0.6           |
| (1,942)  | 1:93:A:THR:HB    | 1:95:A:VAL:HG13  | 11       | 0.6           |
| (1,697)  | 1:57:A:VAL:HG12  | 1:56:A:LEU:H     | 11       | 0.6           |
| (1,561)  | 1:116:A:GLN:HE21 | 1:120:A:ALA:H    | 16       | 0.6           |
| (1,554)  | 1:70:A:GLN:HA    | 1:70:A:GLN:HE21  | 14       | 0.6           |
| (1,524)  | 1:20:A:LYS:HB3   | 1:22:A:ASN:HD22  | 4        | 0.6           |
| (1,370)  | 1:71:A:LEU:HD12  | 1:61:A:ALA:H     | 12       | 0.6           |
| (1,275)  | 1:85:A:LEU:HD22  | 1:87:A:GLY:H     | 17       | 0.6           |
| (1,222)  | 1:102:A:CYS:H    | 1:95:A:VAL:HG12  | 2        | 0.6           |
| (1,222)  | 1:102:A:CYS:H    | 1:95:A:VAL:HG12  | 3        | 0.6           |
| (1,222)  | 1:102:A:CYS:H    | 1:95:A:VAL:HG12  | 5        | 0.6           |
| (3,150)  | 1:77:A:LEU:H     | 1:79:A:THR:HG22  | 15       | 0.59          |
| (3,117)  | 1:48:A:LEU:HD23  | 1:39:A:PHE:HD2   | 12       | 0.59          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (3,97)   | 1:31:A:LEU:HD22  | 1:30:A:PHE:HB3   | 3        | 0.59          |
| (3,97)   | 1:31:A:LEU:HD22  | 1:30:A:PHE:HB3   | 11       | 0.59          |
| (3,96)   | 1:110:A:VAL:HG21 | 1:109:A:HIS:HA   | 4        | 0.59          |
| (3,96)   | 1:110:A:VAL:HG21 | 1:109:A:HIS:HA   | 17       | 0.59          |
| (3,78)   | 1:77:A:LEU:HD23  | 1:77:A:LEU:H     | 3        | 0.59          |
| (3,78)   | 1:77:A:LEU:HD22  | 1:77:A:LEU:H     | 5        | 0.59          |
| (3,78)   | 1:77:A:LEU:HD21  | 1:77:A:LEU:H     | 7        | 0.59          |
| (3,78)   | 1:77:A:LEU:HD22  | 1:77:A:LEU:H     | 15       | 0.59          |
| (3,78)   | 1:77:A:LEU:HD22  | 1:77:A:LEU:H     | 16       | 0.59          |
| (1,4259) | 1:57:A:VAL:HG12  | 1:56:A:LEU:H     | 4        | 0.59          |
| (1,4259) | 1:57:A:VAL:HG12  | 1:56:A:LEU:H     | 9        | 0.59          |
| (1,4171) | 1:48:A:LEU:HD21  | 1:49:A:LYS:H     | 10       | 0.59          |
| (1,4164) | 1:32:A:ALA:HB1   | 1:41:A:ALA:H     | 10       | 0.59          |
| (1,4132) | 1:60:A:VAL:HG12  | 1:34:A:ARG:HE    | 8        | 0.59          |
| (1,4082) | 1:22:A:ASN:HD21  | 1:22:A:ASN:HB3   | 3        | 0.59          |
| (1,4082) | 1:22:A:ASN:HD21  | 1:22:A:ASN:HB3   | 14       | 0.59          |
| (1,4082) | 1:22:A:ASN:HD21  | 1:22:A:ASN:HB3   | 16       | 0.59          |
| (1,4028) | 1:31:A:LEU:HD21  | 1:32:A:ALA:H     | 17       | 0.59          |
| (1,3957) | 1:58:A:ASP:H     | 1:57:A:VAL:HG12  | 1        | 0.59          |
| (1,3870) | 1:85:A:LEU:HD23  | 1:87:A:GLY:H     | 13       | 0.59          |
| (1,3870) | 1:85:A:LEU:HD21  | 1:87:A:GLY:H     | 15       | 0.59          |
| (1,3861) | 1:110:A:VAL:HG21 | 1:91:A:GLY:H     | 8        | 0.59          |
| (1,3845) | 1:95:A:VAL:HG11  | 1:96:A:ASP:H     | 9        | 0.59          |
| (1,3799) | 1:105:A:LEU:HD12 | 1:111:A:GLU:H    | 8        | 0.59          |
| (1,3799) | 1:105:A:LEU:HD12 | 1:111:A:GLU:H    | 9        | 0.59          |
| (1,3782) | 1:120:A:ALA:HB3  | 1:119:A:GLU:H    | 17       | 0.59          |
| (1,3742) | 1:28:A:ILE:H     | 1:29:A:ALA:HB1   | 4        | 0.59          |
| (1,3541) | 1:64:A:MET:HB2   | 1:21:A:LEU:HD21  | 8        | 0.59          |
| (1,3489) | 1:21:A:LEU:HD21  | 1:20:A:LYS:HA    | 9        | 0.59          |
| (1,3484) | 1:32:A:ALA:H     | 1:31:A:LEU:HD13  | 4        | 0.59          |
| (1,3463) | 1:35:A:PHE:HE2   | 1:38:A:CYS:HB2   | 9        | 0.59          |
| (1,3452) | 1:95:A:VAL:HA    | 1:93:A:THR:HG22  | 13       | 0.59          |
| (1,3377) | 1:40:A:SER:HB2   | 1:41:A:ALA:HB2   | 8        | 0.59          |
| (1,3376) | 1:41:A:ALA:HB1   | 1:40:A:SER:HB3   | 9        | 0.59          |
| (1,3362) | 1:56:A:LEU:HD22  | 1:56:A:LEU:HA    | 9        | 0.59          |
| (1,3302) | 1:83:A:ARG:HB2   | 1:86:A:TYR:HD2   | 8        | 0.59          |
| (1,3281) | 1:93:A:THR:HG22  | 1:104:A:GLU:HG2  | 1        | 0.59          |
| (1,3281) | 1:93:A:THR:HG23  | 1:104:A:GLU:HG2  | 15       | 0.59          |
| (1,3204) | 1:121:A:LYS:HB2  | 1:117:A:LEU:HD13 | 14       | 0.59          |
| (1,3045) | 1:52:A:ILE:HG13  | 1:54:A:GLN:HE21  | 15       | 0.59          |
| (1,2991) | 1:54:A:GLN:HE22  | 1:54:A:GLN:HG2   | 4        | 0.59          |
| (1,2962) | 1:97:A:LEU:HD22  | 1:56:A:LEU:HD23  | 1        | 0.59          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2962) | 1:97:A:LEU:HD23  | 1:56:A:LEU:HD23  | 5        | 0.59          |
| (1,2962) | 1:97:A:LEU:HD23  | 1:56:A:LEU:HD23  | 7        | 0.59          |
| (1,2962) | 1:97:A:LEU:HD21  | 1:56:A:LEU:HD21  | 8        | 0.59          |
| (1,2954) | 1:71:A:LEU:HB2   | 1:75:A:LEU:HD12  | 4        | 0.59          |
| (1,2954) | 1:71:A:LEU:HB2   | 1:75:A:LEU:HD13  | 7        | 0.59          |
| (1,2926) | 1:21:A:LEU:HB2   | 1:21:A:LEU:HD23  | 3        | 0.59          |
| (1,2926) | 1:21:A:LEU:HB2   | 1:21:A:LEU:HD21  | 13       | 0.59          |
| (1,2926) | 1:21:A:LEU:HB2   | 1:21:A:LEU:HD23  | 17       | 0.59          |
| (1,2886) | 1:41:A:ALA:HA    | 1:32:A:ALA:HB3   | 7        | 0.59          |
| (1,2886) | 1:41:A:ALA:HA    | 1:32:A:ALA:HB1   | 8        | 0.59          |
| (1,2885) | 1:32:A:ALA:HB2   | 1:31:A:LEU:H     | 12       | 0.59          |
| (1,2880) | 1:61:A:ALA:HB2   | 1:57:A:VAL:HG12  | 2        | 0.59          |
| (1,2880) | 1:61:A:ALA:HB3   | 1:57:A:VAL:HG13  | 13       | 0.59          |
| (1,2864) | 1:78:A:TYR:HE1   | 1:78:A:TYR:HB3   | 15       | 0.59          |
| (1,2845) | 1:22:A:ASN:H     | 1:27:A:VAL:HG11  | 8        | 0.59          |
| (1,2832) | 1:97:A:LEU:HD21  | 1:97:A:LEU:H     | 7        | 0.59          |
| (1,2817) | 1:97:A:LEU:HD12  | 1:97:A:LEU:HA    | 6        | 0.59          |
| (1,2680) | 1:117:A:LEU:HD12 | 1:82:A:TRP:HD1   | 10       | 0.59          |
| (1,2669) | 1:75:A:LEU:HD21  | 1:78:A:TYR:HE1   | 14       | 0.59          |
| (1,2582) | 1:60:A:VAL:HG13  | 1:57:A:VAL:HG12  | 13       | 0.59          |
| (1,2572) | 1:125:A:GLN:H    | 1:124:A:VAL:HG23 | 5        | 0.59          |
| (1,2572) | 1:125:A:GLN:H    | 1:124:A:VAL:HG22 | 6        | 0.59          |
| (1,2400) | 1:28:A:ILE:HB    | 1:28:A:ILE:HD12  | 1        | 0.59          |
| (1,2400) | 1:28:A:ILE:HB    | 1:28:A:ILE:HD12  | 11       | 0.59          |
| (1,2398) | 1:50:A:ILE:HD11  | 1:50:A:ILE:H     | 13       | 0.59          |
| (1,2398) | 1:50:A:ILE:HD11  | 1:50:A:ILE:H     | 14       | 0.59          |
| (1,2324) | 1:97:A:LEU:HD21  | 1:39:A:PHE:H     | 3        | 0.59          |
| (1,2309) | 1:39:A:PHE:HB3   | 1:39:A:PHE:HE2   | 4        | 0.59          |
| (1,2157) | 1:99:A:GLY:HA3   | 1:95:A:VAL:HG22  | 2        | 0.59          |
| (1,2157) | 1:99:A:GLY:HA3   | 1:95:A:VAL:HG21  | 14       | 0.59          |
| (1,2142) | 1:21:A:LEU:HD12  | 1:30:A:PHE:HA    | 1        | 0.59          |
| (1,2142) | 1:21:A:LEU:HD11  | 1:30:A:PHE:HA    | 8        | 0.59          |
| (1,1998) | 1:116:A:GLN:HG3  | 1:116:A:GLN:HE21 | 4        | 0.59          |
| (1,1998) | 1:116:A:GLN:HG3  | 1:116:A:GLN:HE21 | 5        | 0.59          |
| (1,1998) | 1:116:A:GLN:HG3  | 1:116:A:GLN:HE21 | 9        | 0.59          |
| (1,1998) | 1:116:A:GLN:HG3  | 1:116:A:GLN:HE21 | 10       | 0.59          |
| (1,1998) | 1:116:A:GLN:HG3  | 1:116:A:GLN:HE21 | 13       | 0.59          |
| (1,1998) | 1:116:A:GLN:HG3  | 1:116:A:GLN:HE21 | 16       | 0.59          |
| (1,1790) | 1:90:A:PRO:HA    | 1:92:A:ALA:HB1   | 10       | 0.59          |
| (1,1751) | 1:32:A:ALA:HB2   | 1:41:A:ALA:H     | 6        | 0.59          |
| (1,1635) | 1:121:A:LYS:HB2  | 1:117:A:LEU:HD12 | 10       | 0.59          |
| (1,1503) | 1:52:A:ILE:HG12  | 1:54:A:GLN:HE21  | 16       | 0.59          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1490) | 1:78:A:TYR:HH    | 1:45:A:ALA:HB2  | 2        | 0.59          |
| (1,1372) | 1:28:A:ILE:HD11  | 1:31:A:LEU:HB3  | 6        | 0.59          |
| (1,1369) | 1:39:A:PHE:HZ    | 1:28:A:ILE:HD13 | 2        | 0.59          |
| (1,1369) | 1:39:A:PHE:HZ    | 1:28:A:ILE:HD12 | 14       | 0.59          |
| (1,1369) | 1:39:A:PHE:HZ    | 1:28:A:ILE:HD12 | 17       | 0.59          |
| (1,1361) | 1:41:A:ALA:HA    | 1:32:A:ALA:HB2  | 12       | 0.59          |
| (1,1360) | 1:32:A:ALA:HB1   | 1:31:A:LEU:H    | 3        | 0.59          |
| (1,1360) | 1:32:A:ALA:HB2   | 1:31:A:LEU:H    | 13       | 0.59          |
| (1,1360) | 1:32:A:ALA:HB2   | 1:31:A:LEU:H    | 16       | 0.59          |
| (1,1343) | 1:78:A:TYR:HE2   | 1:48:A:LEU:HD12 | 9        | 0.59          |
| (1,1343) | 1:78:A:TYR:HE2   | 1:48:A:LEU:HD12 | 13       | 0.59          |
| (1,1342) | 1:48:A:LEU:HD11  | 1:84:A:TYR:HE1  | 10       | 0.59          |
| (1,1342) | 1:48:A:LEU:HD13  | 1:84:A:TYR:HE1  | 14       | 0.59          |
| (1,1334) | 1:81:A:SER:HB3   | 1:84:A:TYR:HD2  | 9        | 0.59          |
| (1,1334) | 1:81:A:SER:HB3   | 1:84:A:TYR:HD1  | 10       | 0.59          |
| (1,1334) | 1:81:A:SER:HB3   | 1:84:A:TYR:HD2  | 15       | 0.59          |
| (1,1308) | 1:97:A:LEU:HD22  | 1:35:A:PHE:HD1  | 6        | 0.59          |
| (1,1157) | 1:117:A:LEU:HD12 | 1:82:A:TRP:HD1  | 16       | 0.59          |
| (1,1137) | 1:97:A:LEU:HD12  | 1:35:A:PHE:HD1  | 12       | 0.59          |
| (1,1125) | 1:97:A:LEU:HD11  | 1:60:A:VAL:HG11 | 17       | 0.59          |
| (1,1069) | 1:48:A:LEU:HD12  | 1:52:A:ILE:HG12 | 16       | 0.59          |
| (1,815)  | 1:50:A:ILE:HD12  | 1:50:A:ILE:HA   | 16       | 0.59          |
| (1,720)  | 1:120:A:ALA:H    | 1:85:A:LEU:HD23 | 5        | 0.59          |
| (1,697)  | 1:57:A:VAL:HG11  | 1:56:A:LEU:H    | 1        | 0.59          |
| (1,604)  | 1:32:A:ALA:HB3   | 1:41:A:ALA:H    | 17       | 0.59          |
| (1,561)  | 1:116:A:GLN:HE21 | 1:120:A:ALA:H   | 1        | 0.59          |
| (1,561)  | 1:116:A:GLN:HE21 | 1:120:A:ALA:H   | 5        | 0.59          |
| (1,559)  | 1:116:A:GLN:HE21 | 1:113:A:ALA:HA  | 9        | 0.59          |
| (1,389)  | 1:58:A:ASP:H     | 1:57:A:VAL:HG13 | 11       | 0.59          |
| (1,275)  | 1:85:A:LEU:HD22  | 1:87:A:GLY:H    | 1        | 0.59          |
| (1,275)  | 1:85:A:LEU:HD21  | 1:87:A:GLY:H    | 6        | 0.59          |
| (1,126)  | 1:28:A:ILE:H     | 1:29:A:ALA:HB1  | 6        | 0.59          |
| (3,150)  | 1:77:A:LEU:H     | 1:79:A:THR:HG23 | 9        | 0.58          |
| (3,150)  | 1:77:A:LEU:H     | 1:79:A:THR:HG22 | 12       | 0.58          |
| (3,136)  | 1:81:A:SER:H     | 1:82:A:TRP:H    | 3        | 0.58          |
| (3,105)  | 1:64:A:MET:H     | 1:66:A:LEU:HD23 | 12       | 0.58          |
| (3,105)  | 1:64:A:MET:H     | 1:66:A:LEU:HD23 | 17       | 0.58          |
| (3,96)   | 1:110:A:VAL:HG23 | 1:109:A:HIS:HA  | 8        | 0.58          |
| (3,78)   | 1:77:A:LEU:HD23  | 1:77:A:LEU:H    | 13       | 0.58          |
| (3,65)   | 1:49:A:LYS:HB2   | 1:52:A:ILE:HG21 | 1        | 0.58          |
| (3,65)   | 1:52:A:ILE:HG13  | 1:52:A:ILE:HG23 | 6        | 0.58          |
| (3,36)   | 1:50:A:ILE:HG23  | 1:49:A:LYS:HB2  | 8        | 0.58          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (3,11)   | 1:93:A:THR:HB    | 1:104:A:GLU:HG2  | 6        | 0.58          |
| (1,4259) | 1:57:A:VAL:HG12  | 1:56:A:LEU:H     | 3        | 0.58          |
| (1,4259) | 1:57:A:VAL:HG11  | 1:56:A:LEU:H     | 15       | 0.58          |
| (1,4171) | 1:48:A:LEU:HD21  | 1:49:A:LYS:H     | 14       | 0.58          |
| (1,4132) | 1:60:A:VAL:HG12  | 1:34:A:ARG:HE    | 13       | 0.58          |
| (1,4132) | 1:60:A:VAL:HG11  | 1:34:A:ARG:HE    | 15       | 0.58          |
| (1,4082) | 1:22:A:ASN:HD21  | 1:22:A:ASN:HB3   | 10       | 0.58          |
| (1,3957) | 1:58:A:ASP:H     | 1:57:A:VAL:HG12  | 15       | 0.58          |
| (1,3947) | 1:71:A:LEU:HD12  | 1:61:A:ALA:H     | 4        | 0.58          |
| (1,3947) | 1:71:A:LEU:HD11  | 1:61:A:ALA:H     | 6        | 0.58          |
| (1,3947) | 1:71:A:LEU:HD13  | 1:61:A:ALA:H     | 7        | 0.58          |
| (1,3947) | 1:71:A:LEU:HD12  | 1:61:A:ALA:H     | 9        | 0.58          |
| (1,3941) | 1:63:A:GLU:H     | 1:61:A:ALA:HB2   | 3        | 0.58          |
| (1,3870) | 1:85:A:LEU:HD23  | 1:87:A:GLY:H     | 10       | 0.58          |
| (1,3810) | 1:105:A:LEU:HD13 | 1:106:A:ASP:H    | 10       | 0.58          |
| (1,3810) | 1:105:A:LEU:HD12 | 1:106:A:ASP:H    | 14       | 0.58          |
| (1,3810) | 1:105:A:LEU:HD12 | 1:106:A:ASP:H    | 15       | 0.58          |
| (1,3799) | 1:105:A:LEU:HD13 | 1:111:A:GLU:H    | 7        | 0.58          |
| (1,3799) | 1:105:A:LEU:HD13 | 1:111:A:GLU:H    | 10       | 0.58          |
| (1,3799) | 1:105:A:LEU:HD11 | 1:111:A:GLU:H    | 17       | 0.58          |
| (1,3782) | 1:120:A:ALA:HB1  | 1:119:A:GLU:H    | 3        | 0.58          |
| (1,3782) | 1:120:A:ALA:HB1  | 1:119:A:GLU:H    | 7        | 0.58          |
| (1,3782) | 1:120:A:ALA:HB3  | 1:119:A:GLU:H    | 9        | 0.58          |
| (1,3782) | 1:120:A:ALA:HB2  | 1:119:A:GLU:H    | 15       | 0.58          |
| (1,3541) | 1:64:A:MET:HB2   | 1:21:A:LEU:HD23  | 16       | 0.58          |
| (1,3484) | 1:32:A:ALA:H     | 1:31:A:LEU:HD11  | 5        | 0.58          |
| (1,3484) | 1:32:A:ALA:H     | 1:31:A:LEU:HD13  | 6        | 0.58          |
| (1,3484) | 1:32:A:ALA:H     | 1:31:A:LEU:HD12  | 8        | 0.58          |
| (1,3452) | 1:95:A:VAL:HA    | 1:93:A:THR:HG22  | 15       | 0.58          |
| (1,3204) | 1:121:A:LYS:HB2  | 1:117:A:LEU:HD12 | 6        | 0.58          |
| (1,3171) | 1:75:A:LEU:HD22  | 1:31:A:LEU:HD13  | 11       | 0.58          |
| (1,3171) | 1:75:A:LEU:HD22  | 1:31:A:LEU:HD12  | 12       | 0.58          |
| (1,3067) | 1:52:A:ILE:HG22  | 1:53:A:PHE:HB3   | 10       | 0.58          |
| (1,3045) | 1:52:A:ILE:HG13  | 1:54:A:GLN:HE21  | 4        | 0.58          |
| (1,3045) | 1:52:A:ILE:HG13  | 1:54:A:GLN:HE21  | 9        | 0.58          |
| (1,2991) | 1:54:A:GLN:HE22  | 1:54:A:GLN:HG2   | 1        | 0.58          |
| (1,2962) | 1:97:A:LEU:HD21  | 1:56:A:LEU:HD21  | 4        | 0.58          |
| (1,2954) | 1:71:A:LEU:HB2   | 1:75:A:LEU:HD12  | 8        | 0.58          |
| (1,2954) | 1:71:A:LEU:HB2   | 1:75:A:LEU:HD13  | 12       | 0.58          |
| (1,2954) | 1:71:A:LEU:HB2   | 1:75:A:LEU:HD12  | 15       | 0.58          |
| (1,2902) | 1:50:A:ILE:HD12  | 1:76:A:ARG:H     | 13       | 0.58          |
| (1,2886) | 1:41:A:ALA:HA    | 1:32:A:ALA:HB1   | 13       | 0.58          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2880) | 1:61:A:ALA:HB2  | 1:57:A:VAL:HG13  | 4        | 0.58          |
| (1,2880) | 1:61:A:ALA:HB1  | 1:57:A:VAL:HG12  | 15       | 0.58          |
| (1,2880) | 1:61:A:ALA:HB3  | 1:57:A:VAL:HG13  | 16       | 0.58          |
| (1,2865) | 1:78:A:TYR:HE2  | 1:48:A:LEU:HD13  | 6        | 0.58          |
| (1,2673) | 1:97:A:LEU:HD11 | 1:35:A:PHE:HD2   | 10       | 0.58          |
| (1,2669) | 1:75:A:LEU:HD22 | 1:78:A:TYR:HE2   | 6        | 0.58          |
| (1,2669) | 1:75:A:LEU:HD23 | 1:78:A:TYR:HE2   | 13       | 0.58          |
| (1,2664) | 1:97:A:LEU:HD11 | 1:60:A:VAL:HG12  | 10       | 0.58          |
| (1,2600) | 1:105:A:LEU:HA  | 1:105:A:LEU:HD21 | 12       | 0.58          |
| (1,2585) | 1:92:A:ALA:HA   | 1:93:A:THR:HG21  | 10       | 0.58          |
| (1,2585) | 1:92:A:ALA:HA   | 1:93:A:THR:HG21  | 17       | 0.58          |
| (1,2582) | 1:60:A:VAL:HG12 | 1:57:A:VAL:HG12  | 2        | 0.58          |
| (1,2582) | 1:60:A:VAL:HG12 | 1:57:A:VAL:HG12  | 6        | 0.58          |
| (1,2572) | 1:125:A:GLN:H   | 1:124:A:VAL:HG22 | 4        | 0.58          |
| (1,2572) | 1:125:A:GLN:H   | 1:124:A:VAL:HG22 | 11       | 0.58          |
| (1,2572) | 1:125:A:GLN:H   | 1:124:A:VAL:HG22 | 15       | 0.58          |
| (1,2458) | 1:21:A:LEU:HA   | 1:21:A:LEU:HD13  | 2        | 0.58          |
| (1,2398) | 1:50:A:ILE:HD11 | 1:50:A:ILE:H     | 1        | 0.58          |
| (1,2398) | 1:50:A:ILE:HD12 | 1:50:A:ILE:H     | 3        | 0.58          |
| (1,2398) | 1:50:A:ILE:HD12 | 1:50:A:ILE:H     | 10       | 0.58          |
| (1,2309) | 1:39:A:PHE:HB3  | 1:39:A:PHE:HE2   | 3        | 0.58          |
| (1,2305) | 1:45:A:ALA:HB2  | 1:44:A:GLU:HA    | 5        | 0.58          |
| (1,2172) | 1:34:A:ARG:HD3  | 1:60:A:VAL:HG13  | 10       | 0.58          |
| (1,2142) | 1:21:A:LEU:HD13 | 1:30:A:PHE:HA    | 5        | 0.58          |
| (1,2094) | 1:95:A:VAL:HG21 | 1:97:A:LEU:HD21  | 14       | 0.58          |
| (1,2026) | 1:57:A:VAL:HG13 | 1:53:A:PHE:HD1   | 17       | 0.58          |
| (1,1998) | 1:116:A:GLN:HG3 | 1:116:A:GLN:HE21 | 6        | 0.58          |
| (1,1998) | 1:116:A:GLN:HG3 | 1:116:A:GLN:HE21 | 8        | 0.58          |
| (1,1998) | 1:116:A:GLN:HG3 | 1:116:A:GLN:HE21 | 14       | 0.58          |
| (1,1990) | 1:92:A:ALA:HB2  | 1:91:A:GLY:H     | 10       | 0.58          |
| (1,1990) | 1:92:A:ALA:HB2  | 1:91:A:GLY:H     | 15       | 0.58          |
| (1,1851) | 1:35:A:PHE:HE2  | 1:38:A:CYS:HB2   | 3        | 0.58          |
| (1,1682) | 1:41:A:ALA:HB2  | 1:33:A:GLU:H     | 13       | 0.58          |
| (1,1601) | 1:75:A:LEU:HD23 | 1:31:A:LEU:HD12  | 7        | 0.58          |
| (1,1601) | 1:75:A:LEU:HD23 | 1:31:A:LEU:HD11  | 17       | 0.58          |
| (1,1507) | 1:78:A:TYR:HE2  | 1:28:A:ILE:HG23  | 2        | 0.58          |
| (1,1450) | 1:54:A:GLN:HE22 | 1:54:A:GLN:HG2   | 2        | 0.58          |
| (1,1420) | 1:97:A:LEU:HD21 | 1:56:A:LEU:HD23  | 9        | 0.58          |
| (1,1420) | 1:97:A:LEU:HD22 | 1:56:A:LEU:HD22  | 16       | 0.58          |
| (1,1369) | 1:39:A:PHE:HZ   | 1:28:A:ILE:HD12  | 5        | 0.58          |
| (1,1369) | 1:39:A:PHE:HZ   | 1:28:A:ILE:HD13  | 10       | 0.58          |
| (1,1369) | 1:39:A:PHE:HZ   | 1:28:A:ILE:HD12  | 13       | 0.58          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1369) | 1:39:A:PHE:HZ    | 1:28:A:ILE:HD11 | 16       | 0.58          |
| (1,1361) | 1:41:A:ALA:HA    | 1:32:A:ALA:HB3  | 1        | 0.58          |
| (1,1360) | 1:32:A:ALA:HB1   | 1:31:A:LEU:H    | 5        | 0.58          |
| (1,1360) | 1:32:A:ALA:HB2   | 1:31:A:LEU:H    | 8        | 0.58          |
| (1,1356) | 1:61:A:ALA:HB1   | 1:57:A:VAL:HG13 | 6        | 0.58          |
| (1,1342) | 1:48:A:LEU:HD11  | 1:84:A:TYR:HE1  | 5        | 0.58          |
| (1,1308) | 1:97:A:LEU:HD22  | 1:35:A:PHE:HD2  | 15       | 0.58          |
| (1,1301) | 1:97:A:LEU:HD13  | 1:97:A:LEU:HA   | 7        | 0.58          |
| (1,1137) | 1:97:A:LEU:HD12  | 1:35:A:PHE:HD2  | 7        | 0.58          |
| (1,1125) | 1:97:A:LEU:HD12  | 1:60:A:VAL:HG11 | 12       | 0.58          |
| (1,1069) | 1:48:A:LEU:HD12  | 1:52:A:ILE:HG12 | 9        | 0.58          |
| (1,1069) | 1:48:A:LEU:HD12  | 1:52:A:ILE:HG12 | 13       | 0.58          |
| (1,370)  | 1:71:A:LEU:HD13  | 1:61:A:ALA:H    | 8        | 0.58          |
| (1,370)  | 1:71:A:LEU:HD12  | 1:61:A:ALA:H    | 10       | 0.58          |
| (1,241)  | 1:95:A:VAL:HG13  | 1:96:A:ASP:H    | 3        | 0.58          |
| (1,222)  | 1:102:A:CYS:H    | 1:95:A:VAL:HG13 | 16       | 0.58          |
| (3,150)  | 1:77:A:LEU:H     | 1:79:A:THR:HG21 | 6        | 0.57          |
| (3,132)  | 1:113:A:ALA:HB3  | 1:112:A:HIS:H   | 7        | 0.57          |
| (3,126)  | 1:21:A:LEU:HD21  | 1:22:A:ASN:H    | 16       | 0.57          |
| (3,123)  | 1:50:A:ILE:HD13  | 1:79:A:THR:HA   | 9        | 0.57          |
| (3,105)  | 1:64:A:MET:H     | 1:66:A:LEU:HD21 | 2        | 0.57          |
| (3,105)  | 1:64:A:MET:H     | 1:66:A:LEU:HD22 | 10       | 0.57          |
| (3,105)  | 1:64:A:MET:H     | 1:66:A:LEU:HD21 | 16       | 0.57          |
| (3,99)   | 1:72:A:ARG:HG3   | 1:75:A:LEU:HD12 | 15       | 0.57          |
| (3,97)   | 1:31:A:LEU:HD21  | 1:30:A:PHE:HB3  | 5        | 0.57          |
| (3,97)   | 1:31:A:LEU:HD23  | 1:30:A:PHE:HB3  | 12       | 0.57          |
| (3,96)   | 1:110:A:VAL:HG21 | 1:109:A:HIS:HA  | 12       | 0.57          |
| (3,78)   | 1:77:A:LEU:HD22  | 1:77:A:LEU:H    | 1        | 0.57          |
| (3,78)   | 1:77:A:LEU:HD21  | 1:77:A:LEU:H    | 10       | 0.57          |
| (3,65)   | 1:49:A:LYS:HB2   | 1:52:A:ILE:HG22 | 9        | 0.57          |
| (3,40)   | 1:55:A:ASP:H     | 1:52:A:ILE:HD12 | 9        | 0.57          |
| (3,40)   | 1:55:A:ASP:H     | 1:52:A:ILE:HD13 | 16       | 0.57          |
| (3,36)   | 1:50:A:ILE:HG21  | 1:49:A:LYS:HB2  | 7        | 0.57          |
| (1,4171) | 1:48:A:LEU:HD23  | 1:49:A:LYS:H    | 6        | 0.57          |
| (1,4168) | 1:48:A:LEU:H     | 1:48:A:LEU:HD12 | 11       | 0.57          |
| (1,4164) | 1:32:A:ALA:HB2   | 1:41:A:ALA:H    | 6        | 0.57          |
| (1,4164) | 1:32:A:ALA:HB1   | 1:41:A:ALA:H    | 14       | 0.57          |
| (1,4124) | 1:116:A:GLN:HE21 | 1:120:A:ALA:H   | 10       | 0.57          |
| (1,4120) | 1:116:A:GLN:HE21 | 1:119:A:GLU:HB2 | 10       | 0.57          |
| (1,4082) | 1:22:A:ASN:HD21  | 1:22:A:ASN:HB3  | 8        | 0.57          |
| (1,4028) | 1:31:A:LEU:HD22  | 1:32:A:ALA:H    | 2        | 0.57          |
| (1,4028) | 1:31:A:LEU:HD23  | 1:32:A:ALA:H    | 7        | 0.57          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,4028) | 1:31:A:LEU:HD22  | 1:32:A:ALA:H     | 8        | 0.57          |
| (1,4028) | 1:31:A:LEU:HD21  | 1:32:A:ALA:H     | 10       | 0.57          |
| (1,4028) | 1:31:A:LEU:HD21  | 1:32:A:ALA:H     | 13       | 0.57          |
| (1,4028) | 1:31:A:LEU:HD21  | 1:32:A:ALA:H     | 14       | 0.57          |
| (1,4028) | 1:31:A:LEU:HD22  | 1:32:A:ALA:H     | 15       | 0.57          |
| (1,3810) | 1:105:A:LEU:HD13 | 1:106:A:ASP:H    | 5        | 0.57          |
| (1,3541) | 1:64:A:MET:HB2   | 1:21:A:LEU:HD21  | 1        | 0.57          |
| (1,3484) | 1:32:A:ALA:H     | 1:31:A:LEU:HD12  | 17       | 0.57          |
| (1,3452) | 1:95:A:VAL:HA    | 1:93:A:THR:HG23  | 6        | 0.57          |
| (1,3452) | 1:95:A:VAL:HA    | 1:93:A:THR:HG23  | 10       | 0.57          |
| (1,3377) | 1:40:A:SER:HB2   | 1:41:A:ALA:HB2   | 13       | 0.57          |
| (1,3171) | 1:75:A:LEU:HD21  | 1:31:A:LEU:HD13  | 9        | 0.57          |
| (1,3171) | 1:75:A:LEU:HD22  | 1:31:A:LEU:HD11  | 16       | 0.57          |
| (1,2962) | 1:97:A:LEU:HD23  | 1:56:A:LEU:HD23  | 6        | 0.57          |
| (1,2962) | 1:97:A:LEU:HD21  | 1:56:A:LEU:HD23  | 13       | 0.57          |
| (1,2954) | 1:71:A:LEU:HB2   | 1:75:A:LEU:HD11  | 9        | 0.57          |
| (1,2954) | 1:71:A:LEU:HB2   | 1:75:A:LEU:HD12  | 13       | 0.57          |
| (1,2926) | 1:21:A:LEU:HB2   | 1:21:A:LEU:HD22  | 10       | 0.57          |
| (1,2897) | 1:39:A:PHE:HZ    | 1:28:A:ILE:HD11  | 6        | 0.57          |
| (1,2897) | 1:39:A:PHE:HZ    | 1:28:A:ILE:HD13  | 12       | 0.57          |
| (1,2886) | 1:41:A:ALA:HA    | 1:32:A:ALA:HB3   | 3        | 0.57          |
| (1,2885) | 1:32:A:ALA:HB1   | 1:31:A:LEU:H     | 17       | 0.57          |
| (1,2864) | 1:78:A:TYR:HE2   | 1:78:A:TYR:HB3   | 9        | 0.57          |
| (1,2845) | 1:22:A:ASN:H     | 1:27:A:VAL:HG13  | 15       | 0.57          |
| (1,2845) | 1:22:A:ASN:H     | 1:27:A:VAL:HG13  | 17       | 0.57          |
| (1,2680) | 1:117:A:LEU:HD11 | 1:82:A:TRP:HD1   | 1        | 0.57          |
| (1,2669) | 1:75:A:LEU:HD21  | 1:78:A:TYR:HE2   | 9        | 0.57          |
| (1,2664) | 1:97:A:LEU:HD13  | 1:60:A:VAL:HG11  | 13       | 0.57          |
| (1,2600) | 1:105:A:LEU:HA   | 1:105:A:LEU:HD21 | 16       | 0.57          |
| (1,2585) | 1:92:A:ALA:HA    | 1:93:A:THR:HG23  | 6        | 0.57          |
| (1,2577) | 1:60:A:VAL:HG12  | 1:59:A:ARG:HA    | 7        | 0.57          |
| (1,2572) | 1:125:A:GLN:H    | 1:124:A:VAL:HG23 | 3        | 0.57          |
| (1,2572) | 1:125:A:GLN:H    | 1:124:A:VAL:HG21 | 8        | 0.57          |
| (1,2572) | 1:125:A:GLN:H    | 1:124:A:VAL:HG22 | 12       | 0.57          |
| (1,2572) | 1:125:A:GLN:H    | 1:124:A:VAL:HG23 | 17       | 0.57          |
| (1,2363) | 1:48:A:LEU:HD11  | 1:84:A:TYR:HE1   | 11       | 0.57          |
| (1,2309) | 1:39:A:PHE:HB3   | 1:39:A:PHE:HE1   | 5        | 0.57          |
| (1,2309) | 1:39:A:PHE:HB3   | 1:39:A:PHE:HE2   | 6        | 0.57          |
| (1,2309) | 1:39:A:PHE:HB3   | 1:39:A:PHE:HE2   | 7        | 0.57          |
| (1,2309) | 1:39:A:PHE:HB3   | 1:39:A:PHE:HE2   | 17       | 0.57          |
| (1,2147) | 1:85:A:LEU:HA    | 1:85:A:LEU:HD12  | 17       | 0.57          |
| (1,2142) | 1:21:A:LEU:HD11  | 1:30:A:PHE:HA    | 6        | 0.57          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2142) | 1:21:A:LEU:HD13  | 1:30:A:PHE:HA    | 15       | 0.57          |
| (1,2006) | 1:78:A:TYR:HE1   | 1:48:A:LEU:HD11  | 3        | 0.57          |
| (1,1990) | 1:92:A:ALA:HB2   | 1:91:A:GLY:H     | 5        | 0.57          |
| (1,1839) | 1:95:A:VAL:HA    | 1:93:A:THR:HG22  | 11       | 0.57          |
| (1,1839) | 1:95:A:VAL:HA    | 1:93:A:THR:HG21  | 16       | 0.57          |
| (1,1679) | 1:92:A:ALA:HB2   | 1:91:A:GLY:H     | 2        | 0.57          |
| (1,1635) | 1:121:A:LYS:HB2  | 1:117:A:LEU:HD12 | 16       | 0.57          |
| (1,1601) | 1:75:A:LEU:HD21  | 1:31:A:LEU:HD13  | 1        | 0.57          |
| (1,1601) | 1:75:A:LEU:HD21  | 1:31:A:LEU:HD13  | 5        | 0.57          |
| (1,1601) | 1:75:A:LEU:HD21  | 1:31:A:LEU:HD13  | 10       | 0.57          |
| (1,1420) | 1:97:A:LEU:HD21  | 1:56:A:LEU:HD21  | 11       | 0.57          |
| (1,1369) | 1:39:A:PHE:HZ    | 1:28:A:ILE:HD11  | 3        | 0.57          |
| (1,1360) | 1:32:A:ALA:HB3   | 1:31:A:LEU:H     | 15       | 0.57          |
| (1,1342) | 1:48:A:LEU:HD13  | 1:84:A:TYR:HE1   | 9        | 0.57          |
| (1,1334) | 1:81:A:SER:HB3   | 1:84:A:TYR:HD2   | 16       | 0.57          |
| (1,1315) | 1:95:A:VAL:HG21  | 1:97:A:LEU:HD23  | 16       | 0.57          |
| (1,1308) | 1:97:A:LEU:HD22  | 1:35:A:PHE:HD2   | 3        | 0.57          |
| (1,1301) | 1:97:A:LEU:HD11  | 1:97:A:LEU:HA    | 13       | 0.57          |
| (1,1301) | 1:97:A:LEU:HD12  | 1:97:A:LEU:HA    | 17       | 0.57          |
| (1,1125) | 1:97:A:LEU:HD12  | 1:60:A:VAL:HG11  | 7        | 0.57          |
| (1,1043) | 1:78:A:TYR:HE1   | 1:28:A:ILE:HD13  | 12       | 0.57          |
| (1,942)  | 1:93:A:THR:HB    | 1:95:A:VAL:HG12  | 3        | 0.57          |
| (1,720)  | 1:120:A:ALA:H    | 1:85:A:LEU:HD23  | 6        | 0.57          |
| (1,697)  | 1:57:A:VAL:HG12  | 1:56:A:LEU:H     | 13       | 0.57          |
| (1,559)  | 1:116:A:GLN:HE21 | 1:113:A:ALA:HA   | 12       | 0.57          |
| (1,370)  | 1:71:A:LEU:HD11  | 1:61:A:ALA:H     | 1        | 0.57          |
| (1,370)  | 1:71:A:LEU:HD12  | 1:61:A:ALA:H     | 13       | 0.57          |
| (1,370)  | 1:71:A:LEU:HD11  | 1:61:A:ALA:H     | 14       | 0.57          |
| (1,370)  | 1:71:A:LEU:HD12  | 1:61:A:ALA:H     | 16       | 0.57          |
| (1,370)  | 1:71:A:LEU:HD13  | 1:61:A:ALA:H     | 17       | 0.57          |
| (1,275)  | 1:85:A:LEU:HD22  | 1:87:A:GLY:H     | 2        | 0.57          |
| (1,222)  | 1:102:A:CYS:H    | 1:95:A:VAL:HG12  | 1        | 0.57          |
| (1,217)  | 1:93:A:THR:HG21  | 1:103:A:GLY:H    | 2        | 0.57          |
| (1,217)  | 1:93:A:THR:HG23  | 1:103:A:GLY:H    | 4        | 0.57          |
| (1,169)  | 1:120:A:ALA:HB3  | 1:119:A:GLU:H    | 12       | 0.57          |
| (1,12)   | 1:100:A:ASN:H    | 1:100:A:ASN:HD21 | 16       | 0.57          |
| (3,153)  | 1:110:A:VAL:HG23 | 1:114:A:ARG:H    | 12       | 0.56          |
| (3,152)  | 1:27:A:VAL:H     | 1:74:A:ALA:HB2   | 2        | 0.56          |
| (3,152)  | 1:27:A:VAL:H     | 1:74:A:ALA:HB2   | 3        | 0.56          |
| (3,136)  | 1:82:A:TRP:HD1   | 1:82:A:TRP:H     | 16       | 0.56          |
| (3,105)  | 1:64:A:MET:H     | 1:66:A:LEU:HD22  | 1        | 0.56          |
| (3,105)  | 1:64:A:MET:H     | 1:66:A:LEU:HD22  | 6        | 0.56          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (3,100)  | 1:64:A:MET:HB2   | 1:21:A:LEU:HD11 | 7        | 0.56          |
| (3,99)   | 1:72:A:ARG:HG3   | 1:75:A:LEU:HD11 | 1        | 0.56          |
| (3,97)   | 1:31:A:LEU:HD22  | 1:30:A:PHE:HB3  | 2        | 0.56          |
| (3,97)   | 1:31:A:LEU:HD22  | 1:30:A:PHE:HB3  | 9        | 0.56          |
| (3,97)   | 1:31:A:LEU:HD21  | 1:30:A:PHE:HB3  | 14       | 0.56          |
| (3,96)   | 1:110:A:VAL:HG21 | 1:109:A:HIS:HA  | 1        | 0.56          |
| (3,96)   | 1:110:A:VAL:HG21 | 1:109:A:HIS:HA  | 3        | 0.56          |
| (3,96)   | 1:110:A:VAL:HG23 | 1:109:A:HIS:HA  | 6        | 0.56          |
| (3,96)   | 1:110:A:VAL:HG21 | 1:109:A:HIS:HA  | 9        | 0.56          |
| (3,96)   | 1:110:A:VAL:HG22 | 1:109:A:HIS:HA  | 13       | 0.56          |
| (3,96)   | 1:110:A:VAL:HG22 | 1:109:A:HIS:HA  | 15       | 0.56          |
| (3,92)   | 1:88:A:VAL:HG22  | 1:49:A:LYS:HA   | 1        | 0.56          |
| (3,51)   | 1:95:A:VAL:HG21  | 1:49:A:LYS:HA   | 12       | 0.56          |
| (3,40)   | 1:55:A:ASP:H     | 1:52:A:ILE:HD12 | 2        | 0.56          |
| (3,36)   | 1:49:A:LYS:HB2   | 1:52:A:ILE:HD13 | 2        | 0.56          |
| (1,4342) | 1:38:A:CYS:H     | 1:95:A:VAL:HG12 | 4        | 0.56          |
| (1,4283) | 1:120:A:ALA:H    | 1:85:A:LEU:HD23 | 16       | 0.56          |
| (1,4259) | 1:57:A:VAL:HG12  | 1:56:A:LEU:H    | 16       | 0.56          |
| (1,4171) | 1:48:A:LEU:HD23  | 1:49:A:LYS:H    | 5        | 0.56          |
| (1,4171) | 1:48:A:LEU:HD21  | 1:49:A:LYS:H    | 12       | 0.56          |
| (1,4171) | 1:48:A:LEU:HD23  | 1:49:A:LYS:H    | 13       | 0.56          |
| (1,4171) | 1:48:A:LEU:HD22  | 1:49:A:LYS:H    | 15       | 0.56          |
| (1,4132) | 1:60:A:VAL:HG13  | 1:34:A:ARG:HE   | 3        | 0.56          |
| (1,4132) | 1:60:A:VAL:HG12  | 1:34:A:ARG:HE   | 4        | 0.56          |
| (1,4132) | 1:60:A:VAL:HG12  | 1:34:A:ARG:HE   | 9        | 0.56          |
| (1,4122) | 1:116:A:GLN:HE21 | 1:113:A:ALA:HA  | 14       | 0.56          |
| (1,4091) | 1:65:A:ASN:HD22  | 1:20:A:LYS:HA   | 15       | 0.56          |
| (1,4082) | 1:22:A:ASN:HD21  | 1:22:A:ASN:HB3  | 2        | 0.56          |
| (1,4082) | 1:22:A:ASN:HD21  | 1:22:A:ASN:HB3  | 5        | 0.56          |
| (1,4082) | 1:22:A:ASN:HD21  | 1:22:A:ASN:HB3  | 6        | 0.56          |
| (1,4028) | 1:31:A:LEU:HD22  | 1:32:A:ALA:H    | 3        | 0.56          |
| (1,4028) | 1:31:A:LEU:HD21  | 1:32:A:ALA:H    | 5        | 0.56          |
| (1,4028) | 1:31:A:LEU:HD22  | 1:32:A:ALA:H    | 11       | 0.56          |
| (1,4028) | 1:31:A:LEU:HD21  | 1:32:A:ALA:H    | 16       | 0.56          |
| (1,3947) | 1:71:A:LEU:HD11  | 1:61:A:ALA:H    | 11       | 0.56          |
| (1,3810) | 1:105:A:LEU:HD11 | 1:106:A:ASP:H   | 4        | 0.56          |
| (1,3810) | 1:105:A:LEU:HD12 | 1:106:A:ASP:H   | 8        | 0.56          |
| (1,3810) | 1:105:A:LEU:HD12 | 1:106:A:ASP:H   | 9        | 0.56          |
| (1,3810) | 1:105:A:LEU:HD12 | 1:106:A:ASP:H   | 13       | 0.56          |
| (1,3810) | 1:105:A:LEU:HD12 | 1:106:A:ASP:H   | 16       | 0.56          |
| (1,3810) | 1:105:A:LEU:HD11 | 1:106:A:ASP:H   | 17       | 0.56          |
| (1,3799) | 1:105:A:LEU:HD11 | 1:111:A:GLU:H   | 4        | 0.56          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3570) | 1:90:A:PRO:HA   | 1:105:A:LEU:HD11 | 6        | 0.56          |
| (1,3570) | 1:90:A:PRO:HA   | 1:105:A:LEU:HD13 | 14       | 0.56          |
| (1,3541) | 1:64:A:MET:HB2  | 1:21:A:LEU:HD21  | 6        | 0.56          |
| (1,3484) | 1:32:A:ALA:H    | 1:31:A:LEU:HD11  | 9        | 0.56          |
| (1,3484) | 1:32:A:ALA:H    | 1:31:A:LEU:HD11  | 15       | 0.56          |
| (1,3452) | 1:95:A:VAL:HA   | 1:93:A:THR:HG22  | 3        | 0.56          |
| (1,3452) | 1:95:A:VAL:HA   | 1:93:A:THR:HG23  | 17       | 0.56          |
| (1,3446) | 1:65:A:ASN:HD22 | 1:20:A:LYS:HG2   | 6        | 0.56          |
| (1,3302) | 1:83:A:ARG:HB2  | 1:86:A:TYR:HD2   | 6        | 0.56          |
| (1,3281) | 1:93:A:THR:HG22 | 1:104:A:GLU:HG2  | 5        | 0.56          |
| (1,3256) | 1:41:A:ALA:HB1  | 1:33:A:GLU:H     | 4        | 0.56          |
| (1,3204) | 1:121:A:LYS:HB2 | 1:117:A:LEU:HD13 | 5        | 0.56          |
| (1,3204) | 1:121:A:LYS:HB2 | 1:117:A:LEU:HD12 | 13       | 0.56          |
| (1,3171) | 1:75:A:LEU:HD23 | 1:31:A:LEU:HD12  | 4        | 0.56          |
| (1,3171) | 1:75:A:LEU:HD22 | 1:31:A:LEU:HD11  | 8        | 0.56          |
| (1,3171) | 1:75:A:LEU:HD21 | 1:31:A:LEU:HD12  | 14       | 0.56          |
| (1,3171) | 1:75:A:LEU:HD22 | 1:31:A:LEU:HD13  | 15       | 0.56          |
| (1,3021) | 1:64:A:MET:HE1  | 1:63:A:GLU:H     | 7        | 0.56          |
| (1,2902) | 1:50:A:ILE:HD13 | 1:76:A:ARG:H     | 3        | 0.56          |
| (1,2885) | 1:32:A:ALA:HB2  | 1:31:A:LEU:H     | 14       | 0.56          |
| (1,2880) | 1:61:A:ALA:HB3  | 1:57:A:VAL:HG13  | 9        | 0.56          |
| (1,2865) | 1:78:A:TYR:HE1  | 1:48:A:LEU:HD11  | 10       | 0.56          |
| (1,2854) | 1:85:A:LEU:HD23 | 1:84:A:TYR:HD2   | 4        | 0.56          |
| (1,2852) | 1:81:A:SER:HB3  | 1:84:A:TYR:HD1   | 5        | 0.56          |
| (1,2852) | 1:81:A:SER:HB3  | 1:84:A:TYR:HD2   | 11       | 0.56          |
| (1,2845) | 1:22:A:ASN:H    | 1:27:A:VAL:HG12  | 5        | 0.56          |
| (1,2845) | 1:22:A:ASN:H    | 1:27:A:VAL:HG12  | 10       | 0.56          |
| (1,2831) | 1:97:A:LEU:HD22 | 1:35:A:PHE:HD1   | 6        | 0.56          |
| (1,2817) | 1:97:A:LEU:HD11 | 1:97:A:LEU:HA    | 15       | 0.56          |
| (1,2681) | 1:120:A:ALA:HB2 | 1:82:A:TRP:HD1   | 5        | 0.56          |
| (1,2673) | 1:97:A:LEU:HD11 | 1:35:A:PHE:HD2   | 17       | 0.56          |
| (1,2608) | 1:48:A:LEU:HD12 | 1:52:A:ILE:HG12  | 12       | 0.56          |
| (1,2608) | 1:48:A:LEU:HD13 | 1:52:A:ILE:HG12  | 15       | 0.56          |
| (1,2600) | 1:105:A:LEU:HA  | 1:105:A:LEU:HD21 | 4        | 0.56          |
| (1,2582) | 1:60:A:VAL:HG11 | 1:57:A:VAL:HG12  | 1        | 0.56          |
| (1,2572) | 1:125:A:GLN:H   | 1:124:A:VAL:HG21 | 1        | 0.56          |
| (1,2397) | 1:50:A:ILE:HD11 | 1:50:A:ILE:HA    | 15       | 0.56          |
| (1,2324) | 1:97:A:LEU:HD23 | 1:39:A:PHE:H     | 1        | 0.56          |
| (1,2324) | 1:97:A:LEU:HD22 | 1:39:A:PHE:H     | 8        | 0.56          |
| (1,2309) | 1:39:A:PHE:HB3  | 1:39:A:PHE:HE2   | 11       | 0.56          |
| (1,2309) | 1:39:A:PHE:HB3  | 1:39:A:PHE:HE1   | 15       | 0.56          |
| (1,2305) | 1:45:A:ALA:HB2  | 1:44:A:GLU:HA    | 3        | 0.56          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2248) | 1:57:A:VAL:HG21  | 1:57:A:VAL:HA    | 17       | 0.56          |
| (1,2147) | 1:85:A:LEU:HA    | 1:85:A:LEU:HD11  | 7        | 0.56          |
| (1,1790) | 1:90:A:PRO:HA    | 1:92:A:ALA:HB3   | 16       | 0.56          |
| (1,1751) | 1:32:A:ALA:HB2   | 1:41:A:ALA:H     | 7        | 0.56          |
| (1,1751) | 1:32:A:ALA:HB3   | 1:41:A:ALA:H     | 16       | 0.56          |
| (1,1679) | 1:92:A:ALA:HB1   | 1:91:A:GLY:H     | 9        | 0.56          |
| (1,1635) | 1:121:A:LYS:HB2  | 1:117:A:LEU:HD12 | 4        | 0.56          |
| (1,1502) | 1:52:A:ILE:HG13  | 1:54:A:GLN:HE21  | 13       | 0.56          |
| (1,1420) | 1:97:A:LEU:HD23  | 1:56:A:LEU:HD23  | 17       | 0.56          |
| (1,1372) | 1:28:A:ILE:HD13  | 1:31:A:LEU:HB3   | 12       | 0.56          |
| (1,1369) | 1:39:A:PHE:HZ    | 1:28:A:ILE:HD11  | 4        | 0.56          |
| (1,1369) | 1:39:A:PHE:HZ    | 1:28:A:ILE:HD13  | 11       | 0.56          |
| (1,1360) | 1:32:A:ALA:HB1   | 1:31:A:LEU:H     | 6        | 0.56          |
| (1,1360) | 1:32:A:ALA:HB1   | 1:31:A:LEU:H     | 7        | 0.56          |
| (1,1343) | 1:78:A:TYR:HE2   | 1:48:A:LEU:HD11  | 1        | 0.56          |
| (1,1301) | 1:97:A:LEU:HD12  | 1:97:A:LEU:HA    | 11       | 0.56          |
| (1,1158) | 1:120:A:ALA:HB3  | 1:82:A:TRP:HD1   | 10       | 0.56          |
| (1,1137) | 1:97:A:LEU:HD13  | 1:35:A:PHE:HD2   | 14       | 0.56          |
| (1,1069) | 1:48:A:LEU:HD13  | 1:52:A:ILE:HG12  | 3        | 0.56          |
| (1,720)  | 1:120:A:ALA:H    | 1:85:A:LEU:HD21  | 14       | 0.56          |
| (1,697)  | 1:57:A:VAL:HG11  | 1:56:A:LEU:H     | 2        | 0.56          |
| (1,697)  | 1:57:A:VAL:HG12  | 1:56:A:LEU:H     | 4        | 0.56          |
| (1,610)  | 1:48:A:LEU:HD22  | 1:49:A:LYS:H     | 8        | 0.56          |
| (1,604)  | 1:32:A:ALA:HB1   | 1:41:A:ALA:H     | 12       | 0.56          |
| (1,389)  | 1:58:A:ASP:H     | 1:57:A:VAL:HG12  | 2        | 0.56          |
| (1,370)  | 1:71:A:LEU:HD13  | 1:61:A:ALA:H     | 2        | 0.56          |
| (1,370)  | 1:71:A:LEU:HD11  | 1:61:A:ALA:H     | 15       | 0.56          |
| (1,275)  | 1:85:A:LEU:HD23  | 1:87:A:GLY:H     | 4        | 0.56          |
| (1,275)  | 1:85:A:LEU:HD21  | 1:87:A:GLY:H     | 5        | 0.56          |
| (1,263)  | 1:110:A:VAL:HG23 | 1:91:A:GLY:H     | 15       | 0.56          |
| (1,241)  | 1:95:A:VAL:HG13  | 1:96:A:ASP:H     | 1        | 0.56          |
| (1,126)  | 1:28:A:ILE:H     | 1:29:A:ALA:HB1   | 4        | 0.56          |
| (1,126)  | 1:28:A:ILE:H     | 1:29:A:ALA:HB2   | 14       | 0.56          |
| (3,152)  | 1:27:A:VAL:H     | 1:74:A:ALA:HB3   | 11       | 0.55          |
| (3,150)  | 1:77:A:LEU:H     | 1:79:A:THR:HG21  | 11       | 0.55          |
| (3,150)  | 1:77:A:LEU:H     | 1:79:A:THR:HG21  | 17       | 0.55          |
| (3,143)  | 1:25:A:LYS:H     | 1:77:A:LEU:HD21  | 12       | 0.55          |
| (3,136)  | 1:81:A:SER:H     | 1:82:A:TRP:H     | 11       | 0.55          |
| (3,116)  | 1:95:A:VAL:H     | 1:48:A:LEU:HD12  | 11       | 0.55          |
| (3,99)   | 1:72:A:ARG:HG3   | 1:75:A:LEU:HD11  | 3        | 0.55          |
| (3,99)   | 1:72:A:ARG:HG3   | 1:75:A:LEU:HD13  | 12       | 0.55          |
| (3,98)   | 1:64:A:MET:HE3   | 1:63:A:GLU:HG3   | 17       | 0.55          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (3,97)   | 1:31:A:LEU:HD21  | 1:30:A:PHE:HB3  | 6        | 0.55          |
| (3,97)   | 1:31:A:LEU:HD21  | 1:30:A:PHE:HB3  | 10       | 0.55          |
| (3,97)   | 1:31:A:LEU:HD21  | 1:30:A:PHE:HB3  | 16       | 0.55          |
| (3,97)   | 1:31:A:LEU:HD21  | 1:30:A:PHE:HB3  | 17       | 0.55          |
| (3,96)   | 1:110:A:VAL:HG22 | 1:109:A:HIS:HA  | 10       | 0.55          |
| (3,96)   | 1:110:A:VAL:HG22 | 1:109:A:HIS:HA  | 11       | 0.55          |
| (3,96)   | 1:110:A:VAL:HG21 | 1:109:A:HIS:HA  | 16       | 0.55          |
| (3,72)   | 1:117:A:LEU:HG   | 1:117:A:LEU:H   | 6        | 0.55          |
| (3,55)   | 1:97:A:LEU:HD21  | 1:75:A:LEU:HD11 | 11       | 0.55          |
| (3,52)   | 1:95:A:VAL:HG21  | 1:37:A:HIS:HB2  | 3        | 0.55          |
| (3,40)   | 1:55:A:ASP:H     | 1:52:A:ILE:HD12 | 1        | 0.55          |
| (3,40)   | 1:55:A:ASP:H     | 1:52:A:ILE:HD13 | 3        | 0.55          |
| (3,40)   | 1:55:A:ASP:H     | 1:52:A:ILE:HD12 | 4        | 0.55          |
| (3,21)   | 1:22:A:ASN:H     | 1:21:A:LEU:HD11 | 13       | 0.55          |
| (3,18)   | 1:58:A:ASP:HB3   | 1:60:A:VAL:HG13 | 2        | 0.55          |
| (1,4259) | 1:57:A:VAL:HG12  | 1:56:A:LEU:H    | 6        | 0.55          |
| (1,4247) | 1:54:A:GLN:HE22  | 1:57:A:VAL:HG12 | 12       | 0.55          |
| (1,4082) | 1:22:A:ASN:HD21  | 1:22:A:ASN:HB3  | 12       | 0.55          |
| (1,4028) | 1:31:A:LEU:HD21  | 1:32:A:ALA:H    | 6        | 0.55          |
| (1,3957) | 1:58:A:ASP:H     | 1:57:A:VAL:HG12 | 13       | 0.55          |
| (1,3861) | 1:110:A:VAL:HG22 | 1:91:A:GLY:H    | 17       | 0.55          |
| (1,3822) | 1:93:A:THR:HG21  | 1:103:A:GLY:H   | 8        | 0.55          |
| (1,3822) | 1:93:A:THR:HG23  | 1:103:A:GLY:H   | 14       | 0.55          |
| (1,3810) | 1:105:A:LEU:HD13 | 1:106:A:ASP:H   | 6        | 0.55          |
| (1,3810) | 1:105:A:LEU:HD13 | 1:106:A:ASP:H   | 7        | 0.55          |
| (1,3782) | 1:120:A:ALA:HB2  | 1:119:A:GLU:H   | 8        | 0.55          |
| (1,3601) | 1:113:A:ALA:HB3  | 1:111:A:GLU:H   | 7        | 0.55          |
| (1,3554) | 1:66:A:LEU:HB2   | 1:66:A:LEU:HD21 | 5        | 0.55          |
| (1,3554) | 1:66:A:LEU:HB2   | 1:66:A:LEU:HD22 | 11       | 0.55          |
| (1,3541) | 1:64:A:MET:HB2   | 1:21:A:LEU:HD22 | 11       | 0.55          |
| (1,3541) | 1:64:A:MET:HB2   | 1:21:A:LEU:HD22 | 17       | 0.55          |
| (1,3484) | 1:32:A:ALA:H     | 1:31:A:LEU:HD12 | 16       | 0.55          |
| (1,3446) | 1:65:A:ASN:HD22  | 1:20:A:LYS:HG2  | 1        | 0.55          |
| (1,3446) | 1:65:A:ASN:HD22  | 1:20:A:LYS:HG2  | 7        | 0.55          |
| (1,3377) | 1:40:A:SER:HB2   | 1:41:A:ALA:HB2  | 16       | 0.55          |
| (1,3376) | 1:41:A:ALA:HB2   | 1:40:A:SER:HB3  | 11       | 0.55          |
| (1,3366) | 1:72:A:ARG:HA    | 1:56:A:LEU:HD22 | 4        | 0.55          |
| (1,3171) | 1:75:A:LEU:HD21  | 1:31:A:LEU:HD12 | 3        | 0.55          |
| (1,3171) | 1:75:A:LEU:HD23  | 1:31:A:LEU:HD12 | 13       | 0.55          |
| (1,3116) | 1:57:A:VAL:HG23  | 1:53:A:PHE:HE2  | 1        | 0.55          |
| (1,3052) | 1:39:A:PHE:HZ    | 1:52:A:ILE:HG21 | 12       | 0.55          |
| (1,3023) | 1:64:A:MET:HE1   | 1:27:A:VAL:HA   | 10       | 0.55          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3023) | 1:64:A:MET:HE1  | 1:27:A:VAL:HA    | 12       | 0.55          |
| (1,3021) | 1:64:A:MET:HE1  | 1:63:A:GLU:H     | 1        | 0.55          |
| (1,3002) | 1:57:A:VAL:HG13 | 1:60:A:VAL:HB    | 12       | 0.55          |
| (1,2991) | 1:54:A:GLN:HE22 | 1:54:A:GLN:HG2   | 2        | 0.55          |
| (1,2962) | 1:97:A:LEU:HD22 | 1:56:A:LEU:HD22  | 16       | 0.55          |
| (1,2954) | 1:71:A:LEU:HB2  | 1:75:A:LEU:HD11  | 2        | 0.55          |
| (1,2954) | 1:71:A:LEU:HB2  | 1:75:A:LEU:HD11  | 3        | 0.55          |
| (1,2954) | 1:71:A:LEU:HB2  | 1:75:A:LEU:HD11  | 14       | 0.55          |
| (1,2926) | 1:21:A:LEU:HB2  | 1:21:A:LEU:HD21  | 14       | 0.55          |
| (1,2900) | 1:28:A:ILE:HD11 | 1:31:A:LEU:HB3   | 6        | 0.55          |
| (1,2897) | 1:39:A:PHE:HZ   | 1:28:A:ILE:HD13  | 7        | 0.55          |
| (1,2885) | 1:32:A:ALA:HB3  | 1:31:A:LEU:H     | 10       | 0.55          |
| (1,2865) | 1:78:A:TYR:HE2  | 1:48:A:LEU:HD12  | 9        | 0.55          |
| (1,2865) | 1:78:A:TYR:HE2  | 1:48:A:LEU:HD12  | 13       | 0.55          |
| (1,2854) | 1:85:A:LEU:HD22 | 1:84:A:TYR:HD1   | 1        | 0.55          |
| (1,2673) | 1:97:A:LEU:HD12 | 1:35:A:PHE:HD1   | 12       | 0.55          |
| (1,2669) | 1:75:A:LEU:HD22 | 1:78:A:TYR:HE2   | 8        | 0.55          |
| (1,2669) | 1:75:A:LEU:HD21 | 1:78:A:TYR:HE1   | 10       | 0.55          |
| (1,2669) | 1:75:A:LEU:HD22 | 1:78:A:TYR:HE1   | 16       | 0.55          |
| (1,2608) | 1:48:A:LEU:HD12 | 1:52:A:ILE:HG12  | 16       | 0.55          |
| (1,2585) | 1:92:A:ALA:HA   | 1:93:A:THR:HG22  | 5        | 0.55          |
| (1,2585) | 1:92:A:ALA:HA   | 1:93:A:THR:HG22  | 9        | 0.55          |
| (1,2585) | 1:92:A:ALA:HA   | 1:93:A:THR:HG22  | 15       | 0.55          |
| (1,2577) | 1:60:A:VAL:HG11 | 1:59:A:ARG:HA    | 4        | 0.55          |
| (1,2577) | 1:60:A:VAL:HG11 | 1:59:A:ARG:HA    | 9        | 0.55          |
| (1,2572) | 1:125:A:GLN:H   | 1:124:A:VAL:HG21 | 9        | 0.55          |
| (1,2423) | 1:64:A:MET:HA   | 1:64:A:MET:HE1   | 9        | 0.55          |
| (1,2309) | 1:39:A:PHE:HB3  | 1:39:A:PHE:HE2   | 1        | 0.55          |
| (1,2248) | 1:57:A:VAL:HG21 | 1:57:A:VAL:HA    | 7        | 0.55          |
| (1,2248) | 1:57:A:VAL:HG22 | 1:57:A:VAL:HA    | 10       | 0.55          |
| (1,2248) | 1:57:A:VAL:HG22 | 1:57:A:VAL:HA    | 13       | 0.55          |
| (1,2194) | 1:50:A:ILE:HD13 | 1:80:A:SER:H     | 17       | 0.55          |
| (1,2172) | 1:34:A:ARG:HD3  | 1:60:A:VAL:HG12  | 17       | 0.55          |
| (1,1851) | 1:35:A:PHE:HE1  | 1:38:A:CYS:HB2   | 13       | 0.55          |
| (1,1839) | 1:95:A:VAL:HA   | 1:93:A:THR:HG22  | 9        | 0.55          |
| (1,1839) | 1:95:A:VAL:HA   | 1:93:A:THR:HG22  | 12       | 0.55          |
| (1,1838) | 1:93:A:THR:HA   | 1:93:A:THR:HG23  | 7        | 0.55          |
| (1,1751) | 1:32:A:ALA:HB1  | 1:41:A:ALA:H     | 1        | 0.55          |
| (1,1751) | 1:32:A:ALA:HB2  | 1:41:A:ALA:H     | 3        | 0.55          |
| (1,1751) | 1:32:A:ALA:HB3  | 1:41:A:ALA:H     | 13       | 0.55          |
| (1,1740) | 1:77:A:LEU:HD12 | 1:78:A:TYR:H     | 8        | 0.55          |
| (1,1682) | 1:41:A:ALA:HB3  | 1:33:A:GLU:H     | 3        | 0.55          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1682) | 1:41:A:ALA:HB2  | 1:33:A:GLU:H     | 6        | 0.55          |
| (1,1682) | 1:41:A:ALA:HB2  | 1:33:A:GLU:H     | 9        | 0.55          |
| (1,1679) | 1:92:A:ALA:HB1  | 1:91:A:GLY:H     | 17       | 0.55          |
| (1,1635) | 1:121:A:LYS:HB2 | 1:117:A:LEU:HD12 | 8        | 0.55          |
| (1,1507) | 1:78:A:TYR:HE2  | 1:28:A:ILE:HG21  | 11       | 0.55          |
| (1,1482) | 1:64:A:MET:HE3  | 1:27:A:VAL:HA    | 3        | 0.55          |
| (1,1480) | 1:64:A:MET:HE1  | 1:63:A:GLU:H     | 9        | 0.55          |
| (1,1420) | 1:97:A:LEU:HD23 | 1:56:A:LEU:HD22  | 3        | 0.55          |
| (1,1369) | 1:39:A:PHE:HZ   | 1:28:A:ILE:HD13  | 1        | 0.55          |
| (1,1361) | 1:41:A:ALA:HA   | 1:32:A:ALA:HB2   | 14       | 0.55          |
| (1,1360) | 1:32:A:ALA:HB3  | 1:31:A:LEU:H     | 1        | 0.55          |
| (1,1343) | 1:78:A:TYR:HE1  | 1:48:A:LEU:HD13  | 7        | 0.55          |
| (1,1343) | 1:78:A:TYR:HE1  | 1:48:A:LEU:HD13  | 14       | 0.55          |
| (1,1334) | 1:81:A:SER:HB3  | 1:84:A:TYR:HD2   | 3        | 0.55          |
| (1,1334) | 1:81:A:SER:HB3  | 1:84:A:TYR:HD2   | 7        | 0.55          |
| (1,1334) | 1:81:A:SER:HB3  | 1:84:A:TYR:HD1   | 13       | 0.55          |
| (1,1305) | 1:97:A:LEU:HD23 | 1:52:A:ILE:HB    | 5        | 0.55          |
| (1,1069) | 1:48:A:LEU:HD12 | 1:52:A:ILE:HG12  | 8        | 0.55          |
| (1,720)  | 1:120:A:ALA:H   | 1:85:A:LEU:HD22  | 13       | 0.55          |
| (1,697)  | 1:57:A:VAL:HG12 | 1:56:A:LEU:H     | 9        | 0.55          |
| (1,610)  | 1:48:A:LEU:HD21 | 1:49:A:LYS:H     | 10       | 0.55          |
| (1,604)  | 1:32:A:ALA:HB1  | 1:41:A:ALA:H     | 10       | 0.55          |
| (1,467)  | 1:31:A:LEU:HD23 | 1:32:A:ALA:H     | 12       | 0.55          |
| (1,389)  | 1:58:A:ASP:H    | 1:57:A:VAL:HG12  | 1        | 0.55          |
| (1,389)  | 1:58:A:ASP:H    | 1:57:A:VAL:HG12  | 15       | 0.55          |
| (1,370)  | 1:71:A:LEU:HD13 | 1:61:A:ALA:H     | 3        | 0.55          |
| (1,370)  | 1:71:A:LEU:HD13 | 1:61:A:ALA:H     | 5        | 0.55          |
| (1,275)  | 1:85:A:LEU:HD23 | 1:87:A:GLY:H     | 13       | 0.55          |
| (1,275)  | 1:85:A:LEU:HD21 | 1:87:A:GLY:H     | 15       | 0.55          |
| (1,241)  | 1:95:A:VAL:HG11 | 1:96:A:ASP:H     | 9        | 0.55          |
| (1,222)  | 1:102:A:CYS:H   | 1:95:A:VAL:HG13  | 11       | 0.55          |
| (1,169)  | 1:120:A:ALA:HB1 | 1:119:A:GLU:H    | 7        | 0.55          |
| (1,169)  | 1:120:A:ALA:HB3 | 1:119:A:GLU:H    | 9        | 0.55          |
| (1,169)  | 1:120:A:ALA:HB3 | 1:119:A:GLU:H    | 17       | 0.55          |
| (3,152)  | 1:27:A:VAL:H    | 1:74:A:ALA:HB1   | 8        | 0.54          |
| (3,136)  | 1:82:A:TRP:HD1  | 1:82:A:TRP:H     | 5        | 0.54          |
| (3,136)  | 1:81:A:SER:H    | 1:82:A:TRP:H     | 9        | 0.54          |
| (3,132)  | 1:113:A:ALA:HB1 | 1:112:A:HIS:H    | 8        | 0.54          |
| (3,132)  | 1:113:A:ALA:HB3 | 1:112:A:HIS:H    | 12       | 0.54          |
| (3,126)  | 1:21:A:LEU:HD22 | 1:22:A:ASN:H     | 15       | 0.54          |
| (3,123)  | 1:50:A:ILE:HD11 | 1:79:A:THR:HA    | 6        | 0.54          |
| (3,105)  | 1:64:A:MET:H    | 1:66:A:LEU:HD22  | 15       | 0.54          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (3,98)   | 1:64:A:MET:HE3   | 1:63:A:GLU:HG3  | 10       | 0.54          |
| (3,96)   | 1:110:A:VAL:HG22 | 1:109:A:HIS:HA  | 2        | 0.54          |
| (3,96)   | 1:110:A:VAL:HG23 | 1:109:A:HIS:HA  | 7        | 0.54          |
| (3,78)   | 1:77:A:LEU:HD22  | 1:77:A:LEU:H    | 14       | 0.54          |
| (3,72)   | 1:117:A:LEU:HG   | 1:117:A:LEU:H   | 1        | 0.54          |
| (3,65)   | 1:52:A:ILE:HG13  | 1:52:A:ILE:HG22 | 11       | 0.54          |
| (3,51)   | 1:95:A:VAL:HG23  | 1:49:A:LYS:HA   | 13       | 0.54          |
| (3,40)   | 1:55:A:ASP:H     | 1:52:A:ILE:HD13 | 11       | 0.54          |
| (1,4283) | 1:120:A:ALA:H    | 1:85:A:LEU:HD22 | 4        | 0.54          |
| (1,4168) | 1:48:A:LEU:H     | 1:48:A:LEU:HD11 | 1        | 0.54          |
| (1,4164) | 1:32:A:ALA:HB2   | 1:41:A:ALA:H    | 7        | 0.54          |
| (1,4132) | 1:60:A:VAL:HG11  | 1:34:A:ARG:HE   | 6        | 0.54          |
| (1,4028) | 1:31:A:LEU:HD21  | 1:32:A:ALA:H    | 4        | 0.54          |
| (1,4028) | 1:31:A:LEU:HD22  | 1:32:A:ALA:H    | 9        | 0.54          |
| (1,3957) | 1:58:A:ASP:H     | 1:57:A:VAL:HG12 | 3        | 0.54          |
| (1,3957) | 1:58:A:ASP:H     | 1:57:A:VAL:HG12 | 4        | 0.54          |
| (1,3957) | 1:58:A:ASP:H     | 1:57:A:VAL:HG12 | 9        | 0.54          |
| (1,3943) | 1:66:A:LEU:HD12  | 1:62:A:GLY:H    | 1        | 0.54          |
| (1,3943) | 1:66:A:LEU:HD13  | 1:62:A:GLY:H    | 4        | 0.54          |
| (1,3870) | 1:85:A:LEU:HD21  | 1:87:A:GLY:H    | 16       | 0.54          |
| (1,3861) | 1:110:A:VAL:HG23 | 1:91:A:GLY:H    | 13       | 0.54          |
| (1,3861) | 1:110:A:VAL:HG22 | 1:91:A:GLY:H    | 16       | 0.54          |
| (1,3845) | 1:95:A:VAL:HG11  | 1:96:A:ASP:H    | 4        | 0.54          |
| (1,3822) | 1:93:A:THR:HG22  | 1:103:A:GLY:H   | 17       | 0.54          |
| (1,3810) | 1:105:A:LEU:HD13 | 1:106:A:ASP:H   | 2        | 0.54          |
| (1,3810) | 1:105:A:LEU:HD11 | 1:106:A:ASP:H   | 11       | 0.54          |
| (1,3810) | 1:105:A:LEU:HD13 | 1:106:A:ASP:H   | 12       | 0.54          |
| (1,3782) | 1:120:A:ALA:HB1  | 1:119:A:GLU:H   | 13       | 0.54          |
| (1,3601) | 1:113:A:ALA:HB2  | 1:111:A:GLU:H   | 5        | 0.54          |
| (1,3463) | 1:35:A:PHE:HE2   | 1:38:A:CYS:HB2  | 15       | 0.54          |
| (1,3452) | 1:95:A:VAL:HA    | 1:93:A:THR:HG22 | 7        | 0.54          |
| (1,3386) | 1:90:A:PRO:HA    | 1:92:A:ALA:HB1  | 10       | 0.54          |
| (1,3366) | 1:72:A:ARG:HA    | 1:56:A:LEU:HD23 | 3        | 0.54          |
| (1,3366) | 1:72:A:ARG:HA    | 1:56:A:LEU:HD22 | 11       | 0.54          |
| (1,3366) | 1:72:A:ARG:HA    | 1:56:A:LEU:HD22 | 17       | 0.54          |
| (1,3171) | 1:75:A:LEU:HD23  | 1:31:A:LEU:HD12 | 7        | 0.54          |
| (1,3171) | 1:75:A:LEU:HD23  | 1:31:A:LEU:HD11 | 17       | 0.54          |
| (1,3116) | 1:57:A:VAL:HG22  | 1:53:A:PHE:HE2  | 15       | 0.54          |
| (1,3068) | 1:52:A:ILE:HG23  | 1:53:A:PHE:HB2  | 11       | 0.54          |
| (1,3051) | 1:78:A:TYR:HE2   | 1:28:A:ILE:HG23 | 2        | 0.54          |
| (1,3036) | 1:78:A:TYR:HH    | 1:45:A:ALA:HB2  | 2        | 0.54          |
| (1,3023) | 1:64:A:MET:HE1   | 1:27:A:VAL:HA   | 17       | 0.54          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2962) | 1:97:A:LEU:HD21  | 1:56:A:LEU:HD23  | 9        | 0.54          |
| (1,2902) | 1:50:A:ILE:HD12  | 1:76:A:ARG:H     | 1        | 0.54          |
| (1,2902) | 1:50:A:ILE:HD12  | 1:76:A:ARG:H     | 7        | 0.54          |
| (1,2902) | 1:50:A:ILE:HD12  | 1:76:A:ARG:H     | 14       | 0.54          |
| (1,2897) | 1:39:A:PHE:HZ    | 1:28:A:ILE:HD13  | 2        | 0.54          |
| (1,2897) | 1:39:A:PHE:HZ    | 1:28:A:ILE:HD12  | 8        | 0.54          |
| (1,2886) | 1:41:A:ALA:HA    | 1:32:A:ALA:HB3   | 1        | 0.54          |
| (1,2886) | 1:41:A:ALA:HA    | 1:32:A:ALA:HB2   | 12       | 0.54          |
| (1,2880) | 1:61:A:ALA:HB1   | 1:57:A:VAL:HG13  | 6        | 0.54          |
| (1,2864) | 1:78:A:TYR:HE2   | 1:78:A:TYR:HB3   | 6        | 0.54          |
| (1,2852) | 1:81:A:SER:HB3   | 1:84:A:TYR:HD1   | 8        | 0.54          |
| (1,2845) | 1:22:A:ASN:H     | 1:27:A:VAL:HG12  | 13       | 0.54          |
| (1,2831) | 1:97:A:LEU:HD22  | 1:35:A:PHE:HD2   | 3        | 0.54          |
| (1,2831) | 1:97:A:LEU:HD22  | 1:35:A:PHE:HD2   | 15       | 0.54          |
| (1,2817) | 1:97:A:LEU:HD13  | 1:97:A:LEU:HA    | 7        | 0.54          |
| (1,2681) | 1:120:A:ALA:HB2  | 1:82:A:TRP:HD1   | 16       | 0.54          |
| (1,2680) | 1:117:A:LEU:HD12 | 1:82:A:TRP:HD1   | 16       | 0.54          |
| (1,2664) | 1:97:A:LEU:HD12  | 1:60:A:VAL:HG11  | 12       | 0.54          |
| (1,2664) | 1:97:A:LEU:HD11  | 1:60:A:VAL:HG11  | 17       | 0.54          |
| (1,2608) | 1:48:A:LEU:HD12  | 1:52:A:ILE:HG12  | 13       | 0.54          |
| (1,2585) | 1:92:A:ALA:HA    | 1:93:A:THR:HG23  | 2        | 0.54          |
| (1,2585) | 1:92:A:ALA:HA    | 1:93:A:THR:HG22  | 4        | 0.54          |
| (1,2585) | 1:92:A:ALA:HA    | 1:93:A:THR:HG22  | 16       | 0.54          |
| (1,2572) | 1:125:A:GLN:H    | 1:124:A:VAL:HG22 | 7        | 0.54          |
| (1,2458) | 1:21:A:LEU:HA    | 1:21:A:LEU:HD13  | 10       | 0.54          |
| (1,2398) | 1:50:A:ILE:HD12  | 1:50:A:ILE:H     | 5        | 0.54          |
| (1,2398) | 1:50:A:ILE:HD11  | 1:50:A:ILE:H     | 7        | 0.54          |
| (1,2397) | 1:50:A:ILE:HD12  | 1:50:A:ILE:HA    | 16       | 0.54          |
| (1,2309) | 1:39:A:PHE:HB3   | 1:39:A:PHE:HE2   | 9        | 0.54          |
| (1,2147) | 1:85:A:LEU:HA    | 1:85:A:LEU:HD11  | 15       | 0.54          |
| (1,2146) | 1:104:A:GLU:HB3  | 1:93:A:THR:HG21  | 7        | 0.54          |
| (1,2094) | 1:95:A:VAL:HG23  | 1:97:A:LEU:HD21  | 5        | 0.54          |
| (1,1990) | 1:92:A:ALA:HB3   | 1:91:A:GLY:H     | 1        | 0.54          |
| (1,1867) | 1:53:A:PHE:HA    | 1:31:A:LEU:HD12  | 7        | 0.54          |
| (1,1867) | 1:53:A:PHE:HA    | 1:31:A:LEU:HD12  | 12       | 0.54          |
| (1,1867) | 1:53:A:PHE:HA    | 1:31:A:LEU:HD12  | 14       | 0.54          |
| (1,1851) | 1:35:A:PHE:HE2   | 1:38:A:CYS:HB2   | 7        | 0.54          |
| (1,1758) | 1:79:A:THR:HG23  | 1:48:A:LEU:HD13  | 17       | 0.54          |
| (1,1751) | 1:32:A:ALA:HB2   | 1:41:A:ALA:H     | 5        | 0.54          |
| (1,1740) | 1:77:A:LEU:HD13  | 1:78:A:TYR:H     | 2        | 0.54          |
| (1,1740) | 1:77:A:LEU:HD12  | 1:78:A:TYR:H     | 10       | 0.54          |
| (1,1682) | 1:41:A:ALA:HB1   | 1:33:A:GLU:H     | 7        | 0.54          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1682) | 1:41:A:ALA:HB2   | 1:33:A:GLU:H    | 10       | 0.54          |
| (1,1682) | 1:41:A:ALA:HB2   | 1:33:A:GLU:H    | 16       | 0.54          |
| (1,1502) | 1:52:A:ILE:HG13  | 1:54:A:GLN:HE21 | 2        | 0.54          |
| (1,1420) | 1:97:A:LEU:HD23  | 1:56:A:LEU:HD23 | 10       | 0.54          |
| (1,1372) | 1:28:A:ILE:HD12  | 1:31:A:LEU:HB3  | 13       | 0.54          |
| (1,1369) | 1:39:A:PHE:HZ    | 1:28:A:ILE:HD13 | 15       | 0.54          |
| (1,1343) | 1:78:A:TYR:HE2   | 1:48:A:LEU:HD11 | 5        | 0.54          |
| (1,1343) | 1:78:A:TYR:HE2   | 1:48:A:LEU:HD12 | 8        | 0.54          |
| (1,1336) | 1:85:A:LEU:HD22  | 1:84:A:TYR:HD1  | 2        | 0.54          |
| (1,1334) | 1:81:A:SER:HB3   | 1:84:A:TYR:HD1  | 14       | 0.54          |
| (1,1308) | 1:97:A:LEU:HD23  | 1:35:A:PHE:HD2  | 4        | 0.54          |
| (1,1305) | 1:97:A:LEU:HD21  | 1:52:A:ILE:HB   | 11       | 0.54          |
| (1,1301) | 1:97:A:LEU:HD11  | 1:97:A:LEU:HA   | 3        | 0.54          |
| (1,1301) | 1:97:A:LEU:HD13  | 1:97:A:LEU:HA   | 9        | 0.54          |
| (1,1158) | 1:120:A:ALA:HB2  | 1:82:A:TRP:HD1  | 4        | 0.54          |
| (1,1157) | 1:117:A:LEU:HD13 | 1:82:A:TRP:HD1  | 5        | 0.54          |
| (1,1157) | 1:117:A:LEU:HD13 | 1:82:A:TRP:HD1  | 14       | 0.54          |
| (1,1137) | 1:97:A:LEU:HD13  | 1:35:A:PHE:HD1  | 16       | 0.54          |
| (1,1077) | 1:21:A:LEU:HA    | 1:21:A:LEU:HD23 | 9        | 0.54          |
| (1,942)  | 1:93:A:THR:HB    | 1:95:A:VAL:HG11 | 15       | 0.54          |
| (1,815)  | 1:50:A:ILE:HD12  | 1:50:A:ILE:HA   | 12       | 0.54          |
| (1,697)  | 1:57:A:VAL:HG12  | 1:56:A:LEU:H    | 3        | 0.54          |
| (1,697)  | 1:57:A:VAL:HG11  | 1:56:A:LEU:H    | 15       | 0.54          |
| (1,610)  | 1:48:A:LEU:HD21  | 1:49:A:LYS:H    | 14       | 0.54          |
| (1,604)  | 1:32:A:ALA:HB1   | 1:41:A:ALA:H    | 14       | 0.54          |
| (1,467)  | 1:31:A:LEU:HD21  | 1:32:A:ALA:H    | 17       | 0.54          |
| (1,370)  | 1:71:A:LEU:HD12  | 1:61:A:ALA:H    | 4        | 0.54          |
| (1,370)  | 1:71:A:LEU:HD11  | 1:61:A:ALA:H    | 6        | 0.54          |
| (1,370)  | 1:71:A:LEU:HD13  | 1:61:A:ALA:H    | 7        | 0.54          |
| (1,370)  | 1:71:A:LEU:HD12  | 1:61:A:ALA:H    | 9        | 0.54          |
| (1,275)  | 1:85:A:LEU:HD23  | 1:87:A:GLY:H    | 10       | 0.54          |
| (1,263)  | 1:110:A:VAL:HG21 | 1:91:A:GLY:H    | 8        | 0.54          |
| (1,204)  | 1:105:A:LEU:HD13 | 1:106:A:ASP:H   | 10       | 0.54          |
| (1,204)  | 1:105:A:LEU:HD12 | 1:106:A:ASP:H   | 14       | 0.54          |
| (1,204)  | 1:105:A:LEU:HD12 | 1:106:A:ASP:H   | 15       | 0.54          |
| (1,169)  | 1:120:A:ALA:HB1  | 1:119:A:GLU:H   | 3        | 0.54          |
| (1,169)  | 1:120:A:ALA:HB2  | 1:119:A:GLU:H   | 15       | 0.54          |
| (3,136)  | 1:81:A:SER:H     | 1:82:A:TRP:H    | 7        | 0.53          |
| (3,136)  | 1:82:A:TRP:HD1   | 1:82:A:TRP:H    | 10       | 0.53          |
| (3,132)  | 1:113:A:ALA:HB2  | 1:112:A:HIS:H   | 4        | 0.53          |
| (3,132)  | 1:113:A:ALA:HB3  | 1:112:A:HIS:H   | 9        | 0.53          |
| (3,126)  | 1:21:A:LEU:HD22  | 1:22:A:ASN:H    | 8        | 0.53          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (3,123)  | 1:50:A:ILE:HD13  | 1:79:A:THR:HA    | 15       | 0.53          |
| (3,97)   | 1:31:A:LEU:HD23  | 1:30:A:PHE:HB3   | 1        | 0.53          |
| (3,97)   | 1:31:A:LEU:HD22  | 1:30:A:PHE:HB3   | 15       | 0.53          |
| (3,96)   | 1:110:A:VAL:HG21 | 1:109:A:HIS:HA   | 5        | 0.53          |
| (3,96)   | 1:110:A:VAL:HG22 | 1:109:A:HIS:HA   | 14       | 0.53          |
| (3,36)   | 1:50:A:ILE:HG23  | 1:49:A:LYS:HB2   | 13       | 0.53          |
| (1,4283) | 1:120:A:ALA:H    | 1:85:A:LEU:HD22  | 10       | 0.53          |
| (1,4171) | 1:48:A:LEU:HD21  | 1:49:A:LYS:H     | 7        | 0.53          |
| (1,4171) | 1:48:A:LEU:HD22  | 1:49:A:LYS:H     | 9        | 0.53          |
| (1,4164) | 1:32:A:ALA:HB1   | 1:41:A:ALA:H     | 1        | 0.53          |
| (1,4164) | 1:32:A:ALA:HB2   | 1:41:A:ALA:H     | 3        | 0.53          |
| (1,4164) | 1:32:A:ALA:HB3   | 1:41:A:ALA:H     | 13       | 0.53          |
| (1,4164) | 1:32:A:ALA:HB3   | 1:41:A:ALA:H     | 16       | 0.53          |
| (1,4028) | 1:31:A:LEU:HD23  | 1:32:A:ALA:H     | 1        | 0.53          |
| (1,4007) | 1:41:A:ALA:HB2   | 1:41:A:ALA:H     | 1        | 0.53          |
| (1,3957) | 1:58:A:ASP:H     | 1:57:A:VAL:HG12  | 16       | 0.53          |
| (1,3941) | 1:63:A:GLU:H     | 1:61:A:ALA:HB2   | 5        | 0.53          |
| (1,3810) | 1:105:A:LEU:HD11 | 1:106:A:ASP:H    | 3        | 0.53          |
| (1,3782) | 1:120:A:ALA:HB1  | 1:119:A:GLU:H    | 11       | 0.53          |
| (1,3742) | 1:28:A:ILE:H     | 1:29:A:ALA:HB2   | 5        | 0.53          |
| (1,3541) | 1:64:A:MET:HB2   | 1:21:A:LEU:HD21  | 15       | 0.53          |
| (1,3463) | 1:35:A:PHE:HE2   | 1:38:A:CYS:HB2   | 5        | 0.53          |
| (1,3376) | 1:41:A:ALA:HB2   | 1:40:A:SER:HB3   | 2        | 0.53          |
| (1,3376) | 1:41:A:ALA:HB2   | 1:40:A:SER:HB3   | 12       | 0.53          |
| (1,3376) | 1:41:A:ALA:HB1   | 1:40:A:SER:HB3   | 14       | 0.53          |
| (1,3281) | 1:93:A:THR:HG21  | 1:104:A:GLU:HG2  | 11       | 0.53          |
| (1,3256) | 1:41:A:ALA:HB2   | 1:33:A:GLU:H     | 13       | 0.53          |
| (1,3204) | 1:121:A:LYS:HB2  | 1:117:A:LEU:HD12 | 10       | 0.53          |
| (1,3171) | 1:75:A:LEU:HD21  | 1:31:A:LEU:HD13  | 1        | 0.53          |
| (1,3171) | 1:75:A:LEU:HD21  | 1:31:A:LEU:HD13  | 10       | 0.53          |
| (1,3116) | 1:57:A:VAL:HG22  | 1:53:A:PHE:HE2   | 8        | 0.53          |
| (1,3081) | 1:97:A:LEU:HD12  | 1:55:A:ASP:HA    | 6        | 0.53          |
| (1,3068) | 1:52:A:ILE:HG23  | 1:53:A:PHE:HB2   | 7        | 0.53          |
| (1,3046) | 1:52:A:ILE:HG12  | 1:54:A:GLN:HE21  | 16       | 0.53          |
| (1,2962) | 1:97:A:LEU:HD21  | 1:56:A:LEU:HD21  | 11       | 0.53          |
| (1,2962) | 1:97:A:LEU:HD23  | 1:56:A:LEU:HD23  | 17       | 0.53          |
| (1,2954) | 1:71:A:LEU:HB2   | 1:75:A:LEU:HD13  | 11       | 0.53          |
| (1,2926) | 1:21:A:LEU:HB2   | 1:21:A:LEU:HD21  | 5        | 0.53          |
| (1,2926) | 1:21:A:LEU:HB2   | 1:21:A:LEU:HD22  | 6        | 0.53          |
| (1,2902) | 1:50:A:ILE:HD13  | 1:76:A:ARG:H     | 5        | 0.53          |
| (1,2897) | 1:39:A:PHE:HZ    | 1:28:A:ILE:HD12  | 5        | 0.53          |
| (1,2897) | 1:39:A:PHE:HZ    | 1:28:A:ILE:HD13  | 10       | 0.53          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2897) | 1:39:A:PHE:HZ   | 1:28:A:ILE:HD12  | 13       | 0.53          |
| (1,2897) | 1:39:A:PHE:HZ   | 1:28:A:ILE:HD12  | 14       | 0.53          |
| (1,2897) | 1:39:A:PHE:HZ   | 1:28:A:ILE:HD12  | 17       | 0.53          |
| (1,2885) | 1:32:A:ALA:HB1  | 1:31:A:LEU:H     | 3        | 0.53          |
| (1,2885) | 1:32:A:ALA:HB1  | 1:31:A:LEU:H     | 5        | 0.53          |
| (1,2885) | 1:32:A:ALA:HB2  | 1:31:A:LEU:H     | 8        | 0.53          |
| (1,2885) | 1:32:A:ALA:HB2  | 1:31:A:LEU:H     | 13       | 0.53          |
| (1,2885) | 1:32:A:ALA:HB2  | 1:31:A:LEU:H     | 16       | 0.53          |
| (1,2863) | 1:78:A:TYR:HE1  | 1:84:A:TYR:HD1   | 4        | 0.53          |
| (1,2852) | 1:81:A:SER:HB3  | 1:84:A:TYR:HD2   | 9        | 0.53          |
| (1,2852) | 1:81:A:SER:HB3  | 1:84:A:TYR:HD1   | 10       | 0.53          |
| (1,2852) | 1:81:A:SER:HB3  | 1:84:A:TYR:HD2   | 15       | 0.53          |
| (1,2845) | 1:22:A:ASN:H    | 1:27:A:VAL:HG11  | 1        | 0.53          |
| (1,2845) | 1:22:A:ASN:H    | 1:27:A:VAL:HG12  | 11       | 0.53          |
| (1,2836) | 1:95:A:VAL:HG21 | 1:97:A:LEU:HD23  | 16       | 0.53          |
| (1,2817) | 1:97:A:LEU:HD11 | 1:97:A:LEU:HA    | 13       | 0.53          |
| (1,2673) | 1:97:A:LEU:HD12 | 1:35:A:PHE:HD2   | 7        | 0.53          |
| (1,2669) | 1:75:A:LEU:HD21 | 1:78:A:TYR:HE2   | 4        | 0.53          |
| (1,2664) | 1:97:A:LEU:HD12 | 1:60:A:VAL:HG11  | 7        | 0.53          |
| (1,2608) | 1:48:A:LEU:HD12 | 1:52:A:ILE:HG12  | 9        | 0.53          |
| (1,2585) | 1:92:A:ALA:HA   | 1:93:A:THR:HG23  | 8        | 0.53          |
| (1,2585) | 1:92:A:ALA:HA   | 1:93:A:THR:HG23  | 12       | 0.53          |
| (1,2577) | 1:60:A:VAL:HG13 | 1:59:A:ARG:HA    | 6        | 0.53          |
| (1,2577) | 1:60:A:VAL:HG11 | 1:59:A:ARG:HA    | 13       | 0.53          |
| (1,2572) | 1:125:A:GLN:H   | 1:124:A:VAL:HG22 | 13       | 0.53          |
| (1,2572) | 1:125:A:GLN:H   | 1:124:A:VAL:HG23 | 14       | 0.53          |
| (1,2568) | 1:78:A:TYR:HE1  | 1:28:A:ILE:HD13  | 12       | 0.53          |
| (1,2484) | 1:93:A:THR:HB   | 1:95:A:VAL:HG13  | 11       | 0.53          |
| (1,2458) | 1:21:A:LEU:HA   | 1:21:A:LEU:HD11  | 6        | 0.53          |
| (1,2305) | 1:45:A:ALA:HB2  | 1:44:A:GLU:HA    | 13       | 0.53          |
| (1,2305) | 1:45:A:ALA:HB2  | 1:44:A:GLU:HA    | 16       | 0.53          |
| (1,2248) | 1:57:A:VAL:HG22 | 1:57:A:VAL:HA    | 3        | 0.53          |
| (1,2248) | 1:57:A:VAL:HG22 | 1:57:A:VAL:HA    | 5        | 0.53          |
| (1,2248) | 1:57:A:VAL:HG23 | 1:57:A:VAL:HA    | 8        | 0.53          |
| (1,2248) | 1:57:A:VAL:HG23 | 1:57:A:VAL:HA    | 12       | 0.53          |
| (1,2179) | 1:52:A:ILE:HG22 | 1:48:A:LEU:HB3   | 6        | 0.53          |
| (1,2147) | 1:85:A:LEU:HA   | 1:85:A:LEU:HD11  | 3        | 0.53          |
| (1,2147) | 1:85:A:LEU:HA   | 1:85:A:LEU:HD13  | 4        | 0.53          |
| (1,2147) | 1:85:A:LEU:HA   | 1:85:A:LEU:HD12  | 5        | 0.53          |
| (1,2146) | 1:104:A:GLU:HB3 | 1:93:A:THR:HG22  | 10       | 0.53          |
| (1,2146) | 1:104:A:GLU:HB3 | 1:93:A:THR:HG21  | 13       | 0.53          |
| (1,2142) | 1:21:A:LEU:HD13 | 1:30:A:PHE:HA    | 13       | 0.53          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2094) | 1:95:A:VAL:HG22  | 1:97:A:LEU:HD21 | 2        | 0.53          |
| (1,2006) | 1:78:A:TYR:HE2   | 1:48:A:LEU:HD13 | 6        | 0.53          |
| (1,1867) | 1:53:A:PHE:HA    | 1:31:A:LEU:HD13 | 1        | 0.53          |
| (1,1867) | 1:53:A:PHE:HA    | 1:31:A:LEU:HD12 | 3        | 0.53          |
| (1,1867) | 1:53:A:PHE:HA    | 1:31:A:LEU:HD12 | 6        | 0.53          |
| (1,1867) | 1:53:A:PHE:HA    | 1:31:A:LEU:HD13 | 11       | 0.53          |
| (1,1867) | 1:53:A:PHE:HA    | 1:31:A:LEU:HD11 | 17       | 0.53          |
| (1,1790) | 1:90:A:PRO:HA    | 1:92:A:ALA:HB1  | 8        | 0.53          |
| (1,1751) | 1:32:A:ALA:HB1   | 1:41:A:ALA:H    | 15       | 0.53          |
| (1,1740) | 1:77:A:LEU:HD13  | 1:78:A:TYR:H    | 1        | 0.53          |
| (1,1740) | 1:77:A:LEU:HD12  | 1:78:A:TYR:H    | 7        | 0.53          |
| (1,1740) | 1:77:A:LEU:HD12  | 1:78:A:TYR:H    | 14       | 0.53          |
| (1,1682) | 1:41:A:ALA:HB3   | 1:33:A:GLU:H    | 2        | 0.53          |
| (1,1682) | 1:41:A:ALA:HB3   | 1:33:A:GLU:H    | 5        | 0.53          |
| (1,1601) | 1:75:A:LEU:HD23  | 1:31:A:LEU:HD13 | 2        | 0.53          |
| (1,1507) | 1:78:A:TYR:HE1   | 1:28:A:ILE:HG22 | 5        | 0.53          |
| (1,1482) | 1:64:A:MET:HE2   | 1:27:A:VAL:HA   | 14       | 0.53          |
| (1,1372) | 1:28:A:ILE:HD12  | 1:31:A:LEU:HB3  | 8        | 0.53          |
| (1,1369) | 1:39:A:PHE:HZ    | 1:28:A:ILE:HD13 | 9        | 0.53          |
| (1,1360) | 1:32:A:ALA:HB2   | 1:31:A:LEU:H    | 4        | 0.53          |
| (1,1305) | 1:97:A:LEU:HD23  | 1:52:A:ILE:HB   | 6        | 0.53          |
| (1,1158) | 1:120:A:ALA:HB2  | 1:82:A:TRP:HD1  | 13       | 0.53          |
| (1,1155) | 1:53:A:PHE:HB3   | 1:53:A:PHE:HE1  | 11       | 0.53          |
| (1,1155) | 1:53:A:PHE:HB3   | 1:53:A:PHE:HE1  | 17       | 0.53          |
| (1,1137) | 1:97:A:LEU:HD12  | 1:35:A:PHE:HD1  | 2        | 0.53          |
| (1,942)  | 1:93:A:THR:HB    | 1:95:A:VAL:HG12 | 1        | 0.53          |
| (1,942)  | 1:93:A:THR:HB    | 1:95:A:VAL:HG13 | 9        | 0.53          |
| (1,610)  | 1:48:A:LEU:HD23  | 1:49:A:LYS:H    | 6        | 0.53          |
| (1,610)  | 1:48:A:LEU:HD21  | 1:49:A:LYS:H    | 12       | 0.53          |
| (1,610)  | 1:48:A:LEU:HD22  | 1:49:A:LYS:H    | 15       | 0.53          |
| (1,604)  | 1:32:A:ALA:HB2   | 1:41:A:ALA:H    | 6        | 0.53          |
| (1,570)  | 1:60:A:VAL:HG12  | 1:34:A:ARG:HE   | 8        | 0.53          |
| (1,467)  | 1:31:A:LEU:HD23  | 1:32:A:ALA:H    | 7        | 0.53          |
| (1,204)  | 1:105:A:LEU:HD13 | 1:106:A:ASP:H   | 5        | 0.53          |
| (3,152)  | 1:27:A:VAL:H     | 1:74:A:ALA:HB3  | 7        | 0.52          |
| (3,136)  | 1:81:A:SER:H     | 1:82:A:TRP:H    | 2        | 0.52          |
| (3,132)  | 1:113:A:ALA:HB2  | 1:112:A:HIS:H   | 17       | 0.52          |
| (3,123)  | 1:50:A:ILE:HD12  | 1:79:A:THR:HA   | 14       | 0.52          |
| (3,99)   | 1:72:A:ARG:HG3   | 1:75:A:LEU:HD12 | 13       | 0.52          |
| (3,99)   | 1:72:A:ARG:HG3   | 1:75:A:LEU:HD11 | 14       | 0.52          |
| (3,98)   | 1:64:A:MET:HE1   | 1:63:A:GLU:HG3  | 7        | 0.52          |
| (3,65)   | 1:49:A:LYS:HB2   | 1:52:A:ILE:HG22 | 14       | 0.52          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (3,51)   | 1:95:A:VAL:HG21  | 1:49:A:LYS:HA   | 8        | 0.52          |
| (1,4259) | 1:57:A:VAL:HG13  | 1:56:A:LEU:H    | 5        | 0.52          |
| (1,4247) | 1:54:A:GLN:HE22  | 1:57:A:VAL:HG13 | 14       | 0.52          |
| (1,4171) | 1:48:A:LEU:HD21  | 1:49:A:LYS:H    | 11       | 0.52          |
| (1,4171) | 1:48:A:LEU:HD22  | 1:49:A:LYS:H    | 16       | 0.52          |
| (1,4084) | 1:20:A:LYS:HB3   | 1:22:A:ASN:HD22 | 3        | 0.52          |
| (1,4082) | 1:22:A:ASN:HD21  | 1:22:A:ASN:HB3  | 15       | 0.52          |
| (1,3972) | 1:53:A:PHE:H     | 1:56:A:LEU:HB3  | 5        | 0.52          |
| (1,3957) | 1:58:A:ASP:H     | 1:57:A:VAL:HG13 | 5        | 0.52          |
| (1,3943) | 1:66:A:LEU:HD13  | 1:62:A:GLY:H    | 2        | 0.52          |
| (1,3861) | 1:110:A:VAL:HG23 | 1:91:A:GLY:H    | 10       | 0.52          |
| (1,3822) | 1:93:A:THR:HG21  | 1:103:A:GLY:H   | 12       | 0.52          |
| (1,3782) | 1:120:A:ALA:HB1  | 1:119:A:GLU:H   | 1        | 0.52          |
| (1,3742) | 1:28:A:ILE:H     | 1:29:A:ALA:HB2  | 1        | 0.52          |
| (1,3489) | 1:21:A:LEU:HD21  | 1:20:A:LYS:HA   | 4        | 0.52          |
| (1,3376) | 1:41:A:ALA:HB1   | 1:40:A:SER:HB3  | 15       | 0.52          |
| (1,3368) | 1:31:A:LEU:HD13  | 1:31:A:LEU:HA   | 1        | 0.52          |
| (1,3368) | 1:31:A:LEU:HD13  | 1:31:A:LEU:HA   | 2        | 0.52          |
| (1,3368) | 1:31:A:LEU:HD13  | 1:31:A:LEU:HA   | 5        | 0.52          |
| (1,3368) | 1:31:A:LEU:HD13  | 1:31:A:LEU:HA   | 10       | 0.52          |
| (1,3366) | 1:72:A:ARG:HA    | 1:56:A:LEU:HD21 | 2        | 0.52          |
| (1,3366) | 1:72:A:ARG:HA    | 1:56:A:LEU:HD21 | 5        | 0.52          |
| (1,3366) | 1:72:A:ARG:HA    | 1:56:A:LEU:HD22 | 6        | 0.52          |
| (1,3366) | 1:72:A:ARG:HA    | 1:56:A:LEU:HD21 | 9        | 0.52          |
| (1,3366) | 1:72:A:ARG:HA    | 1:56:A:LEU:HD22 | 10       | 0.52          |
| (1,3366) | 1:72:A:ARG:HA    | 1:56:A:LEU:HD21 | 13       | 0.52          |
| (1,3302) | 1:83:A:ARG:HB2   | 1:86:A:TYR:HD2  | 12       | 0.52          |
| (1,3302) | 1:83:A:ARG:HB2   | 1:86:A:TYR:HD2  | 13       | 0.52          |
| (1,3253) | 1:92:A:ALA:HB2   | 1:91:A:GLY:H    | 2        | 0.52          |
| (1,3171) | 1:75:A:LEU:HD21  | 1:31:A:LEU:HD13 | 5        | 0.52          |
| (1,3081) | 1:97:A:LEU:HD13  | 1:55:A:ASP:HA   | 8        | 0.52          |
| (1,3052) | 1:39:A:PHE:HZ    | 1:52:A:ILE:HG22 | 8        | 0.52          |
| (1,2954) | 1:71:A:LEU:HB2   | 1:75:A:LEU:HD11 | 1        | 0.52          |
| (1,2900) | 1:28:A:ILE:HD13  | 1:31:A:LEU:HB3  | 12       | 0.52          |
| (1,2897) | 1:39:A:PHE:HZ    | 1:28:A:ILE:HD11 | 16       | 0.52          |
| (1,2885) | 1:32:A:ALA:HB3   | 1:31:A:LEU:H    | 15       | 0.52          |
| (1,2865) | 1:78:A:TYR:HE2   | 1:48:A:LEU:HD11 | 1        | 0.52          |
| (1,2852) | 1:81:A:SER:HB3   | 1:84:A:TYR:HD2  | 16       | 0.52          |
| (1,2845) | 1:22:A:ASN:H     | 1:27:A:VAL:HG12 | 3        | 0.52          |
| (1,2817) | 1:97:A:LEU:HD12  | 1:97:A:LEU:HA   | 17       | 0.52          |
| (1,2669) | 1:75:A:LEU:HD22  | 1:78:A:TYR:HE1  | 15       | 0.52          |
| (1,2581) | 1:71:A:LEU:HD11  | 1:60:A:VAL:HG11 | 3        | 0.52          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2577) | 1:60:A:VAL:HG11 | 1:59:A:ARG:HA   | 8        | 0.52          |
| (1,2577) | 1:60:A:VAL:HG13 | 1:59:A:ARG:HA   | 14       | 0.52          |
| (1,2577) | 1:60:A:VAL:HG13 | 1:59:A:ARG:HA   | 15       | 0.52          |
| (1,2577) | 1:60:A:VAL:HG13 | 1:59:A:ARG:HA   | 16       | 0.52          |
| (1,2577) | 1:60:A:VAL:HG11 | 1:59:A:ARG:HA   | 17       | 0.52          |
| (1,2458) | 1:21:A:LEU:HA   | 1:21:A:LEU:HD13 | 13       | 0.52          |
| (1,2423) | 1:64:A:MET:HA   | 1:64:A:MET:HE3  | 7        | 0.52          |
| (1,2305) | 1:45:A:ALA:HB3  | 1:44:A:GLU:HA   | 2        | 0.52          |
| (1,2305) | 1:45:A:ALA:HB3  | 1:44:A:GLU:HA   | 14       | 0.52          |
| (1,2248) | 1:57:A:VAL:HG21 | 1:57:A:VAL:HA   | 1        | 0.52          |
| (1,2248) | 1:57:A:VAL:HG23 | 1:57:A:VAL:HA   | 6        | 0.52          |
| (1,2248) | 1:57:A:VAL:HG23 | 1:57:A:VAL:HA   | 15       | 0.52          |
| (1,2248) | 1:57:A:VAL:HG23 | 1:57:A:VAL:HA   | 16       | 0.52          |
| (1,2194) | 1:50:A:ILE:HD13 | 1:80:A:SER:H    | 5        | 0.52          |
| (1,2147) | 1:85:A:LEU:HA   | 1:85:A:LEU:HD11 | 14       | 0.52          |
| (1,1867) | 1:53:A:PHE:HA   | 1:31:A:LEU:HD12 | 4        | 0.52          |
| (1,1867) | 1:53:A:PHE:HA   | 1:31:A:LEU:HD11 | 8        | 0.52          |
| (1,1867) | 1:53:A:PHE:HA   | 1:31:A:LEU:HD13 | 10       | 0.52          |
| (1,1867) | 1:53:A:PHE:HA   | 1:31:A:LEU:HD12 | 13       | 0.52          |
| (1,1867) | 1:53:A:PHE:HA   | 1:31:A:LEU:HD11 | 16       | 0.52          |
| (1,1851) | 1:35:A:PHE:HE2  | 1:38:A:CYS:HB2  | 6        | 0.52          |
| (1,1851) | 1:35:A:PHE:HE2  | 1:38:A:CYS:HB2  | 8        | 0.52          |
| (1,1838) | 1:93:A:THR:HA   | 1:93:A:THR:HG23 | 13       | 0.52          |
| (1,1790) | 1:90:A:PRO:HA   | 1:92:A:ALA:HB2  | 14       | 0.52          |
| (1,1740) | 1:77:A:LEU:HD13 | 1:78:A:TYR:H    | 3        | 0.52          |
| (1,1740) | 1:77:A:LEU:HD13 | 1:78:A:TYR:H    | 11       | 0.52          |
| (1,1740) | 1:77:A:LEU:HD11 | 1:78:A:TYR:H    | 13       | 0.52          |
| (1,1740) | 1:77:A:LEU:HD12 | 1:78:A:TYR:H    | 17       | 0.52          |
| (1,1682) | 1:41:A:ALA:HB2  | 1:33:A:GLU:H    | 1        | 0.52          |
| (1,1679) | 1:92:A:ALA:HB2  | 1:91:A:GLY:H    | 4        | 0.52          |
| (1,1679) | 1:92:A:ALA:HB2  | 1:91:A:GLY:H    | 12       | 0.52          |
| (1,1507) | 1:78:A:TYR:HE2  | 1:28:A:ILE:HG23 | 7        | 0.52          |
| (1,1478) | 1:64:A:MET:HE3  | 1:66:A:LEU:H    | 11       | 0.52          |
| (1,1372) | 1:28:A:ILE:HD13 | 1:31:A:LEU:HB3  | 10       | 0.52          |
| (1,1372) | 1:28:A:ILE:HD12 | 1:31:A:LEU:HB3  | 14       | 0.52          |
| (1,1372) | 1:28:A:ILE:HD11 | 1:31:A:LEU:HB3  | 16       | 0.52          |
| (1,1360) | 1:32:A:ALA:HB2  | 1:31:A:LEU:H    | 9        | 0.52          |
| (1,1360) | 1:32:A:ALA:HB2  | 1:31:A:LEU:H    | 11       | 0.52          |
| (1,1336) | 1:85:A:LEU:HD22 | 1:84:A:TYR:HD1  | 3        | 0.52          |
| (1,1336) | 1:85:A:LEU:HD21 | 1:84:A:TYR:HD2  | 5        | 0.52          |
| (1,1336) | 1:85:A:LEU:HD21 | 1:84:A:TYR:HD2  | 6        | 0.52          |
| (1,1336) | 1:85:A:LEU:HD22 | 1:84:A:TYR:HD1  | 7        | 0.52          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1336) | 1:85:A:LEU:HD22  | 1:84:A:TYR:HD1  | 15       | 0.52          |
| (1,1334) | 1:81:A:SER:HB3   | 1:84:A:TYR:HD1  | 12       | 0.52          |
| (1,1315) | 1:95:A:VAL:HG21  | 1:97:A:LEU:HD21 | 7        | 0.52          |
| (1,1308) | 1:97:A:LEU:HD23  | 1:35:A:PHE:HD1  | 8        | 0.52          |
| (1,1305) | 1:97:A:LEU:HD23  | 1:52:A:ILE:HB   | 14       | 0.52          |
| (1,1077) | 1:21:A:LEU:HA    | 1:21:A:LEU:HD23 | 4        | 0.52          |
| (1,1069) | 1:48:A:LEU:HD12  | 1:52:A:ILE:HG12 | 6        | 0.52          |
| (1,1043) | 1:78:A:TYR:HE2   | 1:28:A:ILE:HD12 | 8        | 0.52          |
| (1,1043) | 1:78:A:TYR:HE1   | 1:28:A:ILE:HD13 | 10       | 0.52          |
| (1,942)  | 1:93:A:THR:HB    | 1:95:A:VAL:HG11 | 4        | 0.52          |
| (1,942)  | 1:93:A:THR:HB    | 1:95:A:VAL:HG12 | 5        | 0.52          |
| (1,697)  | 1:57:A:VAL:HG12  | 1:56:A:LEU:H    | 6        | 0.52          |
| (1,697)  | 1:57:A:VAL:HG12  | 1:56:A:LEU:H    | 16       | 0.52          |
| (1,610)  | 1:48:A:LEU:HD23  | 1:49:A:LYS:H    | 5        | 0.52          |
| (1,610)  | 1:48:A:LEU:HD23  | 1:49:A:LYS:H    | 13       | 0.52          |
| (1,570)  | 1:60:A:VAL:HG12  | 1:34:A:ARG:HE   | 13       | 0.52          |
| (1,570)  | 1:60:A:VAL:HG11  | 1:34:A:ARG:HE   | 15       | 0.52          |
| (1,561)  | 1:116:A:GLN:HE21 | 1:120:A:ALA:H   | 10       | 0.52          |
| (1,559)  | 1:116:A:GLN:HE21 | 1:113:A:ALA:HA  | 14       | 0.52          |
| (1,467)  | 1:31:A:LEU:HD22  | 1:32:A:ALA:H    | 2        | 0.52          |
| (1,467)  | 1:31:A:LEU:HD22  | 1:32:A:ALA:H    | 8        | 0.52          |
| (1,467)  | 1:31:A:LEU:HD21  | 1:32:A:ALA:H    | 10       | 0.52          |
| (1,467)  | 1:31:A:LEU:HD21  | 1:32:A:ALA:H    | 13       | 0.52          |
| (1,467)  | 1:31:A:LEU:HD21  | 1:32:A:ALA:H    | 14       | 0.52          |
| (1,467)  | 1:31:A:LEU:HD22  | 1:32:A:ALA:H    | 15       | 0.52          |
| (1,370)  | 1:71:A:LEU:HD11  | 1:61:A:ALA:H    | 11       | 0.52          |
| (1,204)  | 1:105:A:LEU:HD11 | 1:106:A:ASP:H   | 4        | 0.52          |
| (1,204)  | 1:105:A:LEU:HD12 | 1:106:A:ASP:H   | 8        | 0.52          |
| (1,204)  | 1:105:A:LEU:HD12 | 1:106:A:ASP:H   | 9        | 0.52          |
| (1,204)  | 1:105:A:LEU:HD12 | 1:106:A:ASP:H   | 13       | 0.52          |
| (1,204)  | 1:105:A:LEU:HD12 | 1:106:A:ASP:H   | 16       | 0.52          |
| (1,204)  | 1:105:A:LEU:HD11 | 1:106:A:ASP:H   | 17       | 0.52          |
| (3,152)  | 1:27:A:VAL:H     | 1:29:A:ALA:HB2  | 10       | 0.51          |
| (3,132)  | 1:113:A:ALA:HB2  | 1:112:A:HIS:H   | 6        | 0.51          |
| (3,124)  | 1:88:A:VAL:HG21  | 1:88:A:VAL:H    | 7        | 0.51          |
| (3,106)  | 1:68:A:LYS:HD2   | 1:68:A:LYS:HA   | 11       | 0.51          |
| (3,102)  | 1:65:A:ASN:HB2   | 1:64:A:MET:HG2  | 10       | 0.51          |
| (3,99)   | 1:72:A:ARG:HG3   | 1:75:A:LEU:HD12 | 4        | 0.51          |
| (3,99)   | 1:72:A:ARG:HG3   | 1:75:A:LEU:HD11 | 6        | 0.51          |
| (3,97)   | 1:31:A:LEU:HD22  | 1:30:A:PHE:HB3  | 8        | 0.51          |
| (3,72)   | 1:117:A:LEU:HG   | 1:117:A:LEU:H   | 13       | 0.51          |
| (3,36)   | 1:49:A:LYS:HB2   | 1:52:A:ILE:HD12 | 10       | 0.51          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,4247) | 1:54:A:GLN:HE22 | 1:57:A:VAL:HG12  | 10       | 0.51          |
| (1,4171) | 1:48:A:LEU:HD21 | 1:49:A:LYS:H     | 3        | 0.51          |
| (1,4164) | 1:32:A:ALA:HB2  | 1:41:A:ALA:H     | 5        | 0.51          |
| (1,4082) | 1:22:A:ASN:HD21 | 1:22:A:ASN:HB3   | 1        | 0.51          |
| (1,4007) | 1:41:A:ALA:HB3  | 1:41:A:ALA:H     | 4        | 0.51          |
| (1,3957) | 1:58:A:ASP:H    | 1:57:A:VAL:HG11  | 7        | 0.51          |
| (1,3943) | 1:66:A:LEU:HD12 | 1:62:A:GLY:H     | 7        | 0.51          |
| (1,3943) | 1:66:A:LEU:HD12 | 1:62:A:GLY:H     | 9        | 0.51          |
| (1,3943) | 1:66:A:LEU:HD13 | 1:62:A:GLY:H     | 10       | 0.51          |
| (1,3943) | 1:66:A:LEU:HD13 | 1:62:A:GLY:H     | 12       | 0.51          |
| (1,3943) | 1:66:A:LEU:HD11 | 1:62:A:GLY:H     | 15       | 0.51          |
| (1,3941) | 1:63:A:GLU:H    | 1:61:A:ALA:HB3   | 11       | 0.51          |
| (1,3870) | 1:85:A:LEU:HD22 | 1:87:A:GLY:H     | 8        | 0.51          |
| (1,3870) | 1:85:A:LEU:HD22 | 1:87:A:GLY:H     | 14       | 0.51          |
| (1,3541) | 1:64:A:MET:HB2  | 1:21:A:LEU:HD23  | 5        | 0.51          |
| (1,3463) | 1:35:A:PHE:HE2  | 1:38:A:CYS:HB2   | 3        | 0.51          |
| (1,3452) | 1:95:A:VAL:HA   | 1:93:A:THR:HG22  | 11       | 0.51          |
| (1,3452) | 1:95:A:VAL:HA   | 1:93:A:THR:HG21  | 16       | 0.51          |
| (1,3451) | 1:93:A:THR:HA   | 1:93:A:THR:HG23  | 7        | 0.51          |
| (1,3368) | 1:31:A:LEU:HD13 | 1:31:A:LEU:HA    | 11       | 0.51          |
| (1,3368) | 1:31:A:LEU:HD12 | 1:31:A:LEU:HA    | 14       | 0.51          |
| (1,3366) | 1:72:A:ARG:HA   | 1:56:A:LEU:HD22  | 7        | 0.51          |
| (1,3366) | 1:72:A:ARG:HA   | 1:56:A:LEU:HD21  | 14       | 0.51          |
| (1,3366) | 1:72:A:ARG:HA   | 1:56:A:LEU:HD23  | 15       | 0.51          |
| (1,3366) | 1:72:A:ARG:HA   | 1:56:A:LEU:HD23  | 16       | 0.51          |
| (1,3302) | 1:83:A:ARG:HB2  | 1:86:A:TYR:HD2   | 2        | 0.51          |
| (1,3253) | 1:92:A:ALA:HB1  | 1:91:A:GLY:H     | 9        | 0.51          |
| (1,3204) | 1:121:A:LYS:HB2 | 1:117:A:LEU:HD12 | 16       | 0.51          |
| (1,3116) | 1:57:A:VAL:HG23 | 1:53:A:PHE:HE1   | 7        | 0.51          |
| (1,3116) | 1:57:A:VAL:HG22 | 1:53:A:PHE:HE1   | 12       | 0.51          |
| (1,3116) | 1:57:A:VAL:HG23 | 1:53:A:PHE:HE1   | 13       | 0.51          |
| (1,3116) | 1:57:A:VAL:HG23 | 1:53:A:PHE:HE1   | 17       | 0.51          |
| (1,3078) | 1:54:A:GLN:HB3  | 1:57:A:VAL:HG13  | 14       | 0.51          |
| (1,3051) | 1:78:A:TYR:HE2  | 1:28:A:ILE:HG21  | 11       | 0.51          |
| (1,3045) | 1:52:A:ILE:HG13 | 1:54:A:GLN:HE21  | 13       | 0.51          |
| (1,3024) | 1:64:A:MET:HE2  | 1:65:A:ASN:HB3   | 5        | 0.51          |
| (1,2962) | 1:97:A:LEU:HD23 | 1:56:A:LEU:HD22  | 3        | 0.51          |
| (1,2954) | 1:71:A:LEU:HB2  | 1:75:A:LEU:HD13  | 5        | 0.51          |
| (1,2897) | 1:39:A:PHE:HZ   | 1:28:A:ILE:HD11  | 3        | 0.51          |
| (1,2897) | 1:39:A:PHE:HZ   | 1:28:A:ILE:HD13  | 11       | 0.51          |
| (1,2885) | 1:32:A:ALA:HB1  | 1:31:A:LEU:H     | 7        | 0.51          |
| (1,2865) | 1:78:A:TYR:HE1  | 1:48:A:LEU:HD13  | 7        | 0.51          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2865) | 1:78:A:TYR:HE1  | 1:48:A:LEU:HD13  | 14       | 0.51          |
| (1,2864) | 1:78:A:TYR:HE1  | 1:78:A:TYR:HB3   | 12       | 0.51          |
| (1,2864) | 1:78:A:TYR:HE2  | 1:78:A:TYR:HB3   | 13       | 0.51          |
| (1,2831) | 1:97:A:LEU:HD23 | 1:35:A:PHE:HD2   | 4        | 0.51          |
| (1,2817) | 1:97:A:LEU:HD12 | 1:97:A:LEU:HA    | 11       | 0.51          |
| (1,2681) | 1:120:A:ALA:HB3 | 1:82:A:TRP:HD1   | 10       | 0.51          |
| (1,2673) | 1:97:A:LEU:HD13 | 1:35:A:PHE:HD2   | 14       | 0.51          |
| (1,2608) | 1:48:A:LEU:HD13 | 1:52:A:ILE:HG12  | 3        | 0.51          |
| (1,2592) | 1:69:A:THR:HG22 | 1:70:A:GLN:H     | 17       | 0.51          |
| (1,2585) | 1:92:A:ALA:HA   | 1:93:A:THR:HG23  | 3        | 0.51          |
| (1,2581) | 1:71:A:LEU:HD11 | 1:60:A:VAL:HG12  | 5        | 0.51          |
| (1,2581) | 1:71:A:LEU:HD13 | 1:60:A:VAL:HG11  | 10       | 0.51          |
| (1,2581) | 1:71:A:LEU:HD11 | 1:60:A:VAL:HG13  | 17       | 0.51          |
| (1,2578) | 1:57:A:VAL:HA   | 1:60:A:VAL:HG11  | 3        | 0.51          |
| (1,2578) | 1:57:A:VAL:HA   | 1:60:A:VAL:HG12  | 5        | 0.51          |
| (1,2578) | 1:57:A:VAL:HA   | 1:60:A:VAL:HG12  | 14       | 0.51          |
| (1,2577) | 1:60:A:VAL:HG13 | 1:59:A:ARG:HA    | 2        | 0.51          |
| (1,2577) | 1:60:A:VAL:HG13 | 1:59:A:ARG:HA    | 5        | 0.51          |
| (1,2577) | 1:60:A:VAL:HG12 | 1:59:A:ARG:HA    | 10       | 0.51          |
| (1,2577) | 1:60:A:VAL:HG11 | 1:59:A:ARG:HA    | 12       | 0.51          |
| (1,2572) | 1:125:A:GLN:H   | 1:124:A:VAL:HG22 | 2        | 0.51          |
| (1,2484) | 1:93:A:THR:HB   | 1:95:A:VAL:HG12  | 3        | 0.51          |
| (1,2423) | 1:64:A:MET:HA   | 1:64:A:MET:HE2   | 4        | 0.51          |
| (1,2309) | 1:39:A:PHE:HB3  | 1:39:A:PHE:HE1   | 8        | 0.51          |
| (1,2309) | 1:39:A:PHE:HB3  | 1:39:A:PHE:HE1   | 10       | 0.51          |
| (1,2305) | 1:45:A:ALA:HB2  | 1:44:A:GLU:HA    | 4        | 0.51          |
| (1,2305) | 1:45:A:ALA:HB1  | 1:44:A:GLU:HA    | 6        | 0.51          |
| (1,2305) | 1:45:A:ALA:HB3  | 1:44:A:GLU:HA    | 15       | 0.51          |
| (1,2248) | 1:57:A:VAL:HG23 | 1:57:A:VAL:HA    | 2        | 0.51          |
| (1,2248) | 1:57:A:VAL:HG22 | 1:57:A:VAL:HA    | 4        | 0.51          |
| (1,2248) | 1:57:A:VAL:HG22 | 1:57:A:VAL:HA    | 9        | 0.51          |
| (1,2248) | 1:57:A:VAL:HG22 | 1:57:A:VAL:HA    | 11       | 0.51          |
| (1,2248) | 1:57:A:VAL:HG23 | 1:57:A:VAL:HA    | 14       | 0.51          |
| (1,2201) | 1:64:A:MET:HB2  | 1:21:A:LEU:HD21  | 10       | 0.51          |
| (1,2172) | 1:34:A:ARG:HD3  | 1:60:A:VAL:HG11  | 14       | 0.51          |
| (1,2147) | 1:85:A:LEU:HA   | 1:85:A:LEU:HD11  | 6        | 0.51          |
| (1,2146) | 1:104:A:GLU:HB3 | 1:93:A:THR:HG21  | 8        | 0.51          |
| (1,2006) | 1:78:A:TYR:HE1  | 1:48:A:LEU:HD11  | 10       | 0.51          |
| (1,1867) | 1:53:A:PHE:HA   | 1:31:A:LEU:HD13  | 2        | 0.51          |
| (1,1867) | 1:53:A:PHE:HA   | 1:31:A:LEU:HD13  | 5        | 0.51          |
| (1,1839) | 1:95:A:VAL:HA   | 1:93:A:THR:HG21  | 4        | 0.51          |
| (1,1839) | 1:95:A:VAL:HA   | 1:93:A:THR:HG22  | 8        | 0.51          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1838) | 1:93:A:THR:HA   | 1:93:A:THR:HG21 | 10       | 0.51          |
| (1,1838) | 1:93:A:THR:HA   | 1:93:A:THR:HG22 | 16       | 0.51          |
| (1,1790) | 1:90:A:PRO:HA   | 1:92:A:ALA:HB1  | 6        | 0.51          |
| (1,1751) | 1:32:A:ALA:HB3  | 1:41:A:ALA:H    | 4        | 0.51          |
| (1,1751) | 1:32:A:ALA:HB3  | 1:41:A:ALA:H    | 9        | 0.51          |
| (1,1740) | 1:77:A:LEU:HD13 | 1:78:A:TYR:H    | 4        | 0.51          |
| (1,1740) | 1:77:A:LEU:HD13 | 1:78:A:TYR:H    | 5        | 0.51          |
| (1,1740) | 1:77:A:LEU:HD11 | 1:78:A:TYR:H    | 6        | 0.51          |
| (1,1740) | 1:77:A:LEU:HD12 | 1:78:A:TYR:H    | 9        | 0.51          |
| (1,1740) | 1:77:A:LEU:HD12 | 1:78:A:TYR:H    | 12       | 0.51          |
| (1,1740) | 1:77:A:LEU:HD11 | 1:78:A:TYR:H    | 16       | 0.51          |
| (1,1684) | 1:48:A:LEU:HD12 | 1:50:A:ILE:HA   | 12       | 0.51          |
| (1,1679) | 1:92:A:ALA:HB3  | 1:91:A:GLY:H    | 7        | 0.51          |
| (1,1545) | 1:56:A:LEU:HD11 | 1:60:A:VAL:HB   | 5        | 0.51          |
| (1,1502) | 1:52:A:ILE:HG13 | 1:54:A:GLN:HE21 | 6        | 0.51          |
| (1,1405) | 1:102:A:CYS:H   | 1:95:A:VAL:HG11 | 15       | 0.51          |
| (1,1372) | 1:28:A:ILE:HD11 | 1:31:A:LEU:HB3  | 3        | 0.51          |
| (1,1372) | 1:28:A:ILE:HD12 | 1:31:A:LEU:HB3  | 17       | 0.51          |
| (1,1361) | 1:41:A:ALA:HA   | 1:32:A:ALA:HB2  | 9        | 0.51          |
| (1,1356) | 1:61:A:ALA:HB1  | 1:57:A:VAL:HG12 | 17       | 0.51          |
| (1,1343) | 1:78:A:TYR:HE1  | 1:48:A:LEU:HD12 | 16       | 0.51          |
| (1,1336) | 1:85:A:LEU:HD23 | 1:84:A:TYR:HD2  | 9        | 0.51          |
| (1,1336) | 1:85:A:LEU:HD23 | 1:84:A:TYR:HD2  | 13       | 0.51          |
| (1,1336) | 1:85:A:LEU:HD22 | 1:84:A:TYR:HD2  | 14       | 0.51          |
| (1,1301) | 1:97:A:LEU:HD11 | 1:97:A:LEU:HA   | 4        | 0.51          |
| (1,1301) | 1:97:A:LEU:HD11 | 1:97:A:LEU:HA   | 16       | 0.51          |
| (1,1158) | 1:120:A:ALA:HB2 | 1:82:A:TRP:HD1  | 1        | 0.51          |
| (1,1155) | 1:53:A:PHE:HB3  | 1:53:A:PHE:HE1  | 4        | 0.51          |
| (1,1075) | 1:31:A:LEU:HD13 | 1:31:A:LEU:HA   | 1        | 0.51          |
| (1,1075) | 1:31:A:LEU:HD13 | 1:31:A:LEU:HA   | 2        | 0.51          |
| (1,1075) | 1:31:A:LEU:HD13 | 1:31:A:LEU:HA   | 10       | 0.51          |
| (1,1043) | 1:78:A:TYR:HE2  | 1:28:A:ILE:HD11 | 6        | 0.51          |
| (1,815)  | 1:50:A:ILE:HD13 | 1:50:A:ILE:HA   | 2        | 0.51          |
| (1,720)  | 1:120:A:ALA:H   | 1:85:A:LEU:HD23 | 16       | 0.51          |
| (1,570)  | 1:60:A:VAL:HG13 | 1:34:A:ARG:HE   | 3        | 0.51          |
| (1,570)  | 1:60:A:VAL:HG12 | 1:34:A:ARG:HE   | 4        | 0.51          |
| (1,467)  | 1:31:A:LEU:HD22 | 1:32:A:ALA:H    | 3        | 0.51          |
| (1,467)  | 1:31:A:LEU:HD21 | 1:32:A:ALA:H    | 5        | 0.51          |
| (1,467)  | 1:31:A:LEU:HD21 | 1:32:A:ALA:H    | 6        | 0.51          |
| (1,467)  | 1:31:A:LEU:HD22 | 1:32:A:ALA:H    | 11       | 0.51          |
| (1,467)  | 1:31:A:LEU:HD21 | 1:32:A:ALA:H    | 16       | 0.51          |
| (1,389)  | 1:58:A:ASP:H    | 1:57:A:VAL:HG12 | 13       | 0.51          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,263)  | 1:110:A:VAL:HG22 | 1:91:A:GLY:H     | 17       | 0.51          |
| (1,217)  | 1:93:A:THR:HG21  | 1:103:A:GLY:H    | 8        | 0.51          |
| (1,217)  | 1:93:A:THR:HG23  | 1:103:A:GLY:H    | 14       | 0.51          |
| (1,204)  | 1:105:A:LEU:HD13 | 1:106:A:ASP:H    | 6        | 0.51          |
| (1,204)  | 1:105:A:LEU:HD13 | 1:106:A:ASP:H    | 7        | 0.51          |
| (1,169)  | 1:120:A:ALA:HB2  | 1:119:A:GLU:H    | 8        | 0.51          |
| (3,153)  | 1:110:A:VAL:HG22 | 1:114:A:ARG:H    | 7        | 0.5           |
| (3,152)  | 1:27:A:VAL:H     | 1:74:A:ALA:HB1   | 1        | 0.5           |
| (3,132)  | 1:113:A:ALA:HB2  | 1:112:A:HIS:H    | 1        | 0.5           |
| (3,132)  | 1:113:A:ALA:HB1  | 1:112:A:HIS:H    | 10       | 0.5           |
| (3,126)  | 1:21:A:LEU:HD22  | 1:22:A:ASN:H     | 10       | 0.5           |
| (3,105)  | 1:64:A:MET:H     | 1:66:A:LEU:HD22  | 13       | 0.5           |
| (3,102)  | 1:65:A:ASN:HB2   | 1:64:A:MET:HG2   | 17       | 0.5           |
| (3,99)   | 1:72:A:ARG:HG3   | 1:75:A:LEU:HD13  | 10       | 0.5           |
| (3,99)   | 1:72:A:ARG:HG3   | 1:75:A:LEU:HD12  | 16       | 0.5           |
| (3,72)   | 1:117:A:LEU:HG   | 1:117:A:LEU:H    | 4        | 0.5           |
| (3,69)   | 1:57:A:VAL:HA    | 1:71:A:LEU:HB2   | 10       | 0.5           |
| (3,50)   | 1:31:A:LEU:HD23  | 1:97:A:LEU:HD22  | 15       | 0.5           |
| (3,18)   | 1:58:A:ASP:HB3   | 1:60:A:VAL:HG11  | 8        | 0.5           |
| (1,4283) | 1:120:A:ALA:H    | 1:85:A:LEU:HD21  | 1        | 0.5           |
| (1,4164) | 1:32:A:ALA:HB1   | 1:41:A:ALA:H     | 15       | 0.5           |
| (1,4119) | 1:66:A:LEU:HB2   | 1:70:A:GLN:HE22  | 14       | 0.5           |
| (1,4084) | 1:20:A:LYS:HB3   | 1:22:A:ASN:HD22  | 10       | 0.5           |
| (1,4007) | 1:41:A:ALA:HB2   | 1:41:A:ALA:H     | 3        | 0.5           |
| (1,4007) | 1:41:A:ALA:HB2   | 1:41:A:ALA:H     | 5        | 0.5           |
| (1,4007) | 1:41:A:ALA:HB2   | 1:41:A:ALA:H     | 6        | 0.5           |
| (1,3957) | 1:58:A:ASP:H     | 1:57:A:VAL:HG12  | 6        | 0.5           |
| (1,3957) | 1:58:A:ASP:H     | 1:57:A:VAL:HG11  | 17       | 0.5           |
| (1,3943) | 1:66:A:LEU:HD11  | 1:62:A:GLY:H     | 13       | 0.5           |
| (1,3943) | 1:66:A:LEU:HD11  | 1:62:A:GLY:H     | 16       | 0.5           |
| (1,3861) | 1:110:A:VAL:HG22 | 1:91:A:GLY:H     | 12       | 0.5           |
| (1,3822) | 1:93:A:THR:HG23  | 1:103:A:GLY:H    | 1        | 0.5           |
| (1,3822) | 1:93:A:THR:HG23  | 1:103:A:GLY:H    | 5        | 0.5           |
| (1,3810) | 1:105:A:LEU:HD13 | 1:106:A:ASP:H    | 1        | 0.5           |
| (1,3742) | 1:28:A:ILE:H     | 1:29:A:ALA:HB2   | 2        | 0.5           |
| (1,3601) | 1:113:A:ALA:HB2  | 1:111:A:GLU:H    | 4        | 0.5           |
| (1,3570) | 1:90:A:PRO:HA    | 1:105:A:LEU:HD11 | 5        | 0.5           |
| (1,3554) | 1:66:A:LEU:HB2   | 1:66:A:LEU:HD21  | 3        | 0.5           |
| (1,3446) | 1:65:A:ASN:HD22  | 1:20:A:LYS:HG2   | 11       | 0.5           |
| (1,3446) | 1:65:A:ASN:HD22  | 1:20:A:LYS:HG2   | 15       | 0.5           |
| (1,3386) | 1:90:A:PRO:HA    | 1:92:A:ALA:HB3   | 16       | 0.5           |
| (1,3373) | 1:88:A:VAL:HA    | 1:93:A:THR:HG23  | 13       | 0.5           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3373) | 1:88:A:VAL:HA    | 1:93:A:THR:HG21  | 17       | 0.5           |
| (1,3366) | 1:72:A:ARG:HA    | 1:56:A:LEU:HD23  | 12       | 0.5           |
| (1,3342) | 1:92:A:ALA:HB2   | 1:88:A:VAL:H     | 11       | 0.5           |
| (1,3329) | 1:77:A:LEU:HD12  | 1:78:A:TYR:H     | 8        | 0.5           |
| (1,3302) | 1:83:A:ARG:HB2   | 1:86:A:TYR:HD1   | 16       | 0.5           |
| (1,3256) | 1:41:A:ALA:HB2   | 1:33:A:GLU:H     | 6        | 0.5           |
| (1,3256) | 1:41:A:ALA:HB2   | 1:33:A:GLU:H     | 9        | 0.5           |
| (1,3253) | 1:92:A:ALA:HB1   | 1:91:A:GLY:H     | 17       | 0.5           |
| (1,3204) | 1:121:A:LYS:HB2  | 1:117:A:LEU:HD12 | 4        | 0.5           |
| (1,3116) | 1:57:A:VAL:HG23  | 1:53:A:PHE:HE1   | 10       | 0.5           |
| (1,3052) | 1:39:A:PHE:HZ    | 1:52:A:ILE:HG22  | 4        | 0.5           |
| (1,3023) | 1:64:A:MET:HE3   | 1:27:A:VAL:HA    | 3        | 0.5           |
| (1,3002) | 1:57:A:VAL:HG13  | 1:60:A:VAL:HB    | 10       | 0.5           |
| (1,2962) | 1:97:A:LEU:HD23  | 1:56:A:LEU:HD23  | 10       | 0.5           |
| (1,2900) | 1:28:A:ILE:HD12  | 1:31:A:LEU:HB3   | 13       | 0.5           |
| (1,2897) | 1:39:A:PHE:HZ    | 1:28:A:ILE:HD11  | 4        | 0.5           |
| (1,2890) | 1:33:A:GLU:HB3   | 1:32:A:ALA:HB2   | 10       | 0.5           |
| (1,2886) | 1:41:A:ALA:HA    | 1:32:A:ALA:HB2   | 14       | 0.5           |
| (1,2885) | 1:32:A:ALA:HB3   | 1:31:A:LEU:H     | 1        | 0.5           |
| (1,2885) | 1:32:A:ALA:HB1   | 1:31:A:LEU:H     | 6        | 0.5           |
| (1,2865) | 1:78:A:TYR:HE2   | 1:48:A:LEU:HD11  | 5        | 0.5           |
| (1,2865) | 1:78:A:TYR:HE2   | 1:48:A:LEU:HD12  | 8        | 0.5           |
| (1,2864) | 1:78:A:TYR:HE2   | 1:78:A:TYR:HB3   | 5        | 0.5           |
| (1,2852) | 1:81:A:SER:HB3   | 1:84:A:TYR:HD1   | 13       | 0.5           |
| (1,2827) | 1:97:A:LEU:HD23  | 1:52:A:ILE:HB    | 5        | 0.5           |
| (1,2817) | 1:97:A:LEU:HD11  | 1:97:A:LEU:HA    | 3        | 0.5           |
| (1,2817) | 1:97:A:LEU:HD13  | 1:97:A:LEU:HA    | 9        | 0.5           |
| (1,2680) | 1:117:A:LEU:HD13 | 1:82:A:TRP:HD1   | 14       | 0.5           |
| (1,2608) | 1:48:A:LEU:HD12  | 1:52:A:ILE:HG12  | 8        | 0.5           |
| (1,2592) | 1:69:A:THR:HG21  | 1:70:A:GLN:H     | 5        | 0.5           |
| (1,2592) | 1:69:A:THR:HG22  | 1:70:A:GLN:H     | 14       | 0.5           |
| (1,2585) | 1:92:A:ALA:HA    | 1:93:A:THR:HG22  | 14       | 0.5           |
| (1,2581) | 1:71:A:LEU:HD11  | 1:60:A:VAL:HG13  | 8        | 0.5           |
| (1,2581) | 1:71:A:LEU:HD12  | 1:60:A:VAL:HG11  | 11       | 0.5           |
| (1,2578) | 1:57:A:VAL:HA    | 1:60:A:VAL:HG12  | 6        | 0.5           |
| (1,2578) | 1:57:A:VAL:HA    | 1:60:A:VAL:HG12  | 16       | 0.5           |
| (1,2577) | 1:60:A:VAL:HG12  | 1:59:A:ARG:HA    | 3        | 0.5           |
| (1,2309) | 1:39:A:PHE:HB3   | 1:39:A:PHE:HE1   | 12       | 0.5           |
| (1,2305) | 1:45:A:ALA:HB2   | 1:44:A:GLU:HA    | 10       | 0.5           |
| (1,2268) | 1:110:A:VAL:HG12 | 1:89:A:LYS:H     | 7        | 0.5           |
| (1,2212) | 1:110:A:VAL:HG21 | 1:114:A:ARG:H    | 11       | 0.5           |
| (1,2150) | 1:105:A:LEU:H    | 1:105:A:LEU:HD11 | 7        | 0.5           |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2147) | 1:85:A:LEU:HA   | 1:85:A:LEU:HD13  | 1        | 0.5           |
| (1,2147) | 1:85:A:LEU:HA   | 1:85:A:LEU:HD12  | 8        | 0.5           |
| (1,2147) | 1:85:A:LEU:HA   | 1:85:A:LEU:HD13  | 10       | 0.5           |
| (1,2147) | 1:85:A:LEU:HA   | 1:85:A:LEU:HD12  | 13       | 0.5           |
| (1,2147) | 1:85:A:LEU:HA   | 1:85:A:LEU:HD11  | 16       | 0.5           |
| (1,2146) | 1:104:A:GLU:HB3 | 1:93:A:THR:HG23  | 16       | 0.5           |
| (1,2146) | 1:104:A:GLU:HB3 | 1:93:A:THR:HG22  | 17       | 0.5           |
| (1,2006) | 1:78:A:TYR:HE2  | 1:48:A:LEU:HD12  | 9        | 0.5           |
| (1,2006) | 1:78:A:TYR:HE2  | 1:48:A:LEU:HD12  | 13       | 0.5           |
| (1,1990) | 1:92:A:ALA:HB1  | 1:91:A:GLY:H     | 11       | 0.5           |
| (1,1950) | 1:105:A:LEU:HB2 | 1:110:A:VAL:HG11 | 11       | 0.5           |
| (1,1867) | 1:53:A:PHE:HA   | 1:31:A:LEU:HD13  | 15       | 0.5           |
| (1,1853) | 1:86:A:TYR:HE1  | 1:85:A:LEU:HD13  | 9        | 0.5           |
| (1,1853) | 1:86:A:TYR:HE1  | 1:85:A:LEU:HD13  | 11       | 0.5           |
| (1,1851) | 1:35:A:PHE:HE2  | 1:38:A:CYS:HB2   | 1        | 0.5           |
| (1,1838) | 1:93:A:THR:HA   | 1:93:A:THR:HG22  | 5        | 0.5           |
| (1,1790) | 1:90:A:PRO:HA   | 1:92:A:ALA:HB2   | 3        | 0.5           |
| (1,1790) | 1:90:A:PRO:HA   | 1:92:A:ALA:HB3   | 13       | 0.5           |
| (1,1682) | 1:41:A:ALA:HB2  | 1:33:A:GLU:H     | 15       | 0.5           |
| (1,1545) | 1:56:A:LEU:HD11 | 1:60:A:VAL:HB    | 11       | 0.5           |
| (1,1507) | 1:78:A:TYR:HE2  | 1:28:A:ILE:HG22  | 15       | 0.5           |
| (1,1482) | 1:64:A:MET:HE2  | 1:27:A:VAL:HA    | 11       | 0.5           |
| (1,1480) | 1:64:A:MET:HE2  | 1:63:A:GLU:H     | 5        | 0.5           |
| (1,1405) | 1:102:A:CYS:H   | 1:95:A:VAL:HG11  | 13       | 0.5           |
| (1,1372) | 1:28:A:ILE:HD11 | 1:31:A:LEU:HB3   | 4        | 0.5           |
| (1,1372) | 1:28:A:ILE:HD12 | 1:31:A:LEU:HB3   | 5        | 0.5           |
| (1,1372) | 1:28:A:ILE:HD13 | 1:31:A:LEU:HB3   | 15       | 0.5           |
| (1,1343) | 1:78:A:TYR:HE1  | 1:48:A:LEU:HD13  | 15       | 0.5           |
| (1,1336) | 1:85:A:LEU:HD22 | 1:84:A:TYR:HD2   | 8        | 0.5           |
| (1,1336) | 1:85:A:LEU:HD23 | 1:84:A:TYR:HD2   | 11       | 0.5           |
| (1,1336) | 1:85:A:LEU:HD22 | 1:84:A:TYR:HD1   | 17       | 0.5           |
| (1,1334) | 1:81:A:SER:HB3  | 1:84:A:TYR:HD1   | 6        | 0.5           |
| (1,1305) | 1:97:A:LEU:HD23 | 1:52:A:ILE:HB    | 7        | 0.5           |
| (1,1305) | 1:97:A:LEU:HD21 | 1:52:A:ILE:HB    | 9        | 0.5           |
| (1,1125) | 1:97:A:LEU:HD12 | 1:60:A:VAL:HG13  | 2        | 0.5           |
| (1,1075) | 1:31:A:LEU:HD13 | 1:31:A:LEU:HA    | 5        | 0.5           |
| (1,1075) | 1:31:A:LEU:HD13 | 1:31:A:LEU:HA    | 11       | 0.5           |
| (1,1069) | 1:48:A:LEU:HD13 | 1:52:A:ILE:HG12  | 1        | 0.5           |
| (1,1069) | 1:48:A:LEU:HD12 | 1:52:A:ILE:HG12  | 7        | 0.5           |
| (1,1069) | 1:48:A:LEU:HD13 | 1:52:A:ILE:HG12  | 10       | 0.5           |
| (1,604)  | 1:32:A:ALA:HB2  | 1:41:A:ALA:H     | 7        | 0.5           |
| (1,604)  | 1:32:A:ALA:HB3  | 1:41:A:ALA:H     | 16       | 0.5           |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,570)  | 1:60:A:VAL:HG12  | 1:34:A:ARG:HE   | 9        | 0.5           |
| (1,467)  | 1:31:A:LEU:HD22  | 1:32:A:ALA:H    | 9        | 0.5           |
| (1,442)  | 1:41:A:ALA:HB2   | 1:41:A:ALA:H    | 1        | 0.5           |
| (1,389)  | 1:58:A:ASP:H     | 1:57:A:VAL:HG12 | 3        | 0.5           |
| (1,389)  | 1:58:A:ASP:H     | 1:57:A:VAL:HG12 | 4        | 0.5           |
| (1,389)  | 1:58:A:ASP:H     | 1:57:A:VAL:HG12 | 9        | 0.5           |
| (1,363)  | 1:66:A:LEU:HD13  | 1:62:A:GLY:H    | 4        | 0.5           |
| (1,275)  | 1:85:A:LEU:HD21  | 1:87:A:GLY:H    | 16       | 0.5           |
| (1,263)  | 1:110:A:VAL:HG23 | 1:91:A:GLY:H    | 13       | 0.5           |
| (1,263)  | 1:110:A:VAL:HG22 | 1:91:A:GLY:H    | 16       | 0.5           |
| (1,241)  | 1:95:A:VAL:HG11  | 1:96:A:ASP:H    | 4        | 0.5           |
| (1,217)  | 1:93:A:THR:HG22  | 1:103:A:GLY:H   | 17       | 0.5           |
| (1,204)  | 1:105:A:LEU:HD13 | 1:106:A:ASP:H   | 2        | 0.5           |
| (1,204)  | 1:105:A:LEU:HD11 | 1:106:A:ASP:H   | 11       | 0.5           |
| (1,204)  | 1:105:A:LEU:HD13 | 1:106:A:ASP:H   | 12       | 0.5           |
| (1,169)  | 1:120:A:ALA:HB1  | 1:119:A:GLU:H   | 11       | 0.5           |
| (1,169)  | 1:120:A:ALA:HB1  | 1:119:A:GLU:H   | 13       | 0.5           |
| (3,148)  | 1:22:A:ASN:H     | 1:22:A:ASN:HB2  | 1        | 0.49          |
| (3,148)  | 1:22:A:ASN:H     | 1:65:A:ASN:HB3  | 8        | 0.49          |
| (3,132)  | 1:113:A:ALA:HB2  | 1:112:A:HIS:H   | 16       | 0.49          |
| (3,126)  | 1:21:A:LEU:HD23  | 1:22:A:ASN:H    | 17       | 0.49          |
| (3,124)  | 1:88:A:VAL:HG22  | 1:88:A:VAL:H    | 16       | 0.49          |
| (3,107)  | 1:95:A:VAL:HG22  | 1:102:A:CYS:HB3 | 14       | 0.49          |
| (3,102)  | 1:65:A:ASN:HB2   | 1:64:A:MET:HG2  | 12       | 0.49          |
| (3,99)   | 1:72:A:ARG:HG3   | 1:75:A:LEU:HD13 | 11       | 0.49          |
| (3,98)   | 1:64:A:MET:HE3   | 1:63:A:GLU:HG3  | 12       | 0.49          |
| (3,95)   | 1:75:A:LEU:HD11  | 1:50:A:ILE:H    | 4        | 0.49          |
| (3,95)   | 1:75:A:LEU:HD11  | 1:50:A:ILE:H    | 17       | 0.49          |
| (3,84)   | 1:84:A:TYR:HE1   | 1:84:A:TYR:HA   | 12       | 0.49          |
| (3,72)   | 1:117:A:LEU:HG   | 1:117:A:LEU:H   | 14       | 0.49          |
| (3,62)   | 1:52:A:ILE:HG22  | 1:56:A:LEU:H    | 17       | 0.49          |
| (3,51)   | 1:95:A:VAL:HG23  | 1:49:A:LYS:HA   | 10       | 0.49          |
| (1,4176) | 1:97:A:LEU:HD13  | 1:97:A:LEU:H    | 12       | 0.49          |
| (1,4176) | 1:97:A:LEU:HD12  | 1:97:A:LEU:H    | 17       | 0.49          |
| (1,4118) | 1:71:A:LEU:H     | 1:70:A:GLN:HE21 | 5        | 0.49          |
| (1,4007) | 1:41:A:ALA:HB2   | 1:41:A:ALA:H    | 12       | 0.49          |
| (1,3957) | 1:58:A:ASP:H     | 1:57:A:VAL:HG13 | 8        | 0.49          |
| (1,3943) | 1:66:A:LEU:HD12  | 1:62:A:GLY:H    | 6        | 0.49          |
| (1,3943) | 1:66:A:LEU:HD11  | 1:62:A:GLY:H    | 14       | 0.49          |
| (1,3943) | 1:66:A:LEU:HD11  | 1:62:A:GLY:H    | 17       | 0.49          |
| (1,3822) | 1:93:A:THR:HG21  | 1:103:A:GLY:H   | 9        | 0.49          |
| (1,3822) | 1:93:A:THR:HG23  | 1:103:A:GLY:H   | 16       | 0.49          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3782) | 1:120:A:ALA:HB1  | 1:119:A:GLU:H    | 2        | 0.49          |
| (1,3782) | 1:120:A:ALA:HB1  | 1:119:A:GLU:H    | 5        | 0.49          |
| (1,3782) | 1:120:A:ALA:HB1  | 1:119:A:GLU:H    | 14       | 0.49          |
| (1,3601) | 1:113:A:ALA:HB2  | 1:111:A:GLU:H    | 1        | 0.49          |
| (1,3483) | 1:53:A:PHE:HA    | 1:31:A:LEU:HD12  | 14       | 0.49          |
| (1,3452) | 1:95:A:VAL:HA    | 1:93:A:THR:HG22  | 9        | 0.49          |
| (1,3452) | 1:95:A:VAL:HA    | 1:93:A:THR:HG22  | 12       | 0.49          |
| (1,3446) | 1:65:A:ASN:HD22  | 1:20:A:LYS:HG2   | 5        | 0.49          |
| (1,3405) | 1:55:A:ASP:HB2   | 1:56:A:LEU:HD22  | 2        | 0.49          |
| (1,3373) | 1:88:A:VAL:HA    | 1:93:A:THR:HG23  | 8        | 0.49          |
| (1,3373) | 1:88:A:VAL:HA    | 1:93:A:THR:HG21  | 10       | 0.49          |
| (1,3368) | 1:31:A:LEU:HD11  | 1:31:A:LEU:HA    | 17       | 0.49          |
| (1,3342) | 1:92:A:ALA:HB1   | 1:88:A:VAL:H     | 3        | 0.49          |
| (1,3329) | 1:77:A:LEU:HD13  | 1:78:A:TYR:H     | 2        | 0.49          |
| (1,3329) | 1:77:A:LEU:HD12  | 1:78:A:TYR:H     | 7        | 0.49          |
| (1,3329) | 1:77:A:LEU:HD12  | 1:78:A:TYR:H     | 10       | 0.49          |
| (1,3256) | 1:41:A:ALA:HB3   | 1:33:A:GLU:H     | 3        | 0.49          |
| (1,3256) | 1:41:A:ALA:HB1   | 1:33:A:GLU:H     | 7        | 0.49          |
| (1,3204) | 1:121:A:LYS:HB2  | 1:117:A:LEU:HD12 | 8        | 0.49          |
| (1,3171) | 1:75:A:LEU:HD23  | 1:31:A:LEU:HD13  | 2        | 0.49          |
| (1,3116) | 1:57:A:VAL:HG21  | 1:53:A:PHE:HE1   | 11       | 0.49          |
| (1,3052) | 1:39:A:PHE:HZ    | 1:52:A:ILE:HG22  | 15       | 0.49          |
| (1,3051) | 1:78:A:TYR:HE1   | 1:28:A:ILE:HG22  | 5        | 0.49          |
| (1,3045) | 1:52:A:ILE:HG13  | 1:54:A:GLN:HE21  | 2        | 0.49          |
| (1,3024) | 1:64:A:MET:HE1   | 1:65:A:ASN:HB3   | 6        | 0.49          |
| (1,3021) | 1:64:A:MET:HE1   | 1:63:A:GLU:H     | 9        | 0.49          |
| (1,3002) | 1:57:A:VAL:HG11  | 1:60:A:VAL:HB    | 14       | 0.49          |
| (1,2897) | 1:39:A:PHE:HZ    | 1:28:A:ILE:HD13  | 1        | 0.49          |
| (1,2894) | 1:52:A:ILE:HD11  | 1:53:A:PHE:HB2   | 3        | 0.49          |
| (1,2894) | 1:52:A:ILE:HD11  | 1:53:A:PHE:HB2   | 11       | 0.49          |
| (1,2864) | 1:78:A:TYR:HE1   | 1:78:A:TYR:HB3   | 3        | 0.49          |
| (1,2854) | 1:85:A:LEU:HD22  | 1:84:A:TYR:HD1   | 2        | 0.49          |
| (1,2852) | 1:81:A:SER:HB3   | 1:84:A:TYR:HD2   | 3        | 0.49          |
| (1,2852) | 1:81:A:SER:HB3   | 1:84:A:TYR:HD2   | 7        | 0.49          |
| (1,2852) | 1:81:A:SER:HB3   | 1:84:A:TYR:HD1   | 14       | 0.49          |
| (1,2845) | 1:22:A:ASN:H     | 1:27:A:VAL:HG12  | 4        | 0.49          |
| (1,2831) | 1:97:A:LEU:HD23  | 1:35:A:PHE:HD1   | 8        | 0.49          |
| (1,2827) | 1:97:A:LEU:HD21  | 1:52:A:ILE:HB    | 11       | 0.49          |
| (1,2681) | 1:120:A:ALA:HB2  | 1:82:A:TRP:HD1   | 4        | 0.49          |
| (1,2680) | 1:117:A:LEU:HD13 | 1:82:A:TRP:HD1   | 5        | 0.49          |
| (1,2673) | 1:97:A:LEU:HD13  | 1:35:A:PHE:HD1   | 16       | 0.49          |
| (1,2616) | 1:21:A:LEU:HA    | 1:21:A:LEU:HD23  | 9        | 0.49          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2592) | 1:69:A:THR:HG22 | 1:70:A:GLN:H     | 1        | 0.49          |
| (1,2592) | 1:69:A:THR:HG23 | 1:70:A:GLN:H     | 4        | 0.49          |
| (1,2592) | 1:69:A:THR:HG22 | 1:70:A:GLN:H     | 7        | 0.49          |
| (1,2592) | 1:69:A:THR:HG23 | 1:70:A:GLN:H     | 8        | 0.49          |
| (1,2592) | 1:69:A:THR:HG21 | 1:70:A:GLN:H     | 9        | 0.49          |
| (1,2592) | 1:69:A:THR:HG22 | 1:70:A:GLN:H     | 10       | 0.49          |
| (1,2592) | 1:69:A:THR:HG21 | 1:70:A:GLN:H     | 11       | 0.49          |
| (1,2592) | 1:69:A:THR:HG22 | 1:70:A:GLN:H     | 12       | 0.49          |
| (1,2592) | 1:69:A:THR:HG21 | 1:70:A:GLN:H     | 15       | 0.49          |
| (1,2592) | 1:69:A:THR:HG22 | 1:70:A:GLN:H     | 16       | 0.49          |
| (1,2581) | 1:71:A:LEU:HD13 | 1:60:A:VAL:HG13  | 12       | 0.49          |
| (1,2581) | 1:71:A:LEU:HD12 | 1:60:A:VAL:HG12  | 15       | 0.49          |
| (1,2581) | 1:71:A:LEU:HD13 | 1:60:A:VAL:HG12  | 16       | 0.49          |
| (1,2578) | 1:57:A:VAL:HA   | 1:60:A:VAL:HG12  | 2        | 0.49          |
| (1,2578) | 1:57:A:VAL:HA   | 1:60:A:VAL:HG13  | 4        | 0.49          |
| (1,2578) | 1:57:A:VAL:HA   | 1:60:A:VAL:HG13  | 9        | 0.49          |
| (1,2411) | 1:45:A:ALA:HB3  | 1:84:A:TYR:HB3   | 11       | 0.49          |
| (1,2397) | 1:50:A:ILE:HD12 | 1:50:A:ILE:HA    | 12       | 0.49          |
| (1,2336) | 1:64:A:MET:HE1  | 1:31:A:LEU:HA    | 7        | 0.49          |
| (1,2305) | 1:45:A:ALA:HB2  | 1:44:A:GLU:HA    | 1        | 0.49          |
| (1,2305) | 1:45:A:ALA:HB3  | 1:44:A:GLU:HA    | 8        | 0.49          |
| (1,2305) | 1:45:A:ALA:HB2  | 1:44:A:GLU:HA    | 9        | 0.49          |
| (1,2271) | 1:113:A:ALA:HB2 | 1:112:A:HIS:HD2  | 1        | 0.49          |
| (1,2228) | 1:25:A:LYS:HD3  | 1:25:A:LYS:HG3   | 2        | 0.49          |
| (1,2228) | 1:25:A:LYS:HD3  | 1:25:A:LYS:HG3   | 14       | 0.49          |
| (1,2194) | 1:50:A:ILE:HD13 | 1:80:A:SER:H     | 10       | 0.49          |
| (1,2147) | 1:85:A:LEU:HA   | 1:85:A:LEU:HD13  | 12       | 0.49          |
| (1,1990) | 1:92:A:ALA:HB2  | 1:91:A:GLY:H     | 6        | 0.49          |
| (1,1950) | 1:105:A:LEU:HB2 | 1:110:A:VAL:HG12 | 4        | 0.49          |
| (1,1950) | 1:105:A:LEU:HB2 | 1:110:A:VAL:HG13 | 7        | 0.49          |
| (1,1881) | 1:113:A:ALA:HB3 | 1:88:A:VAL:HA    | 11       | 0.49          |
| (1,1874) | 1:70:A:GLN:HE21 | 1:27:A:VAL:HG12  | 9        | 0.49          |
| (1,1867) | 1:53:A:PHE:HA   | 1:31:A:LEU:HD13  | 9        | 0.49          |
| (1,1865) | 1:45:A:ALA:HB1  | 1:44:A:GLU:HB3   | 9        | 0.49          |
| (1,1853) | 1:86:A:TYR:HE1  | 1:85:A:LEU:HD13  | 2        | 0.49          |
| (1,1853) | 1:86:A:TYR:HE2  | 1:85:A:LEU:HD13  | 12       | 0.49          |
| (1,1851) | 1:35:A:PHE:HE2  | 1:38:A:CYS:HB2   | 10       | 0.49          |
| (1,1839) | 1:95:A:VAL:HA   | 1:93:A:THR:HG21  | 14       | 0.49          |
| (1,1838) | 1:93:A:THR:HA   | 1:93:A:THR:HG22  | 1        | 0.49          |
| (1,1838) | 1:93:A:THR:HA   | 1:93:A:THR:HG22  | 4        | 0.49          |
| (1,1838) | 1:93:A:THR:HA   | 1:93:A:THR:HG21  | 11       | 0.49          |
| (1,1838) | 1:93:A:THR:HA   | 1:93:A:THR:HG23  | 12       | 0.49          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1838) | 1:93:A:THR:HA    | 1:93:A:THR:HG21 | 17       | 0.49          |
| (1,1790) | 1:90:A:PRO:HA    | 1:92:A:ALA:HB1  | 12       | 0.49          |
| (1,1740) | 1:77:A:LEU:HD13  | 1:78:A:TYR:H    | 15       | 0.49          |
| (1,1679) | 1:92:A:ALA:HB3   | 1:91:A:GLY:H    | 3        | 0.49          |
| (1,1545) | 1:56:A:LEU:HD11  | 1:60:A:VAL:HB   | 6        | 0.49          |
| (1,1510) | 1:52:A:ILE:HG23  | 1:50:A:ILE:H    | 7        | 0.49          |
| (1,1507) | 1:78:A:TYR:HE1   | 1:28:A:ILE:HG22 | 4        | 0.49          |
| (1,1481) | 1:64:A:MET:HE3   | 1:30:A:PHE:HA   | 9        | 0.49          |
| (1,1480) | 1:64:A:MET:HE2   | 1:63:A:GLU:H    | 4        | 0.49          |
| (1,1372) | 1:28:A:ILE:HD13  | 1:31:A:LEU:HB3  | 9        | 0.49          |
| (1,1336) | 1:85:A:LEU:HD23  | 1:84:A:TYR:HD2  | 10       | 0.49          |
| (1,1336) | 1:85:A:LEU:HD21  | 1:84:A:TYR:HD1  | 16       | 0.49          |
| (1,1334) | 1:81:A:SER:HB3   | 1:84:A:TYR:HD2  | 1        | 0.49          |
| (1,1305) | 1:97:A:LEU:HD23  | 1:52:A:ILE:HB   | 3        | 0.49          |
| (1,1305) | 1:97:A:LEU:HD21  | 1:52:A:ILE:HB   | 4        | 0.49          |
| (1,1155) | 1:53:A:PHE:HB3   | 1:53:A:PHE:HE1  | 9        | 0.49          |
| (1,1075) | 1:31:A:LEU:HD12  | 1:31:A:LEU:HA   | 14       | 0.49          |
| (1,1069) | 1:48:A:LEU:HD13  | 1:52:A:ILE:HG12 | 5        | 0.49          |
| (1,1043) | 1:78:A:TYR:HE1   | 1:28:A:ILE:HD12 | 17       | 0.49          |
| (1,789)  | 1:50:A:ILE:HG13  | 1:50:A:ILE:HG21 | 2        | 0.49          |
| (1,789)  | 1:50:A:ILE:HG13  | 1:50:A:ILE:HG21 | 4        | 0.49          |
| (1,789)  | 1:50:A:ILE:HG13  | 1:50:A:ILE:HG22 | 8        | 0.49          |
| (1,788)  | 1:52:A:ILE:HD11  | 1:56:A:LEU:H    | 10       | 0.49          |
| (1,720)  | 1:120:A:ALA:H    | 1:85:A:LEU:HD22 | 4        | 0.49          |
| (1,610)  | 1:48:A:LEU:HD21  | 1:49:A:LYS:H    | 7        | 0.49          |
| (1,610)  | 1:48:A:LEU:HD22  | 1:49:A:LYS:H    | 9        | 0.49          |
| (1,604)  | 1:32:A:ALA:HB1   | 1:41:A:ALA:H    | 1        | 0.49          |
| (1,604)  | 1:32:A:ALA:HB2   | 1:41:A:ALA:H    | 3        | 0.49          |
| (1,604)  | 1:32:A:ALA:HB3   | 1:41:A:ALA:H    | 13       | 0.49          |
| (1,467)  | 1:31:A:LEU:HD23  | 1:32:A:ALA:H    | 1        | 0.49          |
| (1,467)  | 1:31:A:LEU:HD21  | 1:32:A:ALA:H    | 4        | 0.49          |
| (1,389)  | 1:58:A:ASP:H     | 1:57:A:VAL:HG12 | 16       | 0.49          |
| (1,363)  | 1:66:A:LEU:HD12  | 1:62:A:GLY:H    | 1        | 0.49          |
| (1,204)  | 1:105:A:LEU:HD11 | 1:106:A:ASP:H   | 3        | 0.49          |
| (1,126)  | 1:28:A:ILE:H     | 1:29:A:ALA:HB2  | 5        | 0.49          |
| (3,136)  | 1:82:A:TRP:HD1   | 1:82:A:TRP:H    | 4        | 0.48          |
| (3,132)  | 1:113:A:ALA:HB1  | 1:112:A:HIS:H   | 14       | 0.48          |
| (3,126)  | 1:21:A:LEU:HD21  | 1:22:A:ASN:H    | 12       | 0.48          |
| (3,123)  | 1:50:A:ILE:HD11  | 1:79:A:THR:HA   | 16       | 0.48          |
| (3,117)  | 1:48:A:LEU:HD22  | 1:39:A:PHE:HD1  | 6        | 0.48          |
| (3,99)   | 1:72:A:ARG:HG3   | 1:75:A:LEU:HD11 | 2        | 0.48          |
| (3,72)   | 1:117:A:LEU:HG   | 1:117:A:LEU:H   | 5        | 0.48          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (3,72)   | 1:117:A:LEU:HG  | 1:117:A:LEU:H    | 10       | 0.48          |
| (3,72)   | 1:117:A:LEU:HG  | 1:117:A:LEU:H    | 16       | 0.48          |
| (3,69)   | 1:57:A:VAL:HA   | 1:71:A:LEU:HB2   | 17       | 0.48          |
| (3,65)   | 1:52:A:ILE:HG13 | 1:52:A:ILE:HG22  | 7        | 0.48          |
| (3,62)   | 1:52:A:ILE:HG22 | 1:56:A:LEU:H     | 16       | 0.48          |
| (3,36)   | 1:50:A:ILE:HG23 | 1:49:A:LYS:HB2   | 16       | 0.48          |
| (3,21)   | 1:31:A:LEU:H    | 1:21:A:LEU:HD13  | 12       | 0.48          |
| (3,18)   | 1:58:A:ASP:HB3  | 1:60:A:VAL:HG12  | 10       | 0.48          |
| (1,4180) | 1:95:A:VAL:H    | 1:48:A:LEU:HD12  | 2        | 0.48          |
| (1,4164) | 1:32:A:ALA:HB3  | 1:41:A:ALA:H     | 4        | 0.48          |
| (1,4164) | 1:32:A:ALA:HB3  | 1:41:A:ALA:H     | 9        | 0.48          |
| (1,4007) | 1:41:A:ALA:HB1  | 1:41:A:ALA:H     | 9        | 0.48          |
| (1,4007) | 1:41:A:ALA:HB2  | 1:41:A:ALA:H     | 10       | 0.48          |
| (1,3943) | 1:66:A:LEU:HD12 | 1:62:A:GLY:H     | 8        | 0.48          |
| (1,3834) | 1:95:A:VAL:HG22 | 1:100:A:ASN:H    | 2        | 0.48          |
| (1,3742) | 1:28:A:ILE:H    | 1:29:A:ALA:HB2   | 13       | 0.48          |
| (1,3644) | 1:53:A:PHE:H    | 1:53:A:PHE:HD1   | 5        | 0.48          |
| (1,3627) | 1:100:A:ASN:H   | 1:100:A:ASN:HD21 | 7        | 0.48          |
| (1,3601) | 1:113:A:ALA:HB3 | 1:111:A:GLU:H    | 12       | 0.48          |
| (1,3570) | 1:90:A:PRO:HA   | 1:105:A:LEU:HD13 | 16       | 0.48          |
| (1,3554) | 1:66:A:LEU:HB2  | 1:66:A:LEU:HD22  | 15       | 0.48          |
| (1,3483) | 1:53:A:PHE:HA   | 1:31:A:LEU:HD13  | 1        | 0.48          |
| (1,3483) | 1:53:A:PHE:HA   | 1:31:A:LEU:HD12  | 3        | 0.48          |
| (1,3483) | 1:53:A:PHE:HA   | 1:31:A:LEU:HD12  | 7        | 0.48          |
| (1,3483) | 1:53:A:PHE:HA   | 1:31:A:LEU:HD12  | 12       | 0.48          |
| (1,3483) | 1:53:A:PHE:HA   | 1:31:A:LEU:HD11  | 17       | 0.48          |
| (1,3463) | 1:35:A:PHE:HE1  | 1:38:A:CYS:HB2   | 13       | 0.48          |
| (1,3451) | 1:93:A:THR:HA   | 1:93:A:THR:HG23  | 13       | 0.48          |
| (1,3418) | 1:117:A:LEU:HB2 | 1:117:A:LEU:HD11 | 7        | 0.48          |
| (1,3405) | 1:55:A:ASP:HB2  | 1:56:A:LEU:HD21  | 3        | 0.48          |
| (1,3405) | 1:55:A:ASP:HB2  | 1:56:A:LEU:HD22  | 5        | 0.48          |
| (1,3405) | 1:55:A:ASP:HB2  | 1:56:A:LEU:HD22  | 14       | 0.48          |
| (1,3405) | 1:55:A:ASP:HB2  | 1:56:A:LEU:HD21  | 16       | 0.48          |
| (1,3368) | 1:31:A:LEU:HD12 | 1:31:A:LEU:HA    | 7        | 0.48          |
| (1,3368) | 1:31:A:LEU:HD13 | 1:31:A:LEU:HA    | 15       | 0.48          |
| (1,3366) | 1:72:A:ARG:HA   | 1:56:A:LEU:HD21  | 1        | 0.48          |
| (1,3352) | 1:79:A:THR:HG23 | 1:48:A:LEU:HD13  | 17       | 0.48          |
| (1,3329) | 1:77:A:LEU:HD13 | 1:78:A:TYR:H     | 1        | 0.48          |
| (1,3329) | 1:77:A:LEU:HD11 | 1:78:A:TYR:H     | 13       | 0.48          |
| (1,3329) | 1:77:A:LEU:HD12 | 1:78:A:TYR:H     | 14       | 0.48          |
| (1,3256) | 1:41:A:ALA:HB3  | 1:33:A:GLU:H     | 2        | 0.48          |
| (1,3256) | 1:41:A:ALA:HB2  | 1:33:A:GLU:H     | 10       | 0.48          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3256) | 1:41:A:ALA:HB2  | 1:33:A:GLU:H     | 16       | 0.48          |
| (1,3199) | 1:113:A:ALA:HB2 | 1:112:A:HIS:HB2  | 5        | 0.48          |
| (1,3116) | 1:57:A:VAL:HG23 | 1:53:A:PHE:HE1   | 3        | 0.48          |
| (1,3116) | 1:57:A:VAL:HG21 | 1:53:A:PHE:HE2   | 5        | 0.48          |
| (1,3081) | 1:97:A:LEU:HD13 | 1:55:A:ASP:HA    | 12       | 0.48          |
| (1,3052) | 1:39:A:PHE:HZ   | 1:52:A:ILE:HG21  | 13       | 0.48          |
| (1,3051) | 1:78:A:TYR:HE2  | 1:28:A:ILE:HG23  | 7        | 0.48          |
| (1,2900) | 1:28:A:ILE:HD12 | 1:31:A:LEU:HB3   | 8        | 0.48          |
| (1,2897) | 1:39:A:PHE:HZ   | 1:28:A:ILE:HD13  | 15       | 0.48          |
| (1,2894) | 1:52:A:ILE:HD13 | 1:53:A:PHE:HB2   | 9        | 0.48          |
| (1,2890) | 1:33:A:GLU:HB3  | 1:32:A:ALA:HB1   | 4        | 0.48          |
| (1,2885) | 1:32:A:ALA:HB2  | 1:31:A:LEU:H     | 4        | 0.48          |
| (1,2864) | 1:78:A:TYR:HE1  | 1:78:A:TYR:HB3   | 10       | 0.48          |
| (1,2845) | 1:22:A:ASN:H    | 1:27:A:VAL:HG11  | 9        | 0.48          |
| (1,2836) | 1:95:A:VAL:HG21 | 1:97:A:LEU:HD21  | 7        | 0.48          |
| (1,2827) | 1:97:A:LEU:HD23 | 1:52:A:ILE:HB    | 6        | 0.48          |
| (1,2678) | 1:53:A:PHE:HB3  | 1:53:A:PHE:HE1   | 17       | 0.48          |
| (1,2673) | 1:97:A:LEU:HD12 | 1:35:A:PHE:HD1   | 2        | 0.48          |
| (1,2669) | 1:75:A:LEU:HD23 | 1:78:A:TYR:HE1   | 12       | 0.48          |
| (1,2669) | 1:75:A:LEU:HD21 | 1:78:A:TYR:HE1   | 17       | 0.48          |
| (1,2592) | 1:69:A:THR:HG21 | 1:70:A:GLN:H     | 6        | 0.48          |
| (1,2592) | 1:69:A:THR:HG21 | 1:70:A:GLN:H     | 13       | 0.48          |
| (1,2581) | 1:71:A:LEU:HD11 | 1:60:A:VAL:HG11  | 7        | 0.48          |
| (1,2578) | 1:57:A:VAL:HA   | 1:60:A:VAL:HG12  | 15       | 0.48          |
| (1,2568) | 1:78:A:TYR:HE2  | 1:28:A:ILE:HD12  | 8        | 0.48          |
| (1,2568) | 1:78:A:TYR:HE1  | 1:28:A:ILE:HD13  | 10       | 0.48          |
| (1,2484) | 1:93:A:THR:HB   | 1:95:A:VAL:HG11  | 15       | 0.48          |
| (1,2309) | 1:39:A:PHE:HB3  | 1:39:A:PHE:HE1   | 13       | 0.48          |
| (1,2228) | 1:25:A:LYS:HD3  | 1:25:A:LYS:HG3   | 1        | 0.48          |
| (1,2201) | 1:64:A:MET:HB2  | 1:21:A:LEU:HD23  | 12       | 0.48          |
| (1,2150) | 1:105:A:LEU:H   | 1:105:A:LEU:HD11 | 5        | 0.48          |
| (1,2150) | 1:105:A:LEU:H   | 1:105:A:LEU:HD11 | 6        | 0.48          |
| (1,2147) | 1:85:A:LEU:HA   | 1:85:A:LEU:HD13  | 9        | 0.48          |
| (1,2147) | 1:85:A:LEU:HA   | 1:85:A:LEU:HD13  | 11       | 0.48          |
| (1,1955) | 1:92:A:ALA:HB3  | 1:113:A:ALA:HB3  | 10       | 0.48          |
| (1,1950) | 1:105:A:LEU:HB2 | 1:110:A:VAL:HG12 | 3        | 0.48          |
| (1,1874) | 1:70:A:GLN:HE21 | 1:27:A:VAL:HG13  | 4        | 0.48          |
| (1,1851) | 1:35:A:PHE:HE1  | 1:38:A:CYS:HB2   | 12       | 0.48          |
| (1,1851) | 1:35:A:PHE:HE2  | 1:38:A:CYS:HB2   | 17       | 0.48          |
| (1,1838) | 1:93:A:THR:HA   | 1:93:A:THR:HG23  | 2        | 0.48          |
| (1,1838) | 1:93:A:THR:HA   | 1:93:A:THR:HG23  | 8        | 0.48          |
| (1,1838) | 1:93:A:THR:HA   | 1:93:A:THR:HG23  | 15       | 0.48          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1751) | 1:32:A:ALA:HB3   | 1:41:A:ALA:H    | 8        | 0.48          |
| (1,1682) | 1:41:A:ALA:HB3   | 1:33:A:GLU:H    | 11       | 0.48          |
| (1,1679) | 1:92:A:ALA:HB1   | 1:91:A:GLY:H    | 16       | 0.48          |
| (1,1545) | 1:56:A:LEU:HD11  | 1:60:A:VAL:HB   | 3        | 0.48          |
| (1,1507) | 1:78:A:TYR:HE2   | 1:28:A:ILE:HG22 | 16       | 0.48          |
| (1,1502) | 1:52:A:ILE:HG13  | 1:54:A:GLN:HE21 | 7        | 0.48          |
| (1,1372) | 1:28:A:ILE:HD13  | 1:31:A:LEU:HB3  | 1        | 0.48          |
| (1,1372) | 1:28:A:ILE:HD13  | 1:31:A:LEU:HB3  | 11       | 0.48          |
| (1,1356) | 1:61:A:ALA:HB1   | 1:57:A:VAL:HG12 | 7        | 0.48          |
| (1,1356) | 1:61:A:ALA:HB1   | 1:57:A:VAL:HG11 | 8        | 0.48          |
| (1,1356) | 1:61:A:ALA:HB3   | 1:57:A:VAL:HG12 | 14       | 0.48          |
| (1,1308) | 1:97:A:LEU:HD22  | 1:35:A:PHE:HD2  | 5        | 0.48          |
| (1,1155) | 1:53:A:PHE:HB3   | 1:53:A:PHE:HE2  | 2        | 0.48          |
| (1,1155) | 1:53:A:PHE:HB3   | 1:53:A:PHE:HE1  | 6        | 0.48          |
| (1,1155) | 1:53:A:PHE:HB3   | 1:53:A:PHE:HE1  | 10       | 0.48          |
| (1,1155) | 1:53:A:PHE:HB3   | 1:53:A:PHE:HE2  | 14       | 0.48          |
| (1,1155) | 1:53:A:PHE:HB3   | 1:53:A:PHE:HE2  | 16       | 0.48          |
| (1,1076) | 1:30:A:PHE:HD1   | 1:31:A:LEU:HD11 | 12       | 0.48          |
| (1,1075) | 1:31:A:LEU:HD11  | 1:31:A:LEU:HA   | 17       | 0.48          |
| (1,1069) | 1:48:A:LEU:HD12  | 1:52:A:ILE:HG12 | 14       | 0.48          |
| (1,1043) | 1:78:A:TYR:HE2   | 1:28:A:ILE:HD13 | 1        | 0.48          |
| (1,789)  | 1:50:A:ILE:HG13  | 1:50:A:ILE:HG23 | 12       | 0.48          |
| (1,720)  | 1:120:A:ALA:H    | 1:85:A:LEU:HD22 | 10       | 0.48          |
| (1,697)  | 1:57:A:VAL:HG13  | 1:56:A:LEU:H    | 5        | 0.48          |
| (1,610)  | 1:48:A:LEU:HD21  | 1:49:A:LYS:H    | 11       | 0.48          |
| (1,610)  | 1:48:A:LEU:HD22  | 1:49:A:LYS:H    | 16       | 0.48          |
| (1,576)  | 1:50:A:ILE:HD11  | 1:50:A:ILE:H    | 11       | 0.48          |
| (1,576)  | 1:50:A:ILE:HD13  | 1:50:A:ILE:H    | 12       | 0.48          |
| (1,570)  | 1:60:A:VAL:HG11  | 1:34:A:ARG:HE   | 6        | 0.48          |
| (1,442)  | 1:41:A:ALA:HB3   | 1:41:A:ALA:H    | 4        | 0.48          |
| (1,389)  | 1:58:A:ASP:H     | 1:57:A:VAL:HG13 | 5        | 0.48          |
| (1,363)  | 1:66:A:LEU:HD13  | 1:62:A:GLY:H    | 2        | 0.48          |
| (1,263)  | 1:110:A:VAL:HG23 | 1:91:A:GLY:H    | 10       | 0.48          |
| (1,217)  | 1:93:A:THR:HG21  | 1:103:A:GLY:H   | 12       | 0.48          |
| (1,169)  | 1:120:A:ALA:HB1  | 1:119:A:GLU:H   | 1        | 0.48          |
| (1,126)  | 1:28:A:ILE:H     | 1:29:A:ALA:HB2  | 1        | 0.48          |
| (3,150)  | 1:77:A:LEU:H     | 1:79:A:THR:HG23 | 16       | 0.47          |
| (3,147)  | 1:71:A:LEU:H     | 1:66:A:LEU:HD21 | 8        | 0.47          |
| (3,132)  | 1:113:A:ALA:HB1  | 1:112:A:HIS:H   | 3        | 0.47          |
| (3,126)  | 1:21:A:LEU:HD22  | 1:22:A:ASN:H    | 2        | 0.47          |
| (3,126)  | 1:21:A:LEU:HD21  | 1:22:A:ASN:H    | 13       | 0.47          |
| (3,124)  | 1:88:A:VAL:HG23  | 1:88:A:VAL:H    | 2        | 0.47          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (3,124)  | 1:88:A:VAL:HG21 | 1:88:A:VAL:H     | 5        | 0.47          |
| (3,124)  | 1:88:A:VAL:HG23 | 1:88:A:VAL:H     | 14       | 0.47          |
| (3,99)   | 1:72:A:ARG:HG3  | 1:75:A:LEU:HD12  | 17       | 0.47          |
| (3,84)   | 1:84:A:TYR:HE1  | 1:84:A:TYR:HA    | 10       | 0.47          |
| (3,84)   | 1:84:A:TYR:HE1  | 1:84:A:TYR:HA    | 14       | 0.47          |
| (3,72)   | 1:117:A:LEU:HG  | 1:117:A:LEU:H    | 8        | 0.47          |
| (3,69)   | 1:57:A:VAL:HA   | 1:71:A:LEU:HB2   | 8        | 0.47          |
| (3,69)   | 1:57:A:VAL:HA   | 1:71:A:LEU:HB2   | 12       | 0.47          |
| (3,65)   | 1:49:A:LYS:HB2  | 1:52:A:ILE:HG23  | 5        | 0.47          |
| (3,50)   | 1:31:A:LEU:HD22 | 1:97:A:LEU:HD22  | 5        | 0.47          |
| (3,50)   | 1:31:A:LEU:HD23 | 1:97:A:LEU:HD23  | 9        | 0.47          |
| (3,29)   | 1:48:A:LEU:HD23 | 1:39:A:PHE:HD2   | 8        | 0.47          |
| (3,18)   | 1:58:A:ASP:HB3  | 1:60:A:VAL:HG11  | 17       | 0.47          |
| (1,4259) | 1:57:A:VAL:HG11 | 1:56:A:LEU:H     | 7        | 0.47          |
| (1,4259) | 1:57:A:VAL:HG11 | 1:56:A:LEU:H     | 14       | 0.47          |
| (1,4247) | 1:54:A:GLN:HE22 | 1:57:A:VAL:HG13  | 7        | 0.47          |
| (1,4180) | 1:95:A:VAL:H    | 1:48:A:LEU:HD13  | 4        | 0.47          |
| (1,4180) | 1:95:A:VAL:H    | 1:48:A:LEU:HD11  | 8        | 0.47          |
| (1,4180) | 1:95:A:VAL:H    | 1:48:A:LEU:HD12  | 17       | 0.47          |
| (1,4171) | 1:48:A:LEU:HD23 | 1:49:A:LYS:H     | 1        | 0.47          |
| (1,4132) | 1:60:A:VAL:HG11 | 1:34:A:ARG:HE    | 5        | 0.47          |
| (1,4007) | 1:41:A:ALA:HB1  | 1:41:A:ALA:H     | 7        | 0.47          |
| (1,3957) | 1:58:A:ASP:H    | 1:57:A:VAL:HG13  | 10       | 0.47          |
| (1,3957) | 1:58:A:ASP:H    | 1:57:A:VAL:HG11  | 14       | 0.47          |
| (1,3834) | 1:95:A:VAL:HG21 | 1:100:A:ASN:H    | 9        | 0.47          |
| (1,3834) | 1:95:A:VAL:HG21 | 1:100:A:ASN:H    | 14       | 0.47          |
| (1,3782) | 1:120:A:ALA:HB1 | 1:119:A:GLU:H    | 4        | 0.47          |
| (1,3782) | 1:120:A:ALA:HB1 | 1:119:A:GLU:H    | 6        | 0.47          |
| (1,3742) | 1:28:A:ILE:H    | 1:29:A:ALA:HB3   | 17       | 0.47          |
| (1,3627) | 1:100:A:ASN:H   | 1:100:A:ASN:HD21 | 4        | 0.47          |
| (1,3601) | 1:113:A:ALA:HB2 | 1:111:A:GLU:H    | 17       | 0.47          |
| (1,3594) | 1:105:A:LEU:HB2 | 1:110:A:VAL:HG11 | 11       | 0.47          |
| (1,3570) | 1:90:A:PRO:HA   | 1:105:A:LEU:HD12 | 11       | 0.47          |
| (1,3554) | 1:66:A:LEU:HB2  | 1:66:A:LEU:HD22  | 10       | 0.47          |
| (1,3541) | 1:64:A:MET:HB2  | 1:21:A:LEU:HD23  | 14       | 0.47          |
| (1,3483) | 1:53:A:PHE:HA   | 1:31:A:LEU:HD12  | 6        | 0.47          |
| (1,3483) | 1:53:A:PHE:HA   | 1:31:A:LEU:HD13  | 11       | 0.47          |
| (1,3483) | 1:53:A:PHE:HA   | 1:31:A:LEU:HD12  | 13       | 0.47          |
| (1,3463) | 1:35:A:PHE:HE2  | 1:38:A:CYS:HB2   | 7        | 0.47          |
| (1,3451) | 1:93:A:THR:HA   | 1:93:A:THR:HG21  | 10       | 0.47          |
| (1,3451) | 1:93:A:THR:HA   | 1:93:A:THR:HG22  | 16       | 0.47          |
| (1,3405) | 1:55:A:ASP:HB2  | 1:56:A:LEU:HD23  | 4        | 0.47          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3405) | 1:55:A:ASP:HB2  | 1:56:A:LEU:HD23 | 6        | 0.47          |
| (1,3405) | 1:55:A:ASP:HB2  | 1:56:A:LEU:HD22 | 9        | 0.47          |
| (1,3386) | 1:90:A:PRO:HA   | 1:92:A:ALA:HB1  | 8        | 0.47          |
| (1,3386) | 1:90:A:PRO:HA   | 1:92:A:ALA:HB2  | 14       | 0.47          |
| (1,3377) | 1:40:A:SER:HB2  | 1:41:A:ALA:HB1  | 7        | 0.47          |
| (1,3373) | 1:88:A:VAL:HA   | 1:93:A:THR:HG21 | 6        | 0.47          |
| (1,3373) | 1:88:A:VAL:HA   | 1:93:A:THR:HG23 | 12       | 0.47          |
| (1,3373) | 1:88:A:VAL:HA   | 1:93:A:THR:HG23 | 15       | 0.47          |
| (1,3368) | 1:31:A:LEU:HD12 | 1:31:A:LEU:HA   | 16       | 0.47          |
| (1,3366) | 1:72:A:ARG:HA   | 1:56:A:LEU:HD23 | 8        | 0.47          |
| (1,3342) | 1:92:A:ALA:HB1  | 1:88:A:VAL:H    | 14       | 0.47          |
| (1,3329) | 1:77:A:LEU:HD13 | 1:78:A:TYR:H    | 3        | 0.47          |
| (1,3329) | 1:77:A:LEU:HD13 | 1:78:A:TYR:H    | 11       | 0.47          |
| (1,3329) | 1:77:A:LEU:HD11 | 1:78:A:TYR:H    | 16       | 0.47          |
| (1,3329) | 1:77:A:LEU:HD12 | 1:78:A:TYR:H    | 17       | 0.47          |
| (1,3323) | 1:66:A:LEU:HD21 | 1:66:A:LEU:H    | 14       | 0.47          |
| (1,3302) | 1:83:A:ARG:HB2  | 1:86:A:TYR:HD2  | 11       | 0.47          |
| (1,3256) | 1:41:A:ALA:HB2  | 1:33:A:GLU:H    | 1        | 0.47          |
| (1,3256) | 1:41:A:ALA:HB3  | 1:33:A:GLU:H    | 5        | 0.47          |
| (1,3253) | 1:92:A:ALA:HB2  | 1:91:A:GLY:H    | 4        | 0.47          |
| (1,3253) | 1:92:A:ALA:HB2  | 1:91:A:GLY:H    | 12       | 0.47          |
| (1,3199) | 1:113:A:ALA:HB2 | 1:112:A:HIS:HB2 | 2        | 0.47          |
| (1,3199) | 1:113:A:ALA:HB1 | 1:112:A:HIS:HB2 | 13       | 0.47          |
| (1,3081) | 1:97:A:LEU:HD12 | 1:55:A:ASP:HA   | 17       | 0.47          |
| (1,3068) | 1:52:A:ILE:HG23 | 1:53:A:PHE:HB2  | 17       | 0.47          |
| (1,3052) | 1:39:A:PHE:HZ   | 1:52:A:ILE:HG23 | 3        | 0.47          |
| (1,3051) | 1:78:A:TYR:HE2  | 1:28:A:ILE:HG22 | 15       | 0.47          |
| (1,3023) | 1:64:A:MET:HE2  | 1:27:A:VAL:HA   | 14       | 0.47          |
| (1,3002) | 1:57:A:VAL:HG13 | 1:60:A:VAL:HB   | 8        | 0.47          |
| (1,2900) | 1:28:A:ILE:HD11 | 1:31:A:LEU:HB3  | 3        | 0.47          |
| (1,2900) | 1:28:A:ILE:HD13 | 1:31:A:LEU:HB3  | 10       | 0.47          |
| (1,2900) | 1:28:A:ILE:HD12 | 1:31:A:LEU:HB3  | 14       | 0.47          |
| (1,2900) | 1:28:A:ILE:HD11 | 1:31:A:LEU:HB3  | 16       | 0.47          |
| (1,2897) | 1:39:A:PHE:HZ   | 1:28:A:ILE:HD13 | 9        | 0.47          |
| (1,2885) | 1:32:A:ALA:HB2  | 1:31:A:LEU:H    | 9        | 0.47          |
| (1,2885) | 1:32:A:ALA:HB2  | 1:31:A:LEU:H    | 11       | 0.47          |
| (1,2880) | 1:61:A:ALA:HB1  | 1:57:A:VAL:HG12 | 17       | 0.47          |
| (1,2873) | 1:126:A:ALA:HA  | 1:126:A:ALA:HB3 | 11       | 0.47          |
| (1,2872) | 1:129:A:ALA:HB1 | 1:129:A:ALA:HA  | 6        | 0.47          |
| (1,2865) | 1:78:A:TYR:HE1  | 1:48:A:LEU:HD12 | 16       | 0.47          |
| (1,2864) | 1:78:A:TYR:HE1  | 1:78:A:TYR:HB3  | 14       | 0.47          |
| (1,2863) | 1:78:A:TYR:HE2  | 1:84:A:TYR:HD2  | 2        | 0.47          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2863) | 1:78:A:TYR:HE2   | 1:84:A:TYR:HD2   | 17       | 0.47          |
| (1,2854) | 1:85:A:LEU:HD22  | 1:84:A:TYR:HD1   | 3        | 0.47          |
| (1,2854) | 1:85:A:LEU:HD21  | 1:84:A:TYR:HD2   | 6        | 0.47          |
| (1,2854) | 1:85:A:LEU:HD22  | 1:84:A:TYR:HD1   | 7        | 0.47          |
| (1,2854) | 1:85:A:LEU:HD22  | 1:84:A:TYR:HD1   | 15       | 0.47          |
| (1,2827) | 1:97:A:LEU:HD23  | 1:52:A:ILE:HB    | 14       | 0.47          |
| (1,2817) | 1:97:A:LEU:HD11  | 1:97:A:LEU:HA    | 4        | 0.47          |
| (1,2817) | 1:97:A:LEU:HD11  | 1:97:A:LEU:HA    | 16       | 0.47          |
| (1,2681) | 1:120:A:ALA:HB2  | 1:82:A:TRP:HD1   | 13       | 0.47          |
| (1,2678) | 1:53:A:PHE:HB3   | 1:53:A:PHE:HE1   | 11       | 0.47          |
| (1,2616) | 1:21:A:LEU:HA    | 1:21:A:LEU:HD23  | 4        | 0.47          |
| (1,2608) | 1:48:A:LEU:HD12  | 1:52:A:ILE:HG12  | 6        | 0.47          |
| (1,2592) | 1:69:A:THR:HG21  | 1:70:A:GLN:H     | 2        | 0.47          |
| (1,2592) | 1:69:A:THR:HG23  | 1:70:A:GLN:H     | 3        | 0.47          |
| (1,2581) | 1:71:A:LEU:HD13  | 1:60:A:VAL:HG13  | 13       | 0.47          |
| (1,2578) | 1:57:A:VAL:HA    | 1:60:A:VAL:HG11  | 7        | 0.47          |
| (1,2568) | 1:78:A:TYR:HE2   | 1:28:A:ILE:HD11  | 6        | 0.47          |
| (1,2484) | 1:93:A:THR:HB    | 1:95:A:VAL:HG12  | 1        | 0.47          |
| (1,2484) | 1:93:A:THR:HB    | 1:95:A:VAL:HG13  | 9        | 0.47          |
| (1,2405) | 1:29:A:ALA:H     | 1:28:A:ILE:HD13  | 6        | 0.47          |
| (1,2309) | 1:39:A:PHE:HB3   | 1:39:A:PHE:HE2   | 2        | 0.47          |
| (1,2309) | 1:39:A:PHE:HB3   | 1:39:A:PHE:HE1   | 14       | 0.47          |
| (1,2268) | 1:110:A:VAL:HG12 | 1:89:A:LYS:H     | 5        | 0.47          |
| (1,2268) | 1:110:A:VAL:HG11 | 1:89:A:LYS:H     | 12       | 0.47          |
| (1,2194) | 1:50:A:ILE:HD11  | 1:80:A:SER:H     | 6        | 0.47          |
| (1,2194) | 1:50:A:ILE:HD12  | 1:80:A:SER:H     | 7        | 0.47          |
| (1,2179) | 1:52:A:ILE:HG23  | 1:48:A:LEU:HB3   | 9        | 0.47          |
| (1,2150) | 1:105:A:LEU:H    | 1:105:A:LEU:HD11 | 1        | 0.47          |
| (1,2150) | 1:105:A:LEU:H    | 1:105:A:LEU:HD11 | 2        | 0.47          |
| (1,2150) | 1:105:A:LEU:H    | 1:105:A:LEU:HD12 | 3        | 0.47          |
| (1,2150) | 1:105:A:LEU:H    | 1:105:A:LEU:HD13 | 9        | 0.47          |
| (1,2150) | 1:105:A:LEU:H    | 1:105:A:LEU:HD12 | 11       | 0.47          |
| (1,2150) | 1:105:A:LEU:H    | 1:105:A:LEU:HD11 | 12       | 0.47          |
| (1,2150) | 1:105:A:LEU:H    | 1:105:A:LEU:HD13 | 14       | 0.47          |
| (1,2149) | 1:21:A:LEU:HD21  | 1:30:A:PHE:HD1   | 8        | 0.47          |
| (1,2147) | 1:85:A:LEU:HA    | 1:85:A:LEU:HD13  | 2        | 0.47          |
| (1,2146) | 1:104:A:GLU:HB3  | 1:93:A:THR:HG23  | 5        | 0.47          |
| (1,2146) | 1:104:A:GLU:HB3  | 1:93:A:THR:HG21  | 12       | 0.47          |
| (1,2006) | 1:78:A:TYR:HE2   | 1:48:A:LEU:HD11  | 1        | 0.47          |
| (1,2006) | 1:78:A:TYR:HE1   | 1:48:A:LEU:HD13  | 7        | 0.47          |
| (1,2006) | 1:78:A:TYR:HE1   | 1:48:A:LEU:HD13  | 14       | 0.47          |
| (1,1990) | 1:92:A:ALA:HB3   | 1:91:A:GLY:H     | 14       | 0.47          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1950) | 1:105:A:LEU:HB2  | 1:110:A:VAL:HG11 | 2        | 0.47          |
| (1,1950) | 1:105:A:LEU:HB2  | 1:110:A:VAL:HG13 | 9        | 0.47          |
| (1,1950) | 1:105:A:LEU:HB2  | 1:110:A:VAL:HG13 | 10       | 0.47          |
| (1,1950) | 1:105:A:LEU:HB2  | 1:110:A:VAL:HG11 | 15       | 0.47          |
| (1,1874) | 1:70:A:GLN:HE21  | 1:27:A:VAL:HG13  | 10       | 0.47          |
| (1,1874) | 1:70:A:GLN:HE21  | 1:27:A:VAL:HG12  | 12       | 0.47          |
| (1,1853) | 1:86:A:TYR:HE1   | 1:85:A:LEU:HD13  | 10       | 0.47          |
| (1,1851) | 1:35:A:PHE:HE2   | 1:38:A:CYS:HB2   | 14       | 0.47          |
| (1,1838) | 1:93:A:THR:HA    | 1:93:A:THR:HG21  | 3        | 0.47          |
| (1,1838) | 1:93:A:THR:HA    | 1:93:A:THR:HG23  | 9        | 0.47          |
| (1,1838) | 1:93:A:THR:HA    | 1:93:A:THR:HG22  | 14       | 0.47          |
| (1,1751) | 1:32:A:ALA:HB3   | 1:41:A:ALA:H     | 11       | 0.47          |
| (1,1702) | 1:116:A:GLN:HG3  | 1:116:A:GLN:HE21 | 2        | 0.47          |
| (1,1702) | 1:116:A:GLN:HG3  | 1:116:A:GLN:HE21 | 7        | 0.47          |
| (1,1702) | 1:116:A:GLN:HG3  | 1:116:A:GLN:HE21 | 17       | 0.47          |
| (1,1684) | 1:48:A:LEU:HD13  | 1:50:A:ILE:HA    | 15       | 0.47          |
| (1,1679) | 1:92:A:ALA:HB2   | 1:91:A:GLY:H     | 8        | 0.47          |
| (1,1679) | 1:92:A:ALA:HB1   | 1:91:A:GLY:H     | 13       | 0.47          |
| (1,1516) | 1:31:A:LEU:HD12  | 1:28:A:ILE:HG22  | 17       | 0.47          |
| (1,1507) | 1:78:A:TYR:HE1   | 1:28:A:ILE:HG22  | 8        | 0.47          |
| (1,1502) | 1:52:A:ILE:HG13  | 1:54:A:GLN:HE21  | 5        | 0.47          |
| (1,1405) | 1:102:A:CYS:H    | 1:95:A:VAL:HG13  | 10       | 0.47          |
| (1,1372) | 1:28:A:ILE:HD13  | 1:31:A:LEU:HB3   | 2        | 0.47          |
| (1,1343) | 1:78:A:TYR:HE1   | 1:48:A:LEU:HD12  | 12       | 0.47          |
| (1,1305) | 1:97:A:LEU:HD23  | 1:52:A:ILE:HB    | 10       | 0.47          |
| (1,1157) | 1:117:A:LEU:HD12 | 1:82:A:TRP:HD1   | 6        | 0.47          |
| (1,1155) | 1:53:A:PHE:HB3   | 1:53:A:PHE:HE2   | 1        | 0.47          |
| (1,1155) | 1:53:A:PHE:HB3   | 1:53:A:PHE:HE2   | 8        | 0.47          |
| (1,1155) | 1:53:A:PHE:HB3   | 1:53:A:PHE:HE1   | 12       | 0.47          |
| (1,1155) | 1:53:A:PHE:HB3   | 1:53:A:PHE:HE2   | 15       | 0.47          |
| (1,1125) | 1:97:A:LEU:HD13  | 1:60:A:VAL:HG13  | 16       | 0.47          |
| (1,1076) | 1:30:A:PHE:HD1   | 1:31:A:LEU:HD13  | 16       | 0.47          |
| (1,1075) | 1:31:A:LEU:HD12  | 1:31:A:LEU:HA    | 7        | 0.47          |
| (1,1075) | 1:31:A:LEU:HD13  | 1:31:A:LEU:HA    | 15       | 0.47          |
| (1,1043) | 1:78:A:TYR:HE1   | 1:28:A:ILE:HD13  | 11       | 0.47          |
| (1,788)  | 1:52:A:ILE:HD11  | 1:56:A:LEU:H     | 14       | 0.47          |
| (1,610)  | 1:48:A:LEU:HD21  | 1:49:A:LYS:H     | 3        | 0.47          |
| (1,604)  | 1:32:A:ALA:HB2   | 1:41:A:ALA:H     | 5        | 0.47          |
| (1,576)  | 1:50:A:ILE:HD13  | 1:50:A:ILE:H     | 6        | 0.47          |
| (1,576)  | 1:50:A:ILE:HD12  | 1:50:A:ILE:H     | 15       | 0.47          |
| (1,524)  | 1:20:A:LYS:HB3   | 1:22:A:ASN:HD22  | 3        | 0.47          |
| (1,442)  | 1:41:A:ALA:HB2   | 1:41:A:ALA:H     | 3        | 0.47          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,442)  | 1:41:A:ALA:HB2   | 1:41:A:ALA:H    | 5        | 0.47          |
| (1,442)  | 1:41:A:ALA:HB2   | 1:41:A:ALA:H    | 6        | 0.47          |
| (1,389)  | 1:58:A:ASP:H     | 1:57:A:VAL:HG11 | 7        | 0.47          |
| (1,363)  | 1:66:A:LEU:HD12  | 1:62:A:GLY:H    | 7        | 0.47          |
| (1,363)  | 1:66:A:LEU:HD12  | 1:62:A:GLY:H    | 9        | 0.47          |
| (1,363)  | 1:66:A:LEU:HD13  | 1:62:A:GLY:H    | 12       | 0.47          |
| (1,363)  | 1:66:A:LEU:HD11  | 1:62:A:GLY:H    | 15       | 0.47          |
| (1,275)  | 1:85:A:LEU:HD22  | 1:87:A:GLY:H    | 8        | 0.47          |
| (1,275)  | 1:85:A:LEU:HD22  | 1:87:A:GLY:H    | 14       | 0.47          |
| (1,217)  | 1:93:A:THR:HG23  | 1:103:A:GLY:H   | 5        | 0.47          |
| (3,147)  | 1:71:A:LEU:H     | 1:66:A:LEU:HD23 | 1        | 0.46          |
| (3,147)  | 1:71:A:LEU:H     | 1:66:A:LEU:HD21 | 12       | 0.46          |
| (3,136)  | 1:82:A:TRP:HD1   | 1:82:A:TRP:H    | 8        | 0.46          |
| (3,105)  | 1:64:A:MET:H     | 1:66:A:LEU:HD21 | 3        | 0.46          |
| (3,97)   | 1:31:A:LEU:HD21  | 1:30:A:PHE:HB3  | 13       | 0.46          |
| (3,50)   | 1:31:A:LEU:HD21  | 1:97:A:LEU:HD22 | 7        | 0.46          |
| (3,50)   | 1:31:A:LEU:HD23  | 1:97:A:LEU:HD21 | 8        | 0.46          |
| (3,22)   | 1:48:A:LEU:H     | 1:48:A:LEU:HD13 | 16       | 0.46          |
| (1,4259) | 1:57:A:VAL:HG13  | 1:56:A:LEU:H    | 8        | 0.46          |
| (1,4259) | 1:57:A:VAL:HG11  | 1:56:A:LEU:H    | 17       | 0.46          |
| (1,4247) | 1:54:A:GLN:HE22  | 1:57:A:VAL:HG12 | 5        | 0.46          |
| (1,4247) | 1:54:A:GLN:HE22  | 1:57:A:VAL:HG13 | 17       | 0.46          |
| (1,4197) | 1:66:A:LEU:HD23  | 1:67:A:SER:H    | 7        | 0.46          |
| (1,4197) | 1:66:A:LEU:HD22  | 1:67:A:SER:H    | 14       | 0.46          |
| (1,4176) | 1:97:A:LEU:HD13  | 1:97:A:LEU:H    | 8        | 0.46          |
| (1,4164) | 1:32:A:ALA:HB3   | 1:41:A:ALA:H    | 8        | 0.46          |
| (1,4138) | 1:31:A:LEU:H     | 1:28:A:ILE:HD12 | 2        | 0.46          |
| (1,4132) | 1:60:A:VAL:HG13  | 1:34:A:ARG:HE   | 10       | 0.46          |
| (1,4126) | 1:59:A:ARG:HE    | 1:97:A:LEU:HD11 | 16       | 0.46          |
| (1,4109) | 1:97:A:LEU:HD11  | 1:98:A:ASP:H    | 5        | 0.46          |
| (1,4007) | 1:41:A:ALA:HB2   | 1:41:A:ALA:H    | 13       | 0.46          |
| (1,3972) | 1:53:A:PHE:H     | 1:56:A:LEU:HB3  | 3        | 0.46          |
| (1,3972) | 1:53:A:PHE:H     | 1:56:A:LEU:HB3  | 11       | 0.46          |
| (1,3861) | 1:110:A:VAL:HG22 | 1:91:A:GLY:H    | 4        | 0.46          |
| (1,3822) | 1:93:A:THR:HG22  | 1:103:A:GLY:H   | 10       | 0.46          |
| (1,3782) | 1:120:A:ALA:HB1  | 1:119:A:GLU:H   | 16       | 0.46          |
| (1,3742) | 1:28:A:ILE:H     | 1:29:A:ALA:HB2  | 10       | 0.46          |
| (1,3668) | 1:84:A:TYR:H     | 1:84:A:TYR:HD1  | 17       | 0.46          |
| (1,3644) | 1:53:A:PHE:H     | 1:53:A:PHE:HD2  | 3        | 0.46          |
| (1,3644) | 1:53:A:PHE:H     | 1:53:A:PHE:HD1  | 14       | 0.46          |
| (1,3601) | 1:113:A:ALA:HB1  | 1:111:A:GLU:H   | 13       | 0.46          |
| (1,3599) | 1:92:A:ALA:HB3   | 1:113:A:ALA:HB3 | 10       | 0.46          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3594) | 1:105:A:LEU:HB2 | 1:110:A:VAL:HG13 | 7        | 0.46          |
| (1,3554) | 1:66:A:LEU:HB2  | 1:66:A:LEU:HD22  | 1        | 0.46          |
| (1,3554) | 1:66:A:LEU:HB2  | 1:66:A:LEU:HD23  | 12       | 0.46          |
| (1,3541) | 1:64:A:MET:HB2  | 1:21:A:LEU:HD23  | 13       | 0.46          |
| (1,3483) | 1:53:A:PHE:HA   | 1:31:A:LEU:HD13  | 2        | 0.46          |
| (1,3483) | 1:53:A:PHE:HA   | 1:31:A:LEU:HD12  | 4        | 0.46          |
| (1,3483) | 1:53:A:PHE:HA   | 1:31:A:LEU:HD13  | 5        | 0.46          |
| (1,3483) | 1:53:A:PHE:HA   | 1:31:A:LEU:HD11  | 8        | 0.46          |
| (1,3483) | 1:53:A:PHE:HA   | 1:31:A:LEU:HD13  | 10       | 0.46          |
| (1,3483) | 1:53:A:PHE:HA   | 1:31:A:LEU:HD11  | 16       | 0.46          |
| (1,3451) | 1:93:A:THR:HA   | 1:93:A:THR:HG22  | 5        | 0.46          |
| (1,3405) | 1:55:A:ASP:HB2  | 1:56:A:LEU:HD23  | 11       | 0.46          |
| (1,3386) | 1:90:A:PRO:HA   | 1:92:A:ALA:HB1   | 6        | 0.46          |
| (1,3373) | 1:88:A:VAL:HA   | 1:93:A:THR:HG23  | 2        | 0.46          |
| (1,3373) | 1:88:A:VAL:HA   | 1:93:A:THR:HG22  | 4        | 0.46          |
| (1,3368) | 1:31:A:LEU:HD12 | 1:31:A:LEU:HA    | 3        | 0.46          |
| (1,3368) | 1:31:A:LEU:HD12 | 1:31:A:LEU:HA    | 12       | 0.46          |
| (1,3342) | 1:92:A:ALA:HB2  | 1:88:A:VAL:H     | 9        | 0.46          |
| (1,3342) | 1:92:A:ALA:HB2  | 1:88:A:VAL:H     | 13       | 0.46          |
| (1,3342) | 1:92:A:ALA:HB1  | 1:88:A:VAL:H     | 15       | 0.46          |
| (1,3329) | 1:77:A:LEU:HD13 | 1:78:A:TYR:H     | 4        | 0.46          |
| (1,3329) | 1:77:A:LEU:HD13 | 1:78:A:TYR:H     | 5        | 0.46          |
| (1,3329) | 1:77:A:LEU:HD11 | 1:78:A:TYR:H     | 6        | 0.46          |
| (1,3329) | 1:77:A:LEU:HD12 | 1:78:A:TYR:H     | 9        | 0.46          |
| (1,3329) | 1:77:A:LEU:HD12 | 1:78:A:TYR:H     | 12       | 0.46          |
| (1,3302) | 1:83:A:ARG:HB2  | 1:86:A:TYR:HD1   | 7        | 0.46          |
| (1,3258) | 1:48:A:LEU:HD12 | 1:50:A:ILE:HA    | 12       | 0.46          |
| (1,3253) | 1:92:A:ALA:HB3  | 1:91:A:GLY:H     | 7        | 0.46          |
| (1,3199) | 1:113:A:ALA:HB2 | 1:112:A:HIS:HB2  | 15       | 0.46          |
| (1,3116) | 1:57:A:VAL:HG22 | 1:53:A:PHE:HE2   | 2        | 0.46          |
| (1,3116) | 1:57:A:VAL:HG22 | 1:53:A:PHE:HE2   | 16       | 0.46          |
| (1,3103) | 1:56:A:LEU:HD11 | 1:60:A:VAL:HB    | 5        | 0.46          |
| (1,3081) | 1:97:A:LEU:HD12 | 1:55:A:ASP:HA    | 11       | 0.46          |
| (1,3081) | 1:97:A:LEU:HD11 | 1:55:A:ASP:HA    | 15       | 0.46          |
| (1,3078) | 1:54:A:GLN:HB3  | 1:57:A:VAL:HG12  | 5        | 0.46          |
| (1,3052) | 1:39:A:PHE:HZ   | 1:52:A:ILE:HG22  | 1        | 0.46          |
| (1,3052) | 1:39:A:PHE:HZ   | 1:52:A:ILE:HG22  | 10       | 0.46          |
| (1,3052) | 1:39:A:PHE:HZ   | 1:52:A:ILE:HG21  | 16       | 0.46          |
| (1,3045) | 1:52:A:ILE:HG13 | 1:54:A:GLN:HE21  | 6        | 0.46          |
| (1,3019) | 1:64:A:MET:HE3  | 1:66:A:LEU:H     | 11       | 0.46          |
| (1,3002) | 1:57:A:VAL:HG11 | 1:60:A:VAL:HB    | 17       | 0.46          |
| (1,2940) | 1:99:A:GLY:HA3  | 1:95:A:VAL:HG11  | 10       | 0.46          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2940) | 1:99:A:GLY:HA3   | 1:95:A:VAL:HG11  | 14       | 0.46          |
| (1,2900) | 1:28:A:ILE:HD13  | 1:31:A:LEU:HB3   | 15       | 0.46          |
| (1,2900) | 1:28:A:ILE:HD12  | 1:31:A:LEU:HB3   | 17       | 0.46          |
| (1,2886) | 1:41:A:ALA:HA    | 1:32:A:ALA:HB2   | 9        | 0.46          |
| (1,2872) | 1:129:A:ALA:HB2  | 1:129:A:ALA:HA   | 4        | 0.46          |
| (1,2865) | 1:78:A:TYR:HE1   | 1:48:A:LEU:HD13  | 15       | 0.46          |
| (1,2854) | 1:85:A:LEU:HD21  | 1:84:A:TYR:HD2   | 5        | 0.46          |
| (1,2854) | 1:85:A:LEU:HD23  | 1:84:A:TYR:HD2   | 9        | 0.46          |
| (1,2854) | 1:85:A:LEU:HD23  | 1:84:A:TYR:HD2   | 13       | 0.46          |
| (1,2854) | 1:85:A:LEU:HD22  | 1:84:A:TYR:HD2   | 14       | 0.46          |
| (1,2852) | 1:81:A:SER:HB3   | 1:84:A:TYR:HD1   | 12       | 0.46          |
| (1,2785) | 1:50:A:ILE:HG21  | 1:51:A:GLY:HA3   | 11       | 0.46          |
| (1,2681) | 1:120:A:ALA:HB2  | 1:82:A:TRP:HD1   | 1        | 0.46          |
| (1,2608) | 1:48:A:LEU:HD12  | 1:52:A:ILE:HG12  | 7        | 0.46          |
| (1,2608) | 1:48:A:LEU:HD13  | 1:52:A:ILE:HG12  | 10       | 0.46          |
| (1,2578) | 1:57:A:VAL:HA    | 1:60:A:VAL:HG13  | 8        | 0.46          |
| (1,2578) | 1:57:A:VAL:HA    | 1:60:A:VAL:HG13  | 13       | 0.46          |
| (1,2542) | 1:21:A:LEU:HD11  | 1:30:A:PHE:HA    | 11       | 0.46          |
| (1,2484) | 1:93:A:THR:HB    | 1:95:A:VAL:HG11  | 4        | 0.46          |
| (1,2484) | 1:93:A:THR:HB    | 1:95:A:VAL:HG12  | 5        | 0.46          |
| (1,2405) | 1:29:A:ALA:H     | 1:28:A:ILE:HD11  | 5        | 0.46          |
| (1,2397) | 1:50:A:ILE:HD13  | 1:50:A:ILE:HA    | 2        | 0.46          |
| (1,2370) | 1:50:A:ILE:HG13  | 1:50:A:ILE:HG21  | 4        | 0.46          |
| (1,2271) | 1:113:A:ALA:HB2  | 1:112:A:HIS:HD2  | 5        | 0.46          |
| (1,2271) | 1:113:A:ALA:HB1  | 1:112:A:HIS:HD2  | 13       | 0.46          |
| (1,2268) | 1:110:A:VAL:HG11 | 1:89:A:LYS:H     | 4        | 0.46          |
| (1,2268) | 1:110:A:VAL:HG13 | 1:89:A:LYS:H     | 11       | 0.46          |
| (1,2212) | 1:110:A:VAL:HG23 | 1:114:A:ARG:H    | 5        | 0.46          |
| (1,2150) | 1:105:A:LEU:H    | 1:105:A:LEU:HD12 | 4        | 0.46          |
| (1,2150) | 1:105:A:LEU:H    | 1:105:A:LEU:HD13 | 13       | 0.46          |
| (1,2099) | 1:21:A:LEU:HB2   | 1:21:A:LEU:HD22  | 1        | 0.46          |
| (1,2006) | 1:78:A:TYR:HE2   | 1:48:A:LEU:HD12  | 8        | 0.46          |
| (1,1950) | 1:105:A:LEU:HB2  | 1:110:A:VAL:HG13 | 1        | 0.46          |
| (1,1950) | 1:105:A:LEU:HB2  | 1:110:A:VAL:HG13 | 5        | 0.46          |
| (1,1950) | 1:105:A:LEU:HB2  | 1:110:A:VAL:HG12 | 6        | 0.46          |
| (1,1950) | 1:105:A:LEU:HB2  | 1:110:A:VAL:HG11 | 8        | 0.46          |
| (1,1950) | 1:105:A:LEU:HB2  | 1:110:A:VAL:HG13 | 14       | 0.46          |
| (1,1950) | 1:105:A:LEU:HB2  | 1:110:A:VAL:HG12 | 17       | 0.46          |
| (1,1874) | 1:70:A:GLN:HE21  | 1:27:A:VAL:HG11  | 17       | 0.46          |
| (1,1853) | 1:86:A:TYR:HE1   | 1:85:A:LEU:HD11  | 15       | 0.46          |
| (1,1853) | 1:86:A:TYR:HE2   | 1:85:A:LEU:HD11  | 16       | 0.46          |
| (1,1851) | 1:35:A:PHE:HE1   | 1:38:A:CYS:HB2   | 2        | 0.46          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1851) | 1:35:A:PHE:HE1   | 1:38:A:CYS:HB2   | 16       | 0.46          |
| (1,1839) | 1:95:A:VAL:HA    | 1:93:A:THR:HG21  | 1        | 0.46          |
| (1,1839) | 1:95:A:VAL:HA    | 1:93:A:THR:HG22  | 2        | 0.46          |
| (1,1838) | 1:93:A:THR:HA    | 1:93:A:THR:HG21  | 6        | 0.46          |
| (1,1702) | 1:116:A:GLN:HG3  | 1:116:A:GLN:HE21 | 3        | 0.46          |
| (1,1702) | 1:116:A:GLN:HG3  | 1:116:A:GLN:HE21 | 11       | 0.46          |
| (1,1702) | 1:116:A:GLN:HG3  | 1:116:A:GLN:HE21 | 12       | 0.46          |
| (1,1702) | 1:116:A:GLN:HG3  | 1:116:A:GLN:HE21 | 15       | 0.46          |
| (1,1684) | 1:48:A:LEU:HD12  | 1:50:A:ILE:HA    | 16       | 0.46          |
| (1,1545) | 1:56:A:LEU:HD11  | 1:60:A:VAL:HB    | 8        | 0.46          |
| (1,1545) | 1:56:A:LEU:HD11  | 1:60:A:VAL:HB    | 9        | 0.46          |
| (1,1507) | 1:78:A:TYR:HE1   | 1:28:A:ILE:HG21  | 1        | 0.46          |
| (1,1507) | 1:78:A:TYR:HE2   | 1:28:A:ILE:HG22  | 3        | 0.46          |
| (1,1507) | 1:78:A:TYR:HE1   | 1:28:A:ILE:HG21  | 9        | 0.46          |
| (1,1507) | 1:78:A:TYR:HE2   | 1:28:A:ILE:HG21  | 14       | 0.46          |
| (1,1481) | 1:64:A:MET:HE1   | 1:30:A:PHE:HA    | 4        | 0.46          |
| (1,1480) | 1:64:A:MET:HE2   | 1:63:A:GLU:H     | 15       | 0.46          |
| (1,1372) | 1:28:A:ILE:HD13  | 1:31:A:LEU:HB3   | 7        | 0.46          |
| (1,1361) | 1:41:A:ALA:HA    | 1:32:A:ALA:HB1   | 17       | 0.46          |
| (1,1336) | 1:85:A:LEU:HD21  | 1:84:A:TYR:HD2   | 12       | 0.46          |
| (1,1305) | 1:97:A:LEU:HD21  | 1:52:A:ILE:HB    | 8        | 0.46          |
| (1,1155) | 1:53:A:PHE:HB3   | 1:53:A:PHE:HE1   | 3        | 0.46          |
| (1,1155) | 1:53:A:PHE:HB3   | 1:53:A:PHE:HE1   | 7        | 0.46          |
| (1,1155) | 1:53:A:PHE:HB3   | 1:53:A:PHE:HE1   | 13       | 0.46          |
| (1,1076) | 1:30:A:PHE:HD2   | 1:31:A:LEU:HD11  | 3        | 0.46          |
| (1,1076) | 1:30:A:PHE:HD2   | 1:31:A:LEU:HD12  | 11       | 0.46          |
| (1,1076) | 1:30:A:PHE:HD1   | 1:31:A:LEU:HD11  | 14       | 0.46          |
| (1,1075) | 1:31:A:LEU:HD12  | 1:31:A:LEU:HA    | 16       | 0.46          |
| (1,1043) | 1:78:A:TYR:HE1   | 1:28:A:ILE:HD12  | 14       | 0.46          |
| (1,614)  | 1:97:A:LEU:HD12  | 1:97:A:LEU:H     | 17       | 0.46          |
| (1,604)  | 1:32:A:ALA:HB1   | 1:41:A:ALA:H     | 15       | 0.46          |
| (1,442)  | 1:41:A:ALA:HB2   | 1:41:A:ALA:H     | 12       | 0.46          |
| (1,410)  | 1:53:A:PHE:H     | 1:56:A:LEU:HB3   | 5        | 0.46          |
| (1,389)  | 1:58:A:ASP:H     | 1:57:A:VAL:HG12  | 6        | 0.46          |
| (1,389)  | 1:58:A:ASP:H     | 1:57:A:VAL:HG11  | 17       | 0.46          |
| (1,363)  | 1:66:A:LEU:HD13  | 1:62:A:GLY:H     | 10       | 0.46          |
| (1,363)  | 1:66:A:LEU:HD11  | 1:62:A:GLY:H     | 13       | 0.46          |
| (1,363)  | 1:66:A:LEU:HD11  | 1:62:A:GLY:H     | 16       | 0.46          |
| (1,263)  | 1:110:A:VAL:HG22 | 1:91:A:GLY:H     | 12       | 0.46          |
| (1,217)  | 1:93:A:THR:HG23  | 1:103:A:GLY:H    | 1        | 0.46          |
| (1,204)  | 1:105:A:LEU:HD13 | 1:106:A:ASP:H    | 1        | 0.46          |
| (1,169)  | 1:120:A:ALA:HB1  | 1:119:A:GLU:H    | 14       | 0.46          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,126)  | 1:28:A:ILE:H    | 1:29:A:ALA:HB2   | 2        | 0.46          |
| (3,152)  | 1:27:A:VAL:H    | 1:74:A:ALA:HB3   | 17       | 0.45          |
| (3,147)  | 1:71:A:LEU:H    | 1:66:A:LEU:HD22  | 2        | 0.45          |
| (3,132)  | 1:113:A:ALA:HB2 | 1:112:A:HIS:H    | 11       | 0.45          |
| (3,126)  | 1:21:A:LEU:HD23 | 1:22:A:ASN:H     | 11       | 0.45          |
| (3,124)  | 1:88:A:VAL:HG23 | 1:88:A:VAL:H     | 11       | 0.45          |
| (3,99)   | 1:72:A:ARG:HG3  | 1:75:A:LEU:HD13  | 5        | 0.45          |
| (3,65)   | 1:52:A:ILE:HG13 | 1:52:A:ILE:HG22  | 17       | 0.45          |
| (3,62)   | 1:52:A:ILE:HG23 | 1:56:A:LEU:H     | 8        | 0.45          |
| (3,50)   | 1:31:A:LEU:HD22 | 1:97:A:LEU:HD22  | 10       | 0.45          |
| (3,50)   | 1:31:A:LEU:HD22 | 1:97:A:LEU:HD22  | 17       | 0.45          |
| (1,4197) | 1:66:A:LEU:HD23 | 1:67:A:SER:H     | 4        | 0.45          |
| (1,4109) | 1:97:A:LEU:HD13 | 1:98:A:ASP:H     | 2        | 0.45          |
| (1,4007) | 1:41:A:ALA:HB2  | 1:41:A:ALA:H     | 8        | 0.45          |
| (1,3972) | 1:53:A:PHE:H    | 1:56:A:LEU:HB3   | 6        | 0.45          |
| (1,3834) | 1:95:A:VAL:HG22 | 1:100:A:ASN:H    | 3        | 0.45          |
| (1,3834) | 1:95:A:VAL:HG23 | 1:100:A:ASN:H    | 4        | 0.45          |
| (1,3822) | 1:93:A:THR:HG22 | 1:103:A:GLY:H    | 3        | 0.45          |
| (1,3644) | 1:53:A:PHE:H    | 1:53:A:PHE:HD2   | 10       | 0.45          |
| (1,3601) | 1:113:A:ALA:HB2 | 1:111:A:GLU:H    | 2        | 0.45          |
| (1,3594) | 1:105:A:LEU:HB2 | 1:110:A:VAL:HG12 | 3        | 0.45          |
| (1,3594) | 1:105:A:LEU:HB2 | 1:110:A:VAL:HG12 | 4        | 0.45          |
| (1,3570) | 1:90:A:PRO:HA   | 1:105:A:LEU:HD13 | 8        | 0.45          |
| (1,3554) | 1:66:A:LEU:HB2  | 1:66:A:LEU:HD21  | 2        | 0.45          |
| (1,3554) | 1:66:A:LEU:HB2  | 1:66:A:LEU:HD22  | 7        | 0.45          |
| (1,3541) | 1:64:A:MET:HB2  | 1:21:A:LEU:HD22  | 3        | 0.45          |
| (1,3479) | 1:45:A:ALA:HB1  | 1:44:A:GLU:HB3   | 9        | 0.45          |
| (1,3463) | 1:35:A:PHE:HE2  | 1:38:A:CYS:HB2   | 6        | 0.45          |
| (1,3463) | 1:35:A:PHE:HE2  | 1:38:A:CYS:HB2   | 8        | 0.45          |
| (1,3452) | 1:95:A:VAL:HA   | 1:93:A:THR:HG21  | 4        | 0.45          |
| (1,3452) | 1:95:A:VAL:HA   | 1:93:A:THR:HG22  | 8        | 0.45          |
| (1,3451) | 1:93:A:THR:HA   | 1:93:A:THR:HG22  | 1        | 0.45          |
| (1,3451) | 1:93:A:THR:HA   | 1:93:A:THR:HG22  | 4        | 0.45          |
| (1,3451) | 1:93:A:THR:HA   | 1:93:A:THR:HG21  | 11       | 0.45          |
| (1,3451) | 1:93:A:THR:HA   | 1:93:A:THR:HG23  | 12       | 0.45          |
| (1,3451) | 1:93:A:THR:HA   | 1:93:A:THR:HG21  | 17       | 0.45          |
| (1,3418) | 1:117:A:LEU:HB2 | 1:117:A:LEU:HD11 | 15       | 0.45          |
| (1,3418) | 1:117:A:LEU:HB2 | 1:117:A:LEU:HD12 | 17       | 0.45          |
| (1,3405) | 1:55:A:ASP:HB2  | 1:56:A:LEU:HD23  | 7        | 0.45          |
| (1,3405) | 1:55:A:ASP:HB2  | 1:56:A:LEU:HD22  | 13       | 0.45          |
| (1,3386) | 1:90:A:PRO:HA   | 1:92:A:ALA:HB3   | 13       | 0.45          |
| (1,3368) | 1:31:A:LEU:HD11 | 1:31:A:LEU:HA    | 8        | 0.45          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3368) | 1:31:A:LEU:HD13 | 1:31:A:LEU:HA   | 9        | 0.45          |
| (1,3342) | 1:92:A:ALA:HB1  | 1:88:A:VAL:H    | 4        | 0.45          |
| (1,3342) | 1:92:A:ALA:HB3  | 1:88:A:VAL:H    | 6        | 0.45          |
| (1,3342) | 1:92:A:ALA:HB1  | 1:88:A:VAL:H    | 7        | 0.45          |
| (1,3329) | 1:77:A:LEU:HD13 | 1:78:A:TYR:H    | 15       | 0.45          |
| (1,3302) | 1:83:A:ARG:HB2  | 1:86:A:TYR:HD2  | 3        | 0.45          |
| (1,3302) | 1:83:A:ARG:HB2  | 1:86:A:TYR:HD1  | 15       | 0.45          |
| (1,3256) | 1:41:A:ALA:HB2  | 1:33:A:GLU:H    | 15       | 0.45          |
| (1,3231) | 1:27:A:VAL:HG22 | 1:27:A:VAL:HA   | 13       | 0.45          |
| (1,3199) | 1:113:A:ALA:HB2 | 1:112:A:HIS:HB2 | 1        | 0.45          |
| (1,3199) | 1:113:A:ALA:HB1 | 1:112:A:HIS:HB2 | 3        | 0.45          |
| (1,3199) | 1:113:A:ALA:HB2 | 1:112:A:HIS:HB2 | 11       | 0.45          |
| (1,3116) | 1:57:A:VAL:HG21 | 1:53:A:PHE:HE1  | 4        | 0.45          |
| (1,3116) | 1:57:A:VAL:HG21 | 1:53:A:PHE:HE1  | 9        | 0.45          |
| (1,3081) | 1:97:A:LEU:HD12 | 1:55:A:ASP:HA   | 10       | 0.45          |
| (1,3078) | 1:54:A:GLN:HB3  | 1:57:A:VAL:HG11 | 6        | 0.45          |
| (1,3078) | 1:54:A:GLN:HB3  | 1:57:A:VAL:HG13 | 7        | 0.45          |
| (1,3078) | 1:54:A:GLN:HB3  | 1:57:A:VAL:HG12 | 12       | 0.45          |
| (1,3078) | 1:54:A:GLN:HB3  | 1:57:A:VAL:HG11 | 16       | 0.45          |
| (1,3070) | 1:55:A:ASP:H    | 1:54:A:GLN:HB2  | 5        | 0.45          |
| (1,3070) | 1:55:A:ASP:H    | 1:54:A:GLN:HB2  | 14       | 0.45          |
| (1,3070) | 1:55:A:ASP:H    | 1:54:A:GLN:HB2  | 16       | 0.45          |
| (1,3067) | 1:52:A:ILE:HG22 | 1:53:A:PHE:HB3  | 12       | 0.45          |
| (1,3052) | 1:39:A:PHE:HZ   | 1:52:A:ILE:HG23 | 2        | 0.45          |
| (1,3051) | 1:78:A:TYR:HE1  | 1:28:A:ILE:HG22 | 4        | 0.45          |
| (1,3024) | 1:64:A:MET:HE2  | 1:65:A:ASN:HB3  | 12       | 0.45          |
| (1,3024) | 1:64:A:MET:HE1  | 1:65:A:ASN:HB3  | 15       | 0.45          |
| (1,3021) | 1:64:A:MET:HE2  | 1:63:A:GLU:H    | 5        | 0.45          |
| (1,2900) | 1:28:A:ILE:HD11 | 1:31:A:LEU:HB3  | 4        | 0.45          |
| (1,2900) | 1:28:A:ILE:HD12 | 1:31:A:LEU:HB3  | 5        | 0.45          |
| (1,2890) | 1:33:A:GLU:HB3  | 1:32:A:ALA:HB3  | 5        | 0.45          |
| (1,2872) | 1:129:A:ALA:HB2 | 1:129:A:ALA:HA  | 12       | 0.45          |
| (1,2872) | 1:129:A:ALA:HB2 | 1:129:A:ALA:HA  | 17       | 0.45          |
| (1,2854) | 1:85:A:LEU:HD22 | 1:84:A:TYR:HD2  | 8        | 0.45          |
| (1,2854) | 1:85:A:LEU:HD23 | 1:84:A:TYR:HD2  | 11       | 0.45          |
| (1,2854) | 1:85:A:LEU:HD22 | 1:84:A:TYR:HD1  | 17       | 0.45          |
| (1,2845) | 1:22:A:ASN:H    | 1:27:A:VAL:HG11 | 16       | 0.45          |
| (1,2827) | 1:97:A:LEU:HD23 | 1:52:A:ILE:HB   | 7        | 0.45          |
| (1,2827) | 1:97:A:LEU:HD21 | 1:52:A:ILE:HB   | 9        | 0.45          |
| (1,2785) | 1:50:A:ILE:HG22 | 1:51:A:GLY:HA3  | 5        | 0.45          |
| (1,2678) | 1:53:A:PHE:HB3  | 1:53:A:PHE:HE1  | 4        | 0.45          |
| (1,2664) | 1:97:A:LEU:HD12 | 1:60:A:VAL:HG13 | 2        | 0.45          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2608) | 1:48:A:LEU:HD13  | 1:52:A:ILE:HG12  | 1        | 0.45          |
| (1,2585) | 1:92:A:ALA:HA    | 1:93:A:THR:HG23  | 11       | 0.45          |
| (1,2581) | 1:71:A:LEU:HD11  | 1:60:A:VAL:HG12  | 2        | 0.45          |
| (1,2578) | 1:57:A:VAL:HA    | 1:60:A:VAL:HG11  | 11       | 0.45          |
| (1,2577) | 1:60:A:VAL:HG12  | 1:59:A:ARG:HA    | 11       | 0.45          |
| (1,2568) | 1:78:A:TYR:HE1   | 1:28:A:ILE:HD12  | 17       | 0.45          |
| (1,2423) | 1:64:A:MET:HA    | 1:64:A:MET:HE3   | 1        | 0.45          |
| (1,2423) | 1:64:A:MET:HA    | 1:64:A:MET:HE2   | 10       | 0.45          |
| (1,2423) | 1:64:A:MET:HA    | 1:64:A:MET:HE2   | 17       | 0.45          |
| (1,2405) | 1:29:A:ALA:H     | 1:28:A:ILE:HD12  | 12       | 0.45          |
| (1,2370) | 1:50:A:ILE:HG13  | 1:50:A:ILE:HG21  | 2        | 0.45          |
| (1,2370) | 1:50:A:ILE:HG13  | 1:50:A:ILE:HG22  | 8        | 0.45          |
| (1,2305) | 1:45:A:ALA:HB3   | 1:44:A:GLU:HA    | 17       | 0.45          |
| (1,2212) | 1:110:A:VAL:HG21 | 1:114:A:ARG:H    | 15       | 0.45          |
| (1,2194) | 1:50:A:ILE:HD13  | 1:80:A:SER:H     | 4        | 0.45          |
| (1,2194) | 1:50:A:ILE:HD12  | 1:80:A:SER:H     | 8        | 0.45          |
| (1,2150) | 1:105:A:LEU:H    | 1:105:A:LEU:HD13 | 8        | 0.45          |
| (1,2150) | 1:105:A:LEU:H    | 1:105:A:LEU:HD11 | 10       | 0.45          |
| (1,2150) | 1:105:A:LEU:H    | 1:105:A:LEU:HD13 | 15       | 0.45          |
| (1,2150) | 1:105:A:LEU:H    | 1:105:A:LEU:HD13 | 16       | 0.45          |
| (1,2006) | 1:78:A:TYR:HE2   | 1:48:A:LEU:HD11  | 5        | 0.45          |
| (1,2003) | 1:48:A:LEU:HB3   | 1:48:A:LEU:HD13  | 6        | 0.45          |
| (1,2003) | 1:48:A:LEU:HB3   | 1:48:A:LEU:HD13  | 7        | 0.45          |
| (1,2003) | 1:48:A:LEU:HB3   | 1:48:A:LEU:HD11  | 15       | 0.45          |
| (1,1950) | 1:105:A:LEU:HB2  | 1:110:A:VAL:HG12 | 13       | 0.45          |
| (1,1950) | 1:105:A:LEU:HB2  | 1:110:A:VAL:HG11 | 16       | 0.45          |
| (1,1874) | 1:70:A:GLN:HE21  | 1:27:A:VAL:HG13  | 14       | 0.45          |
| (1,1853) | 1:86:A:TYR:HE2   | 1:85:A:LEU:HD11  | 3        | 0.45          |
| (1,1853) | 1:86:A:TYR:HE1   | 1:85:A:LEU:HD11  | 7        | 0.45          |
| (1,1853) | 1:86:A:TYR:HE1   | 1:85:A:LEU:HD12  | 8        | 0.45          |
| (1,1853) | 1:86:A:TYR:HE2   | 1:85:A:LEU:HD12  | 17       | 0.45          |
| (1,1790) | 1:90:A:PRO:HA    | 1:92:A:ALA:HB3   | 9        | 0.45          |
| (1,1790) | 1:90:A:PRO:HA    | 1:92:A:ALA:HB3   | 11       | 0.45          |
| (1,1735) | 1:66:A:LEU:HD23  | 1:67:A:SER:H     | 7        | 0.45          |
| (1,1735) | 1:66:A:LEU:HD22  | 1:67:A:SER:H     | 14       | 0.45          |
| (1,1702) | 1:116:A:GLN:HG3  | 1:116:A:GLN:HE21 | 1        | 0.45          |
| (1,1698) | 1:44:A:GLU:HG2   | 1:45:A:ALA:HB1   | 12       | 0.45          |
| (1,1682) | 1:41:A:ALA:HB3   | 1:33:A:GLU:H     | 12       | 0.45          |
| (1,1507) | 1:78:A:TYR:HE1   | 1:28:A:ILE:HG22  | 13       | 0.45          |
| (1,1482) | 1:64:A:MET:HE3   | 1:27:A:VAL:HA    | 16       | 0.45          |
| (1,1481) | 1:64:A:MET:HE1   | 1:30:A:PHE:HA    | 5        | 0.45          |
| (1,1405) | 1:102:A:CYS:H    | 1:95:A:VAL:HG11  | 7        | 0.45          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1398) | 1:88:A:VAL:HG21 | 1:85:A:LEU:H    | 16       | 0.45          |
| (1,1356) | 1:61:A:ALA:HB1  | 1:57:A:VAL:HG11 | 10       | 0.45          |
| (1,1342) | 1:48:A:LEU:HD11 | 1:84:A:TYR:HE1  | 11       | 0.45          |
| (1,1315) | 1:95:A:VAL:HG21 | 1:97:A:LEU:HD21 | 14       | 0.45          |
| (1,1305) | 1:97:A:LEU:HD21 | 1:52:A:ILE:HB   | 13       | 0.45          |
| (1,1305) | 1:97:A:LEU:HD23 | 1:52:A:ILE:HB   | 15       | 0.45          |
| (1,1305) | 1:97:A:LEU:HD23 | 1:52:A:ILE:HB   | 17       | 0.45          |
| (1,1155) | 1:53:A:PHE:HB3  | 1:53:A:PHE:HE2  | 5        | 0.45          |
| (1,1125) | 1:97:A:LEU:HD13 | 1:60:A:VAL:HG13 | 14       | 0.45          |
| (1,1077) | 1:21:A:LEU:HA   | 1:21:A:LEU:HD22 | 7        | 0.45          |
| (1,1076) | 1:30:A:PHE:HD1  | 1:31:A:LEU:HD11 | 7        | 0.45          |
| (1,1076) | 1:30:A:PHE:HD2  | 1:31:A:LEU:HD12 | 10       | 0.45          |
| (1,1075) | 1:31:A:LEU:HD12 | 1:31:A:LEU:HA   | 3        | 0.45          |
| (1,1075) | 1:31:A:LEU:HD12 | 1:31:A:LEU:HA   | 12       | 0.45          |
| (1,1073) | 1:97:A:LEU:HD13 | 1:97:A:LEU:H    | 12       | 0.45          |
| (1,1073) | 1:97:A:LEU:HD12 | 1:97:A:LEU:H    | 17       | 0.45          |
| (1,1043) | 1:78:A:TYR:HE1  | 1:28:A:ILE:HD13 | 7        | 0.45          |
| (1,1043) | 1:78:A:TYR:HE2  | 1:28:A:ILE:HD12 | 13       | 0.45          |
| (1,1043) | 1:78:A:TYR:HE1  | 1:28:A:ILE:HD13 | 15       | 0.45          |
| (1,942)  | 1:93:A:THR:HB   | 1:95:A:VAL:HG12 | 2        | 0.45          |
| (1,942)  | 1:93:A:THR:HB   | 1:95:A:VAL:HG12 | 6        | 0.45          |
| (1,825)  | 1:45:A:ALA:HB2  | 1:78:A:TYR:HB3  | 4        | 0.45          |
| (1,825)  | 1:45:A:ALA:HB3  | 1:78:A:TYR:HB3  | 8        | 0.45          |
| (1,789)  | 1:50:A:ILE:HG13 | 1:50:A:ILE:HG23 | 9        | 0.45          |
| (1,789)  | 1:50:A:ILE:HG13 | 1:50:A:ILE:HG23 | 11       | 0.45          |
| (1,789)  | 1:50:A:ILE:HG13 | 1:50:A:ILE:HG23 | 15       | 0.45          |
| (1,788)  | 1:52:A:ILE:HD11 | 1:56:A:LEU:H    | 5        | 0.45          |
| (1,788)  | 1:52:A:ILE:HD11 | 1:56:A:LEU:H    | 6        | 0.45          |
| (1,614)  | 1:97:A:LEU:HD13 | 1:97:A:LEU:H    | 12       | 0.45          |
| (1,604)  | 1:32:A:ALA:HB3  | 1:41:A:ALA:H    | 9        | 0.45          |
| (1,576)  | 1:50:A:ILE:HD12 | 1:50:A:ILE:H    | 9        | 0.45          |
| (1,576)  | 1:50:A:ILE:HD13 | 1:50:A:ILE:H    | 16       | 0.45          |
| (1,557)  | 1:66:A:LEU:HB2  | 1:70:A:GLN:HE22 | 14       | 0.45          |
| (1,524)  | 1:20:A:LYS:HB3  | 1:22:A:ASN:HD22 | 10       | 0.45          |
| (1,442)  | 1:41:A:ALA:HB1  | 1:41:A:ALA:H    | 9        | 0.45          |
| (1,442)  | 1:41:A:ALA:HB2  | 1:41:A:ALA:H    | 10       | 0.45          |
| (1,389)  | 1:58:A:ASP:H    | 1:57:A:VAL:HG13 | 8        | 0.45          |
| (1,363)  | 1:66:A:LEU:HD12 | 1:62:A:GLY:H    | 6        | 0.45          |
| (1,363)  | 1:66:A:LEU:HD11 | 1:62:A:GLY:H    | 14       | 0.45          |
| (1,363)  | 1:66:A:LEU:HD11 | 1:62:A:GLY:H    | 17       | 0.45          |
| (1,217)  | 1:93:A:THR:HG21 | 1:103:A:GLY:H   | 9        | 0.45          |
| (1,217)  | 1:93:A:THR:HG23 | 1:103:A:GLY:H   | 16       | 0.45          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,169)  | 1:120:A:ALA:HB1  | 1:119:A:GLU:H    | 2        | 0.45          |
| (1,169)  | 1:120:A:ALA:HB1  | 1:119:A:GLU:H    | 5        | 0.45          |
| (3,139)  | 1:66:A:LEU:HD22  | 1:70:A:GLN:H     | 5        | 0.44          |
| (3,139)  | 1:66:A:LEU:HD21  | 1:70:A:GLN:H     | 9        | 0.44          |
| (3,132)  | 1:113:A:ALA:HB2  | 1:112:A:HIS:H    | 2        | 0.44          |
| (3,132)  | 1:113:A:ALA:HB2  | 1:112:A:HIS:H    | 5        | 0.44          |
| (3,123)  | 1:50:A:ILE:HD12  | 1:79:A:THR:HA    | 7        | 0.44          |
| (3,84)   | 1:84:A:TYR:HE1   | 1:84:A:TYR:HA    | 13       | 0.44          |
| (3,84)   | 1:84:A:TYR:HE2   | 1:84:A:TYR:HA    | 16       | 0.44          |
| (3,50)   | 1:31:A:LEU:HD22  | 1:97:A:LEU:HD22  | 6        | 0.44          |
| (3,50)   | 1:31:A:LEU:HD21  | 1:97:A:LEU:HD22  | 12       | 0.44          |
| (3,22)   | 1:48:A:LEU:H     | 1:48:A:LEU:HD12  | 2        | 0.44          |
| (3,18)   | 1:58:A:ASP:HB3   | 1:60:A:VAL:HG11  | 13       | 0.44          |
| (3,16)   | 1:90:A:PRO:HA    | 1:110:A:VAL:HG11 | 6        | 0.44          |
| (1,4259) | 1:57:A:VAL:HG13  | 1:56:A:LEU:H     | 10       | 0.44          |
| (1,4247) | 1:54:A:GLN:HE22  | 1:57:A:VAL:HG12  | 8        | 0.44          |
| (1,4197) | 1:66:A:LEU:HD22  | 1:67:A:SER:H     | 10       | 0.44          |
| (1,4164) | 1:32:A:ALA:HB3   | 1:41:A:ALA:H     | 11       | 0.44          |
| (1,4138) | 1:31:A:LEU:H     | 1:28:A:ILE:HD12  | 11       | 0.44          |
| (1,4087) | 1:65:A:ASN:HB2   | 1:65:A:ASN:HD21  | 6        | 0.44          |
| (1,4007) | 1:41:A:ALA:HB2   | 1:41:A:ALA:H     | 11       | 0.44          |
| (1,3972) | 1:53:A:PHE:H     | 1:56:A:LEU:HB3   | 14       | 0.44          |
| (1,3861) | 1:110:A:VAL:HG23 | 1:91:A:GLY:H     | 2        | 0.44          |
| (1,3834) | 1:95:A:VAL:HG21  | 1:100:A:ASN:H    | 7        | 0.44          |
| (1,3834) | 1:95:A:VAL:HG21  | 1:100:A:ASN:H    | 16       | 0.44          |
| (1,3822) | 1:93:A:THR:HG21  | 1:103:A:GLY:H    | 7        | 0.44          |
| (1,3822) | 1:93:A:THR:HG21  | 1:103:A:GLY:H    | 15       | 0.44          |
| (1,3782) | 1:120:A:ALA:HB2  | 1:119:A:GLU:H    | 10       | 0.44          |
| (1,3742) | 1:28:A:ILE:H     | 1:29:A:ALA:HB2   | 7        | 0.44          |
| (1,3742) | 1:28:A:ILE:H     | 1:29:A:ALA:HB3   | 8        | 0.44          |
| (1,3742) | 1:28:A:ILE:H     | 1:29:A:ALA:HB3   | 11       | 0.44          |
| (1,3742) | 1:28:A:ILE:H     | 1:29:A:ALA:HB3   | 12       | 0.44          |
| (1,3742) | 1:28:A:ILE:H     | 1:29:A:ALA:HB3   | 15       | 0.44          |
| (1,3644) | 1:53:A:PHE:H     | 1:53:A:PHE:HD2   | 6        | 0.44          |
| (1,3644) | 1:53:A:PHE:H     | 1:53:A:PHE:HD2   | 9        | 0.44          |
| (1,3601) | 1:113:A:ALA:HB2  | 1:111:A:GLU:H    | 11       | 0.44          |
| (1,3594) | 1:105:A:LEU:HB2  | 1:110:A:VAL:HG13 | 9        | 0.44          |
| (1,3570) | 1:90:A:PRO:HA    | 1:105:A:LEU:HD13 | 13       | 0.44          |
| (1,3554) | 1:66:A:LEU:HB2   | 1:66:A:LEU:HD22  | 4        | 0.44          |
| (1,3554) | 1:66:A:LEU:HB2   | 1:66:A:LEU:HD22  | 6        | 0.44          |
| (1,3554) | 1:66:A:LEU:HB2   | 1:66:A:LEU:HD23  | 8        | 0.44          |
| (1,3554) | 1:66:A:LEU:HB2   | 1:66:A:LEU:HD21  | 16       | 0.44          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3554) | 1:66:A:LEU:HB2  | 1:66:A:LEU:HD23 | 17       | 0.44          |
| (1,3508) | 1:113:A:ALA:HB3 | 1:88:A:VAL:HA   | 11       | 0.44          |
| (1,3498) | 1:70:A:GLN:HE21 | 1:27:A:VAL:HG13 | 4        | 0.44          |
| (1,3498) | 1:70:A:GLN:HE21 | 1:27:A:VAL:HG12 | 9        | 0.44          |
| (1,3483) | 1:53:A:PHE:HA   | 1:31:A:LEU:HD13 | 9        | 0.44          |
| (1,3483) | 1:53:A:PHE:HA   | 1:31:A:LEU:HD13 | 15       | 0.44          |
| (1,3482) | 1:71:A:LEU:HB2  | 1:31:A:LEU:HD12 | 2        | 0.44          |
| (1,3482) | 1:71:A:LEU:HB2  | 1:31:A:LEU:HD11 | 14       | 0.44          |
| (1,3464) | 1:86:A:TYR:HE1  | 1:85:A:LEU:HD13 | 9        | 0.44          |
| (1,3464) | 1:86:A:TYR:HE1  | 1:85:A:LEU:HD13 | 11       | 0.44          |
| (1,3451) | 1:93:A:THR:HA   | 1:93:A:THR:HG23 | 2        | 0.44          |
| (1,3451) | 1:93:A:THR:HA   | 1:93:A:THR:HG23 | 8        | 0.44          |
| (1,3451) | 1:93:A:THR:HA   | 1:93:A:THR:HG23 | 15       | 0.44          |
| (1,3405) | 1:55:A:ASP:HB2  | 1:56:A:LEU:HD22 | 1        | 0.44          |
| (1,3386) | 1:90:A:PRO:HA   | 1:92:A:ALA:HB2  | 3        | 0.44          |
| (1,3386) | 1:90:A:PRO:HA   | 1:92:A:ALA:HB1  | 12       | 0.44          |
| (1,3373) | 1:88:A:VAL:HA   | 1:93:A:THR:HG22 | 16       | 0.44          |
| (1,3368) | 1:31:A:LEU:HD12 | 1:31:A:LEU:HA   | 6        | 0.44          |
| (1,3368) | 1:31:A:LEU:HD12 | 1:31:A:LEU:HA   | 13       | 0.44          |
| (1,3342) | 1:92:A:ALA:HB2  | 1:88:A:VAL:H    | 16       | 0.44          |
| (1,3253) | 1:92:A:ALA:HB3  | 1:91:A:GLY:H    | 3        | 0.44          |
| (1,3231) | 1:27:A:VAL:HG22 | 1:27:A:VAL:HA   | 4        | 0.44          |
| (1,3231) | 1:27:A:VAL:HG23 | 1:27:A:VAL:HA   | 5        | 0.44          |
| (1,3231) | 1:27:A:VAL:HG23 | 1:27:A:VAL:HA   | 6        | 0.44          |
| (1,3196) | 1:64:A:MET:HB2  | 1:64:A:MET:HA   | 10       | 0.44          |
| (1,3196) | 1:64:A:MET:HB2  | 1:64:A:MET:HA   | 12       | 0.44          |
| (1,3196) | 1:64:A:MET:HB2  | 1:64:A:MET:HA   | 16       | 0.44          |
| (1,3161) | 1:82:A:TRP:HH2  | 1:120:A:ALA:HB2 | 17       | 0.44          |
| (1,3116) | 1:57:A:VAL:HG22 | 1:53:A:PHE:HE2  | 14       | 0.44          |
| (1,3103) | 1:56:A:LEU:HD11 | 1:60:A:VAL:HB   | 11       | 0.44          |
| (1,3070) | 1:55:A:ASP:H    | 1:54:A:GLN:HB2  | 6        | 0.44          |
| (1,3055) | 1:52:A:ILE:HG23 | 1:50:A:ILE:H    | 7        | 0.44          |
| (1,3051) | 1:78:A:TYR:HE2  | 1:28:A:ILE:HG22 | 16       | 0.44          |
| (1,3023) | 1:64:A:MET:HE2  | 1:27:A:VAL:HA   | 11       | 0.44          |
| (1,3022) | 1:64:A:MET:HE3  | 1:30:A:PHE:HA   | 9        | 0.44          |
| (1,3021) | 1:64:A:MET:HE2  | 1:63:A:GLU:H    | 4        | 0.44          |
| (1,3002) | 1:57:A:VAL:HG11 | 1:60:A:VAL:HB   | 7        | 0.44          |
| (1,2900) | 1:28:A:ILE:HD13 | 1:31:A:LEU:HB3  | 9        | 0.44          |
| (1,2894) | 1:52:A:ILE:HD13 | 1:53:A:PHE:HB2  | 1        | 0.44          |
| (1,2890) | 1:33:A:GLU:HB3  | 1:32:A:ALA:HB3  | 6        | 0.44          |
| (1,2890) | 1:33:A:GLU:HB3  | 1:32:A:ALA:HB1  | 11       | 0.44          |
| (1,2880) | 1:61:A:ALA:HB1  | 1:57:A:VAL:HG12 | 7        | 0.44          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2880) | 1:61:A:ALA:HB1   | 1:57:A:VAL:HG11 | 8        | 0.44          |
| (1,2880) | 1:61:A:ALA:HB3   | 1:57:A:VAL:HG12 | 14       | 0.44          |
| (1,2872) | 1:129:A:ALA:HB2  | 1:129:A:ALA:HA  | 2        | 0.44          |
| (1,2872) | 1:129:A:ALA:HB3  | 1:129:A:ALA:HA  | 9        | 0.44          |
| (1,2863) | 1:78:A:TYR:HE2   | 1:84:A:TYR:HD1  | 9        | 0.44          |
| (1,2861) | 1:84:A:TYR:HE1   | 1:84:A:TYR:HA   | 12       | 0.44          |
| (1,2854) | 1:85:A:LEU:HD23  | 1:84:A:TYR:HD2  | 10       | 0.44          |
| (1,2854) | 1:85:A:LEU:HD21  | 1:84:A:TYR:HD1  | 16       | 0.44          |
| (1,2852) | 1:81:A:SER:HB3   | 1:84:A:TYR:HD1  | 6        | 0.44          |
| (1,2845) | 1:22:A:ASN:H     | 1:27:A:VAL:HG12 | 14       | 0.44          |
| (1,2831) | 1:97:A:LEU:HD22  | 1:35:A:PHE:HD2  | 5        | 0.44          |
| (1,2827) | 1:97:A:LEU:HD23  | 1:52:A:ILE:HB   | 3        | 0.44          |
| (1,2785) | 1:50:A:ILE:HG21  | 1:51:A:GLY:HA3  | 3        | 0.44          |
| (1,2678) | 1:53:A:PHE:HB3   | 1:53:A:PHE:HE1  | 9        | 0.44          |
| (1,2608) | 1:48:A:LEU:HD13  | 1:52:A:ILE:HG12 | 5        | 0.44          |
| (1,2581) | 1:71:A:LEU:HD13  | 1:60:A:VAL:HG13 | 4        | 0.44          |
| (1,2581) | 1:71:A:LEU:HD12  | 1:60:A:VAL:HG12 | 6        | 0.44          |
| (1,2581) | 1:71:A:LEU:HD13  | 1:60:A:VAL:HG13 | 9        | 0.44          |
| (1,2578) | 1:57:A:VAL:HA    | 1:60:A:VAL:HG11 | 1        | 0.44          |
| (1,2568) | 1:78:A:TYR:HE2   | 1:28:A:ILE:HD13 | 1        | 0.44          |
| (1,2542) | 1:21:A:LEU:HD12  | 1:30:A:PHE:HA   | 16       | 0.44          |
| (1,2458) | 1:21:A:LEU:HA    | 1:21:A:LEU:HD13 | 15       | 0.44          |
| (1,2458) | 1:21:A:LEU:HA    | 1:21:A:LEU:HD12 | 17       | 0.44          |
| (1,2423) | 1:64:A:MET:HA    | 1:64:A:MET:HE1  | 15       | 0.44          |
| (1,2408) | 1:52:A:ILE:HD11  | 1:96:A:ASP:HA   | 8        | 0.44          |
| (1,2408) | 1:52:A:ILE:HD13  | 1:96:A:ASP:HA   | 10       | 0.44          |
| (1,2405) | 1:29:A:ALA:H     | 1:28:A:ILE:HD13 | 4        | 0.44          |
| (1,2405) | 1:29:A:ALA:H     | 1:28:A:ILE:HD11 | 8        | 0.44          |
| (1,2370) | 1:50:A:ILE:HG13  | 1:50:A:ILE:HG23 | 12       | 0.44          |
| (1,2369) | 1:52:A:ILE:HD11  | 1:56:A:LEU:H    | 10       | 0.44          |
| (1,2271) | 1:113:A:ALA:HB2  | 1:112:A:HIS:HD2 | 2        | 0.44          |
| (1,2271) | 1:113:A:ALA:HB2  | 1:112:A:HIS:HD2 | 4        | 0.44          |
| (1,2271) | 1:113:A:ALA:HB3  | 1:112:A:HIS:HD2 | 7        | 0.44          |
| (1,2271) | 1:113:A:ALA:HB3  | 1:112:A:HIS:HD2 | 9        | 0.44          |
| (1,2268) | 1:110:A:VAL:HG13 | 1:89:A:LYS:H    | 2        | 0.44          |
| (1,2230) | 1:28:A:ILE:H     | 1:28:A:ILE:HG21 | 7        | 0.44          |
| (1,2212) | 1:110:A:VAL:HG23 | 1:114:A:ARG:H   | 1        | 0.44          |
| (1,2212) | 1:110:A:VAL:HG23 | 1:114:A:ARG:H   | 4        | 0.44          |
| (1,2194) | 1:50:A:ILE:HD11  | 1:80:A:SER:H    | 12       | 0.44          |
| (1,2194) | 1:50:A:ILE:HD11  | 1:80:A:SER:H    | 16       | 0.44          |
| (1,2172) | 1:34:A:ARG:HD3   | 1:60:A:VAL:HG11 | 2        | 0.44          |
| (1,2163) | 1:78:A:TYR:HA    | 1:78:A:TYR:HD2  | 5        | 0.44          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2150) | 1:105:A:LEU:H   | 1:105:A:LEU:HD12 | 17       | 0.44          |
| (1,2146) | 1:104:A:GLU:HB3 | 1:93:A:THR:HG21  | 2        | 0.44          |
| (1,2146) | 1:104:A:GLU:HB3 | 1:93:A:THR:HG23  | 14       | 0.44          |
| (1,2146) | 1:104:A:GLU:HB3 | 1:93:A:THR:HG21  | 15       | 0.44          |
| (1,2003) | 1:48:A:LEU:HB3  | 1:48:A:LEU:HD11  | 1        | 0.44          |
| (1,2003) | 1:48:A:LEU:HB3  | 1:48:A:LEU:HD11  | 5        | 0.44          |
| (1,2003) | 1:48:A:LEU:HB3  | 1:48:A:LEU:HD11  | 10       | 0.44          |
| (1,2003) | 1:48:A:LEU:HB3  | 1:48:A:LEU:HD11  | 11       | 0.44          |
| (1,2003) | 1:48:A:LEU:HB3  | 1:48:A:LEU:HD13  | 12       | 0.44          |
| (1,2003) | 1:48:A:LEU:HB3  | 1:48:A:LEU:HD13  | 14       | 0.44          |
| (1,1960) | 1:121:A:LYS:HG3 | 1:117:A:LEU:HD12 | 8        | 0.44          |
| (1,1950) | 1:105:A:LEU:HB2 | 1:110:A:VAL:HG12 | 12       | 0.44          |
| (1,1853) | 1:86:A:TYR:HE2  | 1:85:A:LEU:HD12  | 5        | 0.44          |
| (1,1790) | 1:90:A:PRO:HA   | 1:92:A:ALA:HB2   | 2        | 0.44          |
| (1,1790) | 1:90:A:PRO:HA   | 1:92:A:ALA:HB2   | 7        | 0.44          |
| (1,1735) | 1:66:A:LEU:HD23 | 1:67:A:SER:H     | 4        | 0.44          |
| (1,1702) | 1:116:A:GLN:HG3 | 1:116:A:GLN:HE21 | 4        | 0.44          |
| (1,1702) | 1:116:A:GLN:HG3 | 1:116:A:GLN:HE21 | 5        | 0.44          |
| (1,1702) | 1:116:A:GLN:HG3 | 1:116:A:GLN:HE21 | 9        | 0.44          |
| (1,1702) | 1:116:A:GLN:HG3 | 1:116:A:GLN:HE21 | 10       | 0.44          |
| (1,1702) | 1:116:A:GLN:HG3 | 1:116:A:GLN:HE21 | 13       | 0.44          |
| (1,1702) | 1:116:A:GLN:HG3 | 1:116:A:GLN:HE21 | 16       | 0.44          |
| (1,1516) | 1:31:A:LEU:HD13 | 1:28:A:ILE:HG23  | 12       | 0.44          |
| (1,1481) | 1:64:A:MET:HE1  | 1:30:A:PHE:HA    | 2        | 0.44          |
| (1,1343) | 1:78:A:TYR:HE1  | 1:48:A:LEU:HD11  | 11       | 0.44          |
| (1,1343) | 1:78:A:TYR:HE1  | 1:48:A:LEU:HD13  | 17       | 0.44          |
| (1,1305) | 1:97:A:LEU:HD23 | 1:52:A:ILE:HB    | 2        | 0.44          |
| (1,1301) | 1:97:A:LEU:HD11 | 1:97:A:LEU:HA    | 5        | 0.44          |
| (1,1301) | 1:97:A:LEU:HD11 | 1:97:A:LEU:HA    | 14       | 0.44          |
| (1,1081) | 1:71:A:LEU:HD12 | 1:57:A:VAL:H     | 6        | 0.44          |
| (1,1076) | 1:30:A:PHE:HD2  | 1:31:A:LEU:HD12  | 2        | 0.44          |
| (1,1076) | 1:30:A:PHE:HD2  | 1:31:A:LEU:HD12  | 5        | 0.44          |
| (1,1076) | 1:30:A:PHE:HD2  | 1:31:A:LEU:HD13  | 8        | 0.44          |
| (1,1075) | 1:31:A:LEU:HD11 | 1:31:A:LEU:HA    | 8        | 0.44          |
| (1,1075) | 1:31:A:LEU:HD13 | 1:31:A:LEU:HA    | 9        | 0.44          |
| (1,1069) | 1:48:A:LEU:HD13 | 1:52:A:ILE:HG12  | 11       | 0.44          |
| (1,1043) | 1:78:A:TYR:HE2  | 1:28:A:ILE:HD13  | 9        | 0.44          |
| (1,942)  | 1:93:A:THR:HB   | 1:95:A:VAL:HG11  | 7        | 0.44          |
| (1,825)  | 1:45:A:ALA:HB2  | 1:78:A:TYR:HB3   | 7        | 0.44          |
| (1,822)  | 1:49:A:LYS:H    | 1:52:A:ILE:HD13  | 4        | 0.44          |
| (1,815)  | 1:50:A:ILE:HD13 | 1:50:A:ILE:HA    | 8        | 0.44          |
| (1,789)  | 1:50:A:ILE:HG13 | 1:50:A:ILE:HG23  | 6        | 0.44          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,789)  | 1:50:A:ILE:HG13 | 1:50:A:ILE:HG22  | 16       | 0.44          |
| (1,720)  | 1:120:A:ALA:H   | 1:85:A:LEU:HD21  | 1        | 0.44          |
| (1,604)  | 1:32:A:ALA:HB3  | 1:41:A:ALA:H     | 4        | 0.44          |
| (1,576)  | 1:50:A:ILE:HD11 | 1:50:A:ILE:H     | 13       | 0.44          |
| (1,556)  | 1:71:A:LEU:H    | 1:70:A:GLN:HE21  | 5        | 0.44          |
| (1,442)  | 1:41:A:ALA:HB1  | 1:41:A:ALA:H     | 7        | 0.44          |
| (1,363)  | 1:66:A:LEU:HD12 | 1:62:A:GLY:H     | 8        | 0.44          |
| (1,169)  | 1:120:A:ALA:HB1 | 1:119:A:GLU:H    | 4        | 0.44          |
| (1,126)  | 1:28:A:ILE:H    | 1:29:A:ALA:HB2   | 13       | 0.44          |
| (1,126)  | 1:28:A:ILE:H    | 1:29:A:ALA:HB3   | 17       | 0.44          |
| (1,32)   | 1:53:A:PHE:H    | 1:53:A:PHE:HD1   | 5        | 0.44          |
| (1,12)   | 1:100:A:ASN:H   | 1:100:A:ASN:HD21 | 7        | 0.44          |
| (3,150)  | 1:77:A:LEU:H    | 1:79:A:THR:HG22  | 4        | 0.43          |
| (3,147)  | 1:71:A:LEU:H    | 1:66:A:LEU:HD23  | 11       | 0.43          |
| (3,143)  | 1:25:A:LYS:H    | 1:77:A:LEU:HD22  | 16       | 0.43          |
| (3,139)  | 1:66:A:LEU:HD23 | 1:70:A:GLN:H     | 7        | 0.43          |
| (3,139)  | 1:66:A:LEU:HD23 | 1:70:A:GLN:H     | 11       | 0.43          |
| (3,132)  | 1:113:A:ALA:HB2 | 1:112:A:HIS:H    | 15       | 0.43          |
| (3,111)  | 1:111:A:GLU:HG2 | 1:112:A:HIS:HA   | 13       | 0.43          |
| (3,98)   | 1:64:A:MET:HE2  | 1:63:A:GLU:HG3   | 3        | 0.43          |
| (3,84)   | 1:84:A:TYR:HE2  | 1:84:A:TYR:HA    | 3        | 0.43          |
| (3,84)   | 1:84:A:TYR:HE1  | 1:84:A:TYR:HA    | 8        | 0.43          |
| (3,69)   | 1:57:A:VAL:HA   | 1:71:A:LEU:HB2   | 16       | 0.43          |
| (3,62)   | 1:52:A:ILE:HG23 | 1:56:A:LEU:H     | 15       | 0.43          |
| (3,51)   | 1:95:A:VAL:HG22 | 1:49:A:LYS:HA    | 7        | 0.43          |
| (3,50)   | 1:31:A:LEU:HD23 | 1:97:A:LEU:HD23  | 3        | 0.43          |
| (3,50)   | 1:31:A:LEU:HD22 | 1:97:A:LEU:HD23  | 4        | 0.43          |
| (3,18)   | 1:58:A:ASP:HB3  | 1:60:A:VAL:HG11  | 12       | 0.43          |
| (1,4300) | 1:92:A:ALA:H    | 1:105:A:LEU:HD21 | 15       | 0.43          |
| (1,4138) | 1:31:A:LEU:H    | 1:28:A:ILE:HD12  | 7        | 0.43          |
| (1,4138) | 1:31:A:LEU:H    | 1:28:A:ILE:HD11  | 17       | 0.43          |
| (1,4132) | 1:60:A:VAL:HG11 | 1:34:A:ARG:HE    | 2        | 0.43          |
| (1,4109) | 1:97:A:LEU:HD11 | 1:98:A:ASP:H     | 14       | 0.43          |
| (1,3972) | 1:53:A:PHE:H    | 1:56:A:LEU:HB3   | 9        | 0.43          |
| (1,3957) | 1:58:A:ASP:H    | 1:57:A:VAL:HG13  | 12       | 0.43          |
| (1,3923) | 1:71:A:LEU:HD12 | 1:72:A:ARG:H     | 2        | 0.43          |
| (1,3923) | 1:71:A:LEU:HD12 | 1:72:A:ARG:H     | 3        | 0.43          |
| (1,3923) | 1:71:A:LEU:HD11 | 1:72:A:ARG:H     | 4        | 0.43          |
| (1,3923) | 1:71:A:LEU:HD12 | 1:72:A:ARG:H     | 5        | 0.43          |
| (1,3923) | 1:71:A:LEU:HD12 | 1:72:A:ARG:H     | 7        | 0.43          |
| (1,3923) | 1:71:A:LEU:HD12 | 1:72:A:ARG:H     | 8        | 0.43          |
| (1,3923) | 1:71:A:LEU:HD11 | 1:72:A:ARG:H     | 9        | 0.43          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3923) | 1:71:A:LEU:HD13  | 1:72:A:ARG:H     | 11       | 0.43          |
| (1,3923) | 1:71:A:LEU:HD13  | 1:72:A:ARG:H     | 14       | 0.43          |
| (1,3923) | 1:71:A:LEU:HD13  | 1:72:A:ARG:H     | 15       | 0.43          |
| (1,3923) | 1:71:A:LEU:HD11  | 1:72:A:ARG:H     | 16       | 0.43          |
| (1,3861) | 1:110:A:VAL:HG22 | 1:91:A:GLY:H     | 1        | 0.43          |
| (1,3861) | 1:110:A:VAL:HG22 | 1:91:A:GLY:H     | 9        | 0.43          |
| (1,3839) | 1:65:A:ASN:HB3   | 1:65:A:ASN:HD21  | 2        | 0.43          |
| (1,3834) | 1:95:A:VAL:HG23  | 1:100:A:ASN:H    | 1        | 0.43          |
| (1,3834) | 1:95:A:VAL:HG22  | 1:100:A:ASN:H    | 6        | 0.43          |
| (1,3834) | 1:95:A:VAL:HG21  | 1:100:A:ASN:H    | 11       | 0.43          |
| (1,3822) | 1:93:A:THR:HG22  | 1:103:A:GLY:H    | 6        | 0.43          |
| (1,3742) | 1:28:A:ILE:H     | 1:29:A:ALA:HB3   | 3        | 0.43          |
| (1,3627) | 1:100:A:ASN:H    | 1:100:A:ASN:HD21 | 9        | 0.43          |
| (1,3627) | 1:100:A:ASN:H    | 1:100:A:ASN:HD21 | 12       | 0.43          |
| (1,3612) | 1:120:A:ALA:HB1  | 1:120:A:ALA:HA   | 9        | 0.43          |
| (1,3612) | 1:120:A:ALA:HB1  | 1:120:A:ALA:HA   | 12       | 0.43          |
| (1,3612) | 1:120:A:ALA:HB3  | 1:120:A:ALA:HA   | 15       | 0.43          |
| (1,3601) | 1:113:A:ALA:HB1  | 1:111:A:GLU:H    | 8        | 0.43          |
| (1,3601) | 1:113:A:ALA:HB1  | 1:111:A:GLU:H    | 10       | 0.43          |
| (1,3594) | 1:105:A:LEU:HB2  | 1:110:A:VAL:HG13 | 1        | 0.43          |
| (1,3594) | 1:105:A:LEU:HB2  | 1:110:A:VAL:HG11 | 2        | 0.43          |
| (1,3594) | 1:105:A:LEU:HB2  | 1:110:A:VAL:HG13 | 5        | 0.43          |
| (1,3594) | 1:105:A:LEU:HB2  | 1:110:A:VAL:HG12 | 6        | 0.43          |
| (1,3594) | 1:105:A:LEU:HB2  | 1:110:A:VAL:HG11 | 8        | 0.43          |
| (1,3594) | 1:105:A:LEU:HB2  | 1:110:A:VAL:HG13 | 10       | 0.43          |
| (1,3594) | 1:105:A:LEU:HB2  | 1:110:A:VAL:HG13 | 14       | 0.43          |
| (1,3594) | 1:105:A:LEU:HB2  | 1:110:A:VAL:HG11 | 15       | 0.43          |
| (1,3594) | 1:105:A:LEU:HB2  | 1:110:A:VAL:HG12 | 17       | 0.43          |
| (1,3578) | 1:105:A:LEU:HD13 | 1:109:A:HIS:HA   | 2        | 0.43          |
| (1,3578) | 1:105:A:LEU:HD13 | 1:109:A:HIS:HA   | 7        | 0.43          |
| (1,3578) | 1:105:A:LEU:HD13 | 1:109:A:HIS:HA   | 12       | 0.43          |
| (1,3570) | 1:90:A:PRO:HA    | 1:105:A:LEU:HD11 | 10       | 0.43          |
| (1,3554) | 1:66:A:LEU:HB2   | 1:66:A:LEU:HD23  | 9        | 0.43          |
| (1,3554) | 1:66:A:LEU:HB2   | 1:66:A:LEU:HD22  | 13       | 0.43          |
| (1,3498) | 1:70:A:GLN:HE21  | 1:27:A:VAL:HG13  | 10       | 0.43          |
| (1,3482) | 1:71:A:LEU:HB2   | 1:31:A:LEU:HD12  | 1        | 0.43          |
| (1,3464) | 1:86:A:TYR:HE1   | 1:85:A:LEU:HD13  | 2        | 0.43          |
| (1,3464) | 1:86:A:TYR:HE2   | 1:85:A:LEU:HD13  | 12       | 0.43          |
| (1,3463) | 1:35:A:PHE:HE2   | 1:38:A:CYS:HB2   | 1        | 0.43          |
| (1,3452) | 1:95:A:VAL:HA    | 1:93:A:THR:HG21  | 14       | 0.43          |
| (1,3451) | 1:93:A:THR:HA    | 1:93:A:THR:HG21  | 3        | 0.43          |
| (1,3451) | 1:93:A:THR:HA    | 1:93:A:THR:HG23  | 9        | 0.43          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3451) | 1:93:A:THR:HA   | 1:93:A:THR:HG22  | 14       | 0.43          |
| (1,3418) | 1:117:A:LEU:HB2 | 1:117:A:LEU:HD13 | 3        | 0.43          |
| (1,3418) | 1:117:A:LEU:HB2 | 1:117:A:LEU:HD13 | 12       | 0.43          |
| (1,3401) | 1:86:A:TYR:HE1  | 1:86:A:TYR:HA    | 15       | 0.43          |
| (1,3373) | 1:88:A:VAL:HA   | 1:93:A:THR:HG22  | 14       | 0.43          |
| (1,3342) | 1:92:A:ALA:HB3  | 1:88:A:VAL:H     | 8        | 0.43          |
| (1,3342) | 1:92:A:ALA:HB3  | 1:88:A:VAL:H     | 17       | 0.43          |
| (1,3323) | 1:66:A:LEU:HD22 | 1:66:A:LEU:H     | 1        | 0.43          |
| (1,3323) | 1:66:A:LEU:HD21 | 1:66:A:LEU:H     | 2        | 0.43          |
| (1,3323) | 1:66:A:LEU:HD22 | 1:66:A:LEU:H     | 4        | 0.43          |
| (1,3323) | 1:66:A:LEU:HD22 | 1:66:A:LEU:H     | 6        | 0.43          |
| (1,3323) | 1:66:A:LEU:HD23 | 1:66:A:LEU:H     | 8        | 0.43          |
| (1,3323) | 1:66:A:LEU:HD21 | 1:66:A:LEU:H     | 16       | 0.43          |
| (1,3302) | 1:83:A:ARG:HB2  | 1:86:A:TYR:HD2   | 9        | 0.43          |
| (1,3286) | 1:116:A:GLN:HG3 | 1:116:A:GLN:HE21 | 2        | 0.43          |
| (1,3286) | 1:116:A:GLN:HG3 | 1:116:A:GLN:HE21 | 7        | 0.43          |
| (1,3286) | 1:116:A:GLN:HG3 | 1:116:A:GLN:HE21 | 17       | 0.43          |
| (1,3256) | 1:41:A:ALA:HB3  | 1:33:A:GLU:H     | 11       | 0.43          |
| (1,3253) | 1:92:A:ALA:HB1  | 1:91:A:GLY:H     | 16       | 0.43          |
| (1,3231) | 1:27:A:VAL:HG23 | 1:27:A:VAL:HA    | 3        | 0.43          |
| (1,3231) | 1:27:A:VAL:HG23 | 1:27:A:VAL:HA    | 7        | 0.43          |
| (1,3231) | 1:27:A:VAL:HG22 | 1:27:A:VAL:HA    | 8        | 0.43          |
| (1,3231) | 1:27:A:VAL:HG23 | 1:27:A:VAL:HA    | 9        | 0.43          |
| (1,3199) | 1:113:A:ALA:HB2 | 1:112:A:HIS:HB2  | 16       | 0.43          |
| (1,3196) | 1:64:A:MET:HB2  | 1:64:A:MET:HA    | 11       | 0.43          |
| (1,3196) | 1:64:A:MET:HB2  | 1:64:A:MET:HA    | 13       | 0.43          |
| (1,3196) | 1:64:A:MET:HB2  | 1:64:A:MET:HA    | 17       | 0.43          |
| (1,3116) | 1:57:A:VAL:HG22 | 1:53:A:PHE:HE1   | 6        | 0.43          |
| (1,3115) | 1:58:A:ASP:HA   | 1:57:A:VAL:HG21  | 1        | 0.43          |
| (1,3103) | 1:56:A:LEU:HD11 | 1:60:A:VAL:HB    | 3        | 0.43          |
| (1,3103) | 1:56:A:LEU:HD11 | 1:60:A:VAL:HB    | 6        | 0.43          |
| (1,3081) | 1:97:A:LEU:HD11 | 1:55:A:ASP:HA    | 1        | 0.43          |
| (1,3078) | 1:54:A:GLN:HB3  | 1:57:A:VAL:HG13  | 17       | 0.43          |
| (1,3070) | 1:55:A:ASP:H    | 1:54:A:GLN:HB2   | 7        | 0.43          |
| (1,3070) | 1:55:A:ASP:H    | 1:54:A:GLN:HB2   | 13       | 0.43          |
| (1,3067) | 1:52:A:ILE:HG22 | 1:53:A:PHE:HB3   | 13       | 0.43          |
| (1,3061) | 1:31:A:LEU:HD12 | 1:28:A:ILE:HG22  | 17       | 0.43          |
| (1,3052) | 1:39:A:PHE:HZ   | 1:52:A:ILE:HG23  | 9        | 0.43          |
| (1,3051) | 1:78:A:TYR:HE1  | 1:28:A:ILE:HG21  | 1        | 0.43          |
| (1,3051) | 1:78:A:TYR:HE2  | 1:28:A:ILE:HG22  | 3        | 0.43          |
| (1,3051) | 1:78:A:TYR:HE1  | 1:28:A:ILE:HG22  | 8        | 0.43          |
| (1,2940) | 1:99:A:GLY:HA3  | 1:95:A:VAL:HG13  | 2        | 0.43          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2900) | 1:28:A:ILE:HD13  | 1:31:A:LEU:HB3  | 1        | 0.43          |
| (1,2900) | 1:28:A:ILE:HD13  | 1:31:A:LEU:HB3  | 2        | 0.43          |
| (1,2900) | 1:28:A:ILE:HD13  | 1:31:A:LEU:HB3  | 11       | 0.43          |
| (1,2890) | 1:33:A:GLU:HB3   | 1:32:A:ALA:HB2  | 1        | 0.43          |
| (1,2873) | 1:126:A:ALA:HA   | 1:126:A:ALA:HB3 | 1        | 0.43          |
| (1,2872) | 1:129:A:ALA:HB3  | 1:129:A:ALA:HA  | 8        | 0.43          |
| (1,2852) | 1:81:A:SER:HB3   | 1:84:A:TYR:HD2  | 1        | 0.43          |
| (1,2827) | 1:97:A:LEU:HD21  | 1:52:A:ILE:HB   | 4        | 0.43          |
| (1,2785) | 1:50:A:ILE:HG21  | 1:51:A:GLY:HA3  | 6        | 0.43          |
| (1,2785) | 1:50:A:ILE:HG21  | 1:51:A:GLY:HA3  | 10       | 0.43          |
| (1,2785) | 1:50:A:ILE:HG22  | 1:51:A:GLY:HA3  | 14       | 0.43          |
| (1,2694) | 1:73:A:SER:HB2   | 1:74:A:ALA:H    | 11       | 0.43          |
| (1,2680) | 1:117:A:LEU:HD12 | 1:82:A:TRP:HD1  | 6        | 0.43          |
| (1,2678) | 1:53:A:PHE:HB3   | 1:53:A:PHE:HE2  | 2        | 0.43          |
| (1,2678) | 1:53:A:PHE:HB3   | 1:53:A:PHE:HE1  | 10       | 0.43          |
| (1,2678) | 1:53:A:PHE:HB3   | 1:53:A:PHE:HE2  | 14       | 0.43          |
| (1,2678) | 1:53:A:PHE:HB3   | 1:53:A:PHE:HE2  | 16       | 0.43          |
| (1,2664) | 1:97:A:LEU:HD13  | 1:60:A:VAL:HG13 | 16       | 0.43          |
| (1,2614) | 1:30:A:PHE:HD1   | 1:31:A:LEU:HD11 | 12       | 0.43          |
| (1,2608) | 1:48:A:LEU:HD12  | 1:52:A:ILE:HG12 | 14       | 0.43          |
| (1,2581) | 1:71:A:LEU:HD12  | 1:60:A:VAL:HG12 | 14       | 0.43          |
| (1,2578) | 1:57:A:VAL:HA    | 1:60:A:VAL:HG11 | 10       | 0.43          |
| (1,2568) | 1:78:A:TYR:HE1   | 1:28:A:ILE:HD13 | 11       | 0.43          |
| (1,2458) | 1:21:A:LEU:HA    | 1:21:A:LEU:HD13 | 5        | 0.43          |
| (1,2423) | 1:64:A:MET:HA    | 1:64:A:MET:HE1  | 6        | 0.43          |
| (1,2408) | 1:52:A:ILE:HD12  | 1:96:A:ASP:HA   | 15       | 0.43          |
| (1,2363) | 1:48:A:LEU:HD13  | 1:84:A:TYR:HE2  | 2        | 0.43          |
| (1,2305) | 1:45:A:ALA:HB1   | 1:44:A:GLU:HA   | 12       | 0.43          |
| (1,2271) | 1:113:A:ALA:HB2  | 1:112:A:HIS:HD2 | 6        | 0.43          |
| (1,2271) | 1:113:A:ALA:HB2  | 1:112:A:HIS:HD2 | 11       | 0.43          |
| (1,2212) | 1:110:A:VAL:HG21 | 1:114:A:ARG:H   | 2        | 0.43          |
| (1,2212) | 1:110:A:VAL:HG23 | 1:114:A:ARG:H   | 3        | 0.43          |
| (1,2212) | 1:110:A:VAL:HG23 | 1:114:A:ARG:H   | 16       | 0.43          |
| (1,2194) | 1:50:A:ILE:HD12  | 1:80:A:SER:H    | 1        | 0.43          |
| (1,2194) | 1:50:A:ILE:HD12  | 1:80:A:SER:H    | 13       | 0.43          |
| (1,2179) | 1:52:A:ILE:HG23  | 1:48:A:LEU:HB3  | 3        | 0.43          |
| (1,2003) | 1:48:A:LEU:HB3   | 1:48:A:LEU:HD13 | 13       | 0.43          |
| (1,2003) | 1:48:A:LEU:HB3   | 1:48:A:LEU:HD13 | 16       | 0.43          |
| (1,1955) | 1:92:A:ALA:HB1   | 1:113:A:ALA:HB2 | 13       | 0.43          |
| (1,1874) | 1:70:A:GLN:HE21  | 1:27:A:VAL:HG12 | 1        | 0.43          |
| (1,1866) | 1:83:A:ARG:HD3   | 1:45:A:ALA:HB1  | 7        | 0.43          |
| (1,1866) | 1:83:A:ARG:HD3   | 1:45:A:ALA:HB1  | 16       | 0.43          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1853) | 1:86:A:TYR:HE2  | 1:85:A:LEU:HD13  | 1        | 0.43          |
| (1,1853) | 1:86:A:TYR:HE1  | 1:85:A:LEU:HD13  | 4        | 0.43          |
| (1,1853) | 1:86:A:TYR:HE1  | 1:85:A:LEU:HD11  | 6        | 0.43          |
| (1,1853) | 1:86:A:TYR:HE1  | 1:85:A:LEU:HD12  | 13       | 0.43          |
| (1,1851) | 1:35:A:PHE:HE2  | 1:38:A:CYS:HB2   | 11       | 0.43          |
| (1,1735) | 1:66:A:LEU:HD22 | 1:67:A:SER:H     | 10       | 0.43          |
| (1,1702) | 1:116:A:GLN:HG3 | 1:116:A:GLN:HE21 | 6        | 0.43          |
| (1,1702) | 1:116:A:GLN:HG3 | 1:116:A:GLN:HE21 | 8        | 0.43          |
| (1,1686) | 1:85:A:LEU:HD12 | 1:85:A:LEU:HD21  | 10       | 0.43          |
| (1,1686) | 1:85:A:LEU:HD11 | 1:85:A:LEU:HD22  | 14       | 0.43          |
| (1,1686) | 1:85:A:LEU:HD11 | 1:85:A:LEU:HD21  | 16       | 0.43          |
| (1,1545) | 1:56:A:LEU:HD11 | 1:60:A:VAL:HB    | 1        | 0.43          |
| (1,1507) | 1:78:A:TYR:HE2  | 1:28:A:ILE:HG22  | 10       | 0.43          |
| (1,1507) | 1:78:A:TYR:HE2  | 1:28:A:ILE:HG22  | 17       | 0.43          |
| (1,1356) | 1:61:A:ALA:HB1  | 1:57:A:VAL:HG11  | 12       | 0.43          |
| (1,1308) | 1:97:A:LEU:HD22 | 1:35:A:PHE:HD2   | 7        | 0.43          |
| (1,1305) | 1:97:A:LEU:HD22 | 1:52:A:ILE:HB    | 1        | 0.43          |
| (1,1301) | 1:97:A:LEU:HD13 | 1:97:A:LEU:HA    | 2        | 0.43          |
| (1,1231) | 1:97:A:LEU:HD13 | 1:59:A:ARG:HD3   | 2        | 0.43          |
| (1,1231) | 1:97:A:LEU:HD13 | 1:59:A:ARG:HD3   | 7        | 0.43          |
| (1,1076) | 1:30:A:PHE:HD1  | 1:31:A:LEU:HD11  | 13       | 0.43          |
| (1,1076) | 1:30:A:PHE:HD2  | 1:31:A:LEU:HD12  | 15       | 0.43          |
| (1,1076) | 1:30:A:PHE:HD1  | 1:31:A:LEU:HD13  | 17       | 0.43          |
| (1,1075) | 1:31:A:LEU:HD12 | 1:31:A:LEU:HA    | 6        | 0.43          |
| (1,1061) | 1:21:A:LEU:HD22 | 1:27:A:VAL:HG12  | 7        | 0.43          |
| (1,1043) | 1:78:A:TYR:HE2  | 1:28:A:ILE:HD11  | 4        | 0.43          |
| (1,1043) | 1:78:A:TYR:HE2  | 1:28:A:ILE:HD12  | 5        | 0.43          |
| (1,825)  | 1:45:A:ALA:HB3  | 1:78:A:TYR:HB3   | 15       | 0.43          |
| (1,825)  | 1:45:A:ALA:HB3  | 1:78:A:TYR:HB3   | 17       | 0.43          |
| (1,789)  | 1:50:A:ILE:HG13 | 1:50:A:ILE:HG21  | 17       | 0.43          |
| (1,697)  | 1:57:A:VAL:HG11 | 1:56:A:LEU:H     | 7        | 0.43          |
| (1,697)  | 1:57:A:VAL:HG11 | 1:56:A:LEU:H     | 14       | 0.43          |
| (1,614)  | 1:97:A:LEU:HD13 | 1:97:A:LEU:H     | 8        | 0.43          |
| (1,610)  | 1:48:A:LEU:HD23 | 1:49:A:LYS:H     | 1        | 0.43          |
| (1,576)  | 1:50:A:ILE:HD11 | 1:50:A:ILE:H     | 1        | 0.43          |
| (1,576)  | 1:50:A:ILE:HD12 | 1:50:A:ILE:H     | 3        | 0.43          |
| (1,576)  | 1:50:A:ILE:HD12 | 1:50:A:ILE:H     | 10       | 0.43          |
| (1,576)  | 1:50:A:ILE:HD11 | 1:50:A:ILE:H     | 14       | 0.43          |
| (1,442)  | 1:41:A:ALA:HB2  | 1:41:A:ALA:H     | 13       | 0.43          |
| (1,389)  | 1:58:A:ASP:H    | 1:57:A:VAL:HG13  | 10       | 0.43          |
| (1,389)  | 1:58:A:ASP:H    | 1:57:A:VAL:HG11  | 14       | 0.43          |
| (1,228)  | 1:95:A:VAL:HG22 | 1:100:A:ASN:H    | 2        | 0.43          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,228)  | 1:95:A:VAL:HG21 | 1:100:A:ASN:H    | 9        | 0.43          |
| (1,169)  | 1:120:A:ALA:HB1 | 1:119:A:GLU:H    | 6        | 0.43          |
| (1,169)  | 1:120:A:ALA:HB1 | 1:119:A:GLU:H    | 16       | 0.43          |
| (1,12)   | 1:100:A:ASN:H   | 1:100:A:ASN:HD21 | 4        | 0.43          |
| (3,152)  | 1:27:A:VAL:H    | 1:74:A:ALA:HB3   | 16       | 0.42          |
| (3,147)  | 1:71:A:LEU:H    | 1:66:A:LEU:HD21  | 9        | 0.42          |
| (3,139)  | 1:66:A:LEU:HD22 | 1:70:A:GLN:H     | 2        | 0.42          |
| (3,139)  | 1:66:A:LEU:HD23 | 1:70:A:GLN:H     | 4        | 0.42          |
| (3,132)  | 1:113:A:ALA:HB1 | 1:112:A:HIS:H    | 13       | 0.42          |
| (3,126)  | 1:21:A:LEU:HD21 | 1:22:A:ASN:H     | 14       | 0.42          |
| (3,124)  | 1:88:A:VAL:HG21 | 1:88:A:VAL:H     | 12       | 0.42          |
| (3,124)  | 1:88:A:VAL:HG23 | 1:88:A:VAL:H     | 13       | 0.42          |
| (3,111)  | 1:111:A:GLU:HG2 | 1:112:A:HIS:HA   | 2        | 0.42          |
| (3,99)   | 1:72:A:ARG:HG3  | 1:75:A:LEU:HD12  | 8        | 0.42          |
| (3,69)   | 1:57:A:VAL:HA   | 1:71:A:LEU:HB2   | 13       | 0.42          |
| (3,62)   | 1:52:A:ILE:HG22 | 1:56:A:LEU:H     | 13       | 0.42          |
| (3,36)   | 1:49:A:LYS:HB2  | 1:52:A:ILE:HD11  | 3        | 0.42          |
| (1,4300) | 1:92:A:ALA:H    | 1:105:A:LEU:HD21 | 12       | 0.42          |
| (1,4247) | 1:54:A:GLN:HE22 | 1:57:A:VAL:HG11  | 6        | 0.42          |
| (1,4197) | 1:66:A:LEU:HD23 | 1:67:A:SER:H     | 9        | 0.42          |
| (1,4176) | 1:97:A:LEU:HD12 | 1:97:A:LEU:H     | 10       | 0.42          |
| (1,4138) | 1:31:A:LEU:H    | 1:28:A:ILE:HD12  | 1        | 0.42          |
| (1,4138) | 1:31:A:LEU:H    | 1:28:A:ILE:HD11  | 8        | 0.42          |
| (1,4138) | 1:31:A:LEU:H    | 1:28:A:ILE:HD12  | 10       | 0.42          |
| (1,4138) | 1:31:A:LEU:H    | 1:28:A:ILE:HD12  | 12       | 0.42          |
| (1,4112) | 1:54:A:GLN:HE22 | 1:57:A:VAL:H     | 2        | 0.42          |
| (1,4112) | 1:54:A:GLN:HE22 | 1:57:A:VAL:H     | 3        | 0.42          |
| (1,4112) | 1:54:A:GLN:HE22 | 1:57:A:VAL:H     | 4        | 0.42          |
| (1,4087) | 1:65:A:ASN:HB2  | 1:65:A:ASN:HD21  | 3        | 0.42          |
| (1,4007) | 1:41:A:ALA:HB1  | 1:41:A:ALA:H     | 14       | 0.42          |
| (1,4007) | 1:41:A:ALA:HB2  | 1:41:A:ALA:H     | 16       | 0.42          |
| (1,3923) | 1:71:A:LEU:HD11 | 1:72:A:ARG:H     | 10       | 0.42          |
| (1,3923) | 1:71:A:LEU:HD11 | 1:72:A:ARG:H     | 13       | 0.42          |
| (1,3923) | 1:71:A:LEU:HD12 | 1:72:A:ARG:H     | 17       | 0.42          |
| (1,3839) | 1:65:A:ASN:HB3  | 1:65:A:ASN:HD21  | 8        | 0.42          |
| (1,3834) | 1:95:A:VAL:HG22 | 1:100:A:ASN:H    | 13       | 0.42          |
| (1,3834) | 1:95:A:VAL:HG21 | 1:100:A:ASN:H    | 17       | 0.42          |
| (1,3742) | 1:28:A:ILE:H    | 1:29:A:ALA:HB3   | 9        | 0.42          |
| (1,3742) | 1:28:A:ILE:H    | 1:29:A:ALA:HB2   | 16       | 0.42          |
| (1,3733) | 1:27:A:VAL:HG12 | 1:26:A:GLU:H     | 17       | 0.42          |
| (1,3668) | 1:84:A:TYR:H    | 1:84:A:TYR:HD2   | 4        | 0.42          |
| (1,3644) | 1:53:A:PHE:H    | 1:53:A:PHE:HD2   | 4        | 0.42          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3644) | 1:53:A:PHE:H     | 1:53:A:PHE:HD2   | 7        | 0.42          |
| (1,3644) | 1:53:A:PHE:H     | 1:53:A:PHE:HD2   | 11       | 0.42          |
| (1,3644) | 1:53:A:PHE:H     | 1:53:A:PHE:HD2   | 12       | 0.42          |
| (1,3612) | 1:120:A:ALA:HB1  | 1:120:A:ALA:HA   | 17       | 0.42          |
| (1,3601) | 1:113:A:ALA:HB2  | 1:111:A:GLU:H    | 15       | 0.42          |
| (1,3594) | 1:105:A:LEU:HB2  | 1:110:A:VAL:HG12 | 13       | 0.42          |
| (1,3594) | 1:105:A:LEU:HB2  | 1:110:A:VAL:HG11 | 16       | 0.42          |
| (1,3578) | 1:105:A:LEU:HD13 | 1:109:A:HIS:HA   | 6        | 0.42          |
| (1,3498) | 1:70:A:GLN:HE21  | 1:27:A:VAL:HG12  | 12       | 0.42          |
| (1,3498) | 1:70:A:GLN:HE21  | 1:27:A:VAL:HG11  | 17       | 0.42          |
| (1,3482) | 1:71:A:LEU:HB2   | 1:31:A:LEU:HD11  | 3        | 0.42          |
| (1,3482) | 1:71:A:LEU:HB2   | 1:31:A:LEU:HD11  | 6        | 0.42          |
| (1,3463) | 1:35:A:PHE:HE2   | 1:38:A:CYS:HB2   | 10       | 0.42          |
| (1,3451) | 1:93:A:THR:HA    | 1:93:A:THR:HG21  | 6        | 0.42          |
| (1,3446) | 1:65:A:ASN:HD22  | 1:20:A:LYS:HG2   | 16       | 0.42          |
| (1,3418) | 1:117:A:LEU:HB2  | 1:117:A:LEU:HD11 | 11       | 0.42          |
| (1,3373) | 1:88:A:VAL:HA    | 1:93:A:THR:HG21  | 3        | 0.42          |
| (1,3373) | 1:88:A:VAL:HA    | 1:93:A:THR:HG23  | 9        | 0.42          |
| (1,3342) | 1:92:A:ALA:HB3   | 1:88:A:VAL:H     | 10       | 0.42          |
| (1,3342) | 1:92:A:ALA:HB3   | 1:88:A:VAL:H     | 12       | 0.42          |
| (1,3323) | 1:66:A:LEU:HD21  | 1:66:A:LEU:H     | 3        | 0.42          |
| (1,3323) | 1:66:A:LEU:HD23  | 1:66:A:LEU:H     | 9        | 0.42          |
| (1,3323) | 1:66:A:LEU:HD22  | 1:66:A:LEU:H     | 10       | 0.42          |
| (1,3323) | 1:66:A:LEU:HD22  | 1:66:A:LEU:H     | 13       | 0.42          |
| (1,3319) | 1:66:A:LEU:HD22  | 1:27:A:VAL:HG12  | 12       | 0.42          |
| (1,3286) | 1:116:A:GLN:HG3  | 1:116:A:GLN:HE21 | 3        | 0.42          |
| (1,3286) | 1:116:A:GLN:HG3  | 1:116:A:GLN:HE21 | 11       | 0.42          |
| (1,3286) | 1:116:A:GLN:HG3  | 1:116:A:GLN:HE21 | 12       | 0.42          |
| (1,3286) | 1:116:A:GLN:HG3  | 1:116:A:GLN:HE21 | 15       | 0.42          |
| (1,3258) | 1:48:A:LEU:HD13  | 1:50:A:ILE:HA    | 15       | 0.42          |
| (1,3253) | 1:92:A:ALA:HB2   | 1:91:A:GLY:H     | 8        | 0.42          |
| (1,3253) | 1:92:A:ALA:HB1   | 1:91:A:GLY:H     | 13       | 0.42          |
| (1,3231) | 1:27:A:VAL:HG22  | 1:27:A:VAL:HA    | 11       | 0.42          |
| (1,3231) | 1:27:A:VAL:HG21  | 1:27:A:VAL:HA    | 12       | 0.42          |
| (1,3231) | 1:27:A:VAL:HG22  | 1:27:A:VAL:HA    | 14       | 0.42          |
| (1,3231) | 1:27:A:VAL:HG22  | 1:27:A:VAL:HA    | 16       | 0.42          |
| (1,3231) | 1:27:A:VAL:HG23  | 1:27:A:VAL:HA    | 17       | 0.42          |
| (1,3199) | 1:113:A:ALA:HB1  | 1:112:A:HIS:HB2  | 10       | 0.42          |
| (1,3196) | 1:64:A:MET:HB2   | 1:64:A:MET:HA    | 2        | 0.42          |
| (1,3161) | 1:82:A:TRP:HH2   | 1:120:A:ALA:HB1  | 8        | 0.42          |
| (1,3081) | 1:97:A:LEU:HD13  | 1:55:A:ASP:HA    | 9        | 0.42          |
| (1,3081) | 1:97:A:LEU:HD11  | 1:55:A:ASP:HA    | 13       | 0.42          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3078) | 1:54:A:GLN:HB3  | 1:57:A:VAL:HG12  | 10       | 0.42          |
| (1,3070) | 1:55:A:ASP:H    | 1:54:A:GLN:HB2   | 17       | 0.42          |
| (1,3067) | 1:52:A:ILE:HG23 | 1:53:A:PHE:HB3   | 7        | 0.42          |
| (1,3067) | 1:52:A:ILE:HG23 | 1:53:A:PHE:HB3   | 17       | 0.42          |
| (1,3051) | 1:78:A:TYR:HE1  | 1:28:A:ILE:HG21  | 9        | 0.42          |
| (1,3051) | 1:78:A:TYR:HE2  | 1:28:A:ILE:HG21  | 14       | 0.42          |
| (1,3045) | 1:52:A:ILE:HG13 | 1:54:A:GLN:HE21  | 7        | 0.42          |
| (1,2940) | 1:99:A:GLY:HA3  | 1:95:A:VAL:HG11  | 12       | 0.42          |
| (1,2940) | 1:99:A:GLY:HA3  | 1:95:A:VAL:HG13  | 17       | 0.42          |
| (1,2890) | 1:33:A:GLU:HB3  | 1:32:A:ALA:HB3   | 7        | 0.42          |
| (1,2890) | 1:33:A:GLU:HB3  | 1:32:A:ALA:HB2   | 15       | 0.42          |
| (1,2877) | 1:61:A:ALA:HB3  | 1:61:A:ALA:HA    | 4        | 0.42          |
| (1,2877) | 1:61:A:ALA:HB1  | 1:61:A:ALA:HA    | 7        | 0.42          |
| (1,2877) | 1:61:A:ALA:HB3  | 1:61:A:ALA:HA    | 9        | 0.42          |
| (1,2873) | 1:126:A:ALA:HA  | 1:126:A:ALA:HB1  | 3        | 0.42          |
| (1,2872) | 1:129:A:ALA:HB2 | 1:129:A:ALA:HA   | 3        | 0.42          |
| (1,2872) | 1:129:A:ALA:HB1 | 1:129:A:ALA:HA   | 14       | 0.42          |
| (1,2865) | 1:78:A:TYR:HE1  | 1:48:A:LEU:HD12  | 12       | 0.42          |
| (1,2863) | 1:78:A:TYR:HE1  | 1:84:A:TYR:HD2   | 16       | 0.42          |
| (1,2861) | 1:84:A:TYR:HE1  | 1:84:A:TYR:HA    | 10       | 0.42          |
| (1,2861) | 1:84:A:TYR:HE1  | 1:84:A:TYR:HA    | 14       | 0.42          |
| (1,2827) | 1:97:A:LEU:HD23 | 1:52:A:ILE:HB    | 10       | 0.42          |
| (1,2785) | 1:50:A:ILE:HG22 | 1:51:A:GLY:HA3   | 1        | 0.42          |
| (1,2785) | 1:50:A:ILE:HG21 | 1:51:A:GLY:HA3   | 9        | 0.42          |
| (1,2785) | 1:50:A:ILE:HG21 | 1:51:A:GLY:HA3   | 12       | 0.42          |
| (1,2720) | 1:86:A:TYR:HB3  | 1:117:A:LEU:HD12 | 14       | 0.42          |
| (1,2678) | 1:53:A:PHE:HB3  | 1:53:A:PHE:HE1   | 6        | 0.42          |
| (1,2614) | 1:30:A:PHE:HD1  | 1:31:A:LEU:HD13  | 16       | 0.42          |
| (1,2578) | 1:57:A:VAL:HA   | 1:60:A:VAL:HG13  | 17       | 0.42          |
| (1,2568) | 1:78:A:TYR:HE1  | 1:28:A:ILE:HD13  | 7        | 0.42          |
| (1,2568) | 1:78:A:TYR:HE1  | 1:28:A:ILE:HD12  | 14       | 0.42          |
| (1,2542) | 1:21:A:LEU:HD13 | 1:30:A:PHE:HA    | 12       | 0.42          |
| (1,2542) | 1:21:A:LEU:HD12 | 1:30:A:PHE:HA    | 17       | 0.42          |
| (1,2458) | 1:21:A:LEU:HA   | 1:21:A:LEU:HD11  | 11       | 0.42          |
| (1,2411) | 1:45:A:ALA:HB2  | 1:84:A:TYR:HB3   | 2        | 0.42          |
| (1,2405) | 1:29:A:ALA:H    | 1:28:A:ILE:HD12  | 7        | 0.42          |
| (1,2369) | 1:52:A:ILE:HD11 | 1:56:A:LEU:H     | 14       | 0.42          |
| (1,2309) | 1:39:A:PHE:HB3  | 1:39:A:PHE:HE1   | 16       | 0.42          |
| (1,2271) | 1:113:A:ALA:HB1 | 1:112:A:HIS:HD2  | 8        | 0.42          |
| (1,2271) | 1:113:A:ALA:HB1 | 1:112:A:HIS:HD2  | 10       | 0.42          |
| (1,2271) | 1:113:A:ALA:HB2 | 1:112:A:HIS:HD2  | 15       | 0.42          |
| (1,2271) | 1:113:A:ALA:HB2 | 1:112:A:HIS:HD2  | 17       | 0.42          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2256) | 1:101:A:PRO:HB2  | 1:105:A:LEU:HD23 | 10       | 0.42          |
| (1,2212) | 1:110:A:VAL:HG21 | 1:114:A:ARG:H    | 13       | 0.42          |
| (1,2201) | 1:64:A:MET:HB2   | 1:21:A:LEU:HD21  | 2        | 0.42          |
| (1,2201) | 1:64:A:MET:HB2   | 1:21:A:LEU:HD21  | 8        | 0.42          |
| (1,2196) | 1:107:A:GLU:HA   | 1:110:A:VAL:HG11 | 5        | 0.42          |
| (1,2194) | 1:50:A:ILE:HD13  | 1:80:A:SER:H     | 3        | 0.42          |
| (1,2194) | 1:50:A:ILE:HD12  | 1:80:A:SER:H     | 14       | 0.42          |
| (1,2194) | 1:50:A:ILE:HD13  | 1:80:A:SER:H     | 15       | 0.42          |
| (1,2179) | 1:52:A:ILE:HG21  | 1:48:A:LEU:HB3   | 16       | 0.42          |
| (1,2172) | 1:34:A:ARG:HD3   | 1:60:A:VAL:HG13  | 3        | 0.42          |
| (1,2172) | 1:34:A:ARG:HD3   | 1:60:A:VAL:HG11  | 5        | 0.42          |
| (1,2163) | 1:78:A:TYR:HA    | 1:78:A:TYR:HD2   | 13       | 0.42          |
| (1,2146) | 1:104:A:GLU:HB3  | 1:93:A:THR:HG23  | 4        | 0.42          |
| (1,2099) | 1:21:A:LEU:HB2   | 1:21:A:LEU:HD22  | 15       | 0.42          |
| (1,2099) | 1:21:A:LEU:HB2   | 1:21:A:LEU:HD21  | 16       | 0.42          |
| (1,2006) | 1:78:A:TYR:HE1   | 1:48:A:LEU:HD13  | 15       | 0.42          |
| (1,2006) | 1:78:A:TYR:HE1   | 1:48:A:LEU:HD12  | 16       | 0.42          |
| (1,2003) | 1:48:A:LEU:HB3   | 1:48:A:LEU:HD11  | 3        | 0.42          |
| (1,2003) | 1:48:A:LEU:HB3   | 1:48:A:LEU:HD13  | 8        | 0.42          |
| (1,2003) | 1:48:A:LEU:HB3   | 1:48:A:LEU:HD13  | 9        | 0.42          |
| (1,1881) | 1:113:A:ALA:HB2  | 1:88:A:VAL:HA    | 3        | 0.42          |
| (1,1881) | 1:113:A:ALA:HB3  | 1:88:A:VAL:HA    | 5        | 0.42          |
| (1,1874) | 1:70:A:GLN:HE21  | 1:27:A:VAL:HG13  | 2        | 0.42          |
| (1,1874) | 1:70:A:GLN:HE21  | 1:27:A:VAL:HG12  | 8        | 0.42          |
| (1,1866) | 1:83:A:ARG:HD3   | 1:45:A:ALA:HB3   | 12       | 0.42          |
| (1,1853) | 1:86:A:TYR:HE1   | 1:85:A:LEU:HD11  | 14       | 0.42          |
| (1,1790) | 1:90:A:PRO:HA    | 1:92:A:ALA:HB2   | 4        | 0.42          |
| (1,1790) | 1:90:A:PRO:HA    | 1:92:A:ALA:HB2   | 5        | 0.42          |
| (1,1702) | 1:116:A:GLN:HG3  | 1:116:A:GLN:HE21 | 14       | 0.42          |
| (1,1686) | 1:85:A:LEU:HD11  | 1:85:A:LEU:HD23  | 8        | 0.42          |
| (1,1684) | 1:48:A:LEU:HD12  | 1:50:A:ILE:HA    | 9        | 0.42          |
| (1,1682) | 1:41:A:ALA:HB2   | 1:33:A:GLU:H     | 14       | 0.42          |
| (1,1679) | 1:92:A:ALA:HB2   | 1:91:A:GLY:H     | 10       | 0.42          |
| (1,1679) | 1:92:A:ALA:HB2   | 1:91:A:GLY:H     | 15       | 0.42          |
| (1,1512) | 1:52:A:ILE:HG23  | 1:53:A:PHE:HB2   | 7        | 0.42          |
| (1,1512) | 1:52:A:ILE:HG23  | 1:53:A:PHE:HB2   | 11       | 0.42          |
| (1,1490) | 1:78:A:TYR:HH    | 1:45:A:ALA:HB3   | 5        | 0.42          |
| (1,1405) | 1:102:A:CYS:H    | 1:95:A:VAL:HG12  | 8        | 0.42          |
| (1,1400) | 1:95:A:VAL:HG23  | 1:99:A:GLY:H     | 1        | 0.42          |
| (1,1398) | 1:88:A:VAL:HG21  | 1:85:A:LEU:H     | 3        | 0.42          |
| (1,1361) | 1:41:A:ALA:HA    | 1:32:A:ALA:HB3   | 15       | 0.42          |
| (1,1343) | 1:78:A:TYR:HE1   | 1:48:A:LEU:HD13  | 2        | 0.42          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1305) | 1:97:A:LEU:HD23  | 1:52:A:ILE:HB    | 12       | 0.42          |
| (1,1076) | 1:30:A:PHE:HD1   | 1:31:A:LEU:HD12  | 1        | 0.42          |
| (1,1076) | 1:30:A:PHE:HD2   | 1:31:A:LEU:HD11  | 4        | 0.42          |
| (1,1076) | 1:30:A:PHE:HD2   | 1:31:A:LEU:HD11  | 6        | 0.42          |
| (1,1075) | 1:31:A:LEU:HD12  | 1:31:A:LEU:HA    | 13       | 0.42          |
| (1,1073) | 1:97:A:LEU:HD13  | 1:97:A:LEU:H     | 8        | 0.42          |
| (1,1043) | 1:78:A:TYR:HE1   | 1:28:A:ILE:HD11  | 3        | 0.42          |
| (1,942)  | 1:93:A:THR:HB    | 1:95:A:VAL:HG12  | 8        | 0.42          |
| (1,942)  | 1:93:A:THR:HB    | 1:95:A:VAL:HG13  | 10       | 0.42          |
| (1,942)  | 1:93:A:THR:HB    | 1:95:A:VAL:HG11  | 13       | 0.42          |
| (1,942)  | 1:93:A:THR:HB    | 1:95:A:VAL:HG13  | 14       | 0.42          |
| (1,942)  | 1:93:A:THR:HB    | 1:95:A:VAL:HG12  | 17       | 0.42          |
| (1,822)  | 1:49:A:LYS:H     | 1:52:A:ILE:HD11  | 16       | 0.42          |
| (1,697)  | 1:57:A:VAL:HG13  | 1:56:A:LEU:H     | 8        | 0.42          |
| (1,697)  | 1:57:A:VAL:HG11  | 1:56:A:LEU:H     | 17       | 0.42          |
| (1,618)  | 1:95:A:VAL:H     | 1:48:A:LEU:HD12  | 2        | 0.42          |
| (1,618)  | 1:95:A:VAL:H     | 1:48:A:LEU:HD13  | 4        | 0.42          |
| (1,618)  | 1:95:A:VAL:H     | 1:48:A:LEU:HD12  | 17       | 0.42          |
| (1,604)  | 1:32:A:ALA:HB3   | 1:41:A:ALA:H     | 8        | 0.42          |
| (1,442)  | 1:41:A:ALA:HB2   | 1:41:A:ALA:H     | 8        | 0.42          |
| (1,263)  | 1:110:A:VAL:HG22 | 1:91:A:GLY:H     | 4        | 0.42          |
| (1,228)  | 1:95:A:VAL:HG21  | 1:100:A:ASN:H    | 14       | 0.42          |
| (1,217)  | 1:93:A:THR:HG22  | 1:103:A:GLY:H    | 10       | 0.42          |
| (1,126)  | 1:28:A:ILE:H     | 1:29:A:ALA:HB2   | 10       | 0.42          |
| (1,32)   | 1:53:A:PHE:H     | 1:53:A:PHE:HD2   | 3        | 0.42          |
| (1,32)   | 1:53:A:PHE:H     | 1:53:A:PHE:HD1   | 14       | 0.42          |
| (3,147)  | 1:71:A:LEU:H     | 1:66:A:LEU:HD23  | 6        | 0.41          |
| (3,147)  | 1:71:A:LEU:H     | 1:66:A:LEU:HD21  | 17       | 0.41          |
| (3,139)  | 1:66:A:LEU:HD21  | 1:70:A:GLN:H     | 17       | 0.41          |
| (3,124)  | 1:88:A:VAL:HG23  | 1:88:A:VAL:H     | 10       | 0.41          |
| (3,119)  | 1:98:A:ASP:HB3   | 1:99:A:GLY:HA2   | 5        | 0.41          |
| (3,99)   | 1:72:A:ARG:HG3   | 1:75:A:LEU:HD13  | 7        | 0.41          |
| (3,87)   | 1:117:A:LEU:HD11 | 1:121:A:LYS:H    | 1        | 0.41          |
| (3,87)   | 1:117:A:LEU:HD12 | 1:121:A:LYS:H    | 6        | 0.41          |
| (3,84)   | 1:84:A:TYR:HE1   | 1:84:A:TYR:HA    | 6        | 0.41          |
| (3,84)   | 1:84:A:TYR:HE1   | 1:84:A:TYR:HA    | 9        | 0.41          |
| (3,84)   | 1:84:A:TYR:HE1   | 1:84:A:TYR:HA    | 11       | 0.41          |
| (3,50)   | 1:31:A:LEU:HD21  | 1:97:A:LEU:HD21  | 1        | 0.41          |
| (1,4300) | 1:92:A:ALA:H     | 1:105:A:LEU:HD21 | 1        | 0.41          |
| (1,4176) | 1:97:A:LEU:HD11  | 1:97:A:LEU:H     | 15       | 0.41          |
| (1,4138) | 1:31:A:LEU:H     | 1:28:A:ILE:HD11  | 14       | 0.41          |
| (1,4138) | 1:31:A:LEU:H     | 1:28:A:ILE:HD12  | 15       | 0.41          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,4112) | 1:54:A:GLN:HE22  | 1:57:A:VAL:H     | 9        | 0.41          |
| (1,4112) | 1:54:A:GLN:HE22  | 1:57:A:VAL:H     | 11       | 0.41          |
| (1,4087) | 1:65:A:ASN:HB2   | 1:65:A:ASN:HD21  | 1        | 0.41          |
| (1,4087) | 1:65:A:ASN:HB2   | 1:65:A:ASN:HD21  | 5        | 0.41          |
| (1,4087) | 1:65:A:ASN:HB2   | 1:65:A:ASN:HD21  | 14       | 0.41          |
| (1,4087) | 1:65:A:ASN:HB2   | 1:65:A:ASN:HD21  | 15       | 0.41          |
| (1,4007) | 1:41:A:ALA:HB1   | 1:41:A:ALA:H     | 15       | 0.41          |
| (1,3972) | 1:53:A:PHE:H     | 1:56:A:LEU:HB3   | 4        | 0.41          |
| (1,3972) | 1:53:A:PHE:H     | 1:56:A:LEU:HB3   | 7        | 0.41          |
| (1,3923) | 1:71:A:LEU:HD13  | 1:72:A:ARG:H     | 6        | 0.41          |
| (1,3923) | 1:71:A:LEU:HD11  | 1:72:A:ARG:H     | 12       | 0.41          |
| (1,3861) | 1:110:A:VAL:HG22 | 1:91:A:GLY:H     | 3        | 0.41          |
| (1,3834) | 1:95:A:VAL:HG21  | 1:100:A:ASN:H    | 5        | 0.41          |
| (1,3834) | 1:95:A:VAL:HG22  | 1:100:A:ASN:H    | 15       | 0.41          |
| (1,3826) | 1:102:A:CYS:H    | 1:95:A:VAL:HG11  | 4        | 0.41          |
| (1,3822) | 1:93:A:THR:HG22  | 1:103:A:GLY:H    | 11       | 0.41          |
| (1,3822) | 1:93:A:THR:HG21  | 1:103:A:GLY:H    | 13       | 0.41          |
| (1,3678) | 1:95:A:VAL:H     | 1:96:A:ASP:H     | 15       | 0.41          |
| (1,3644) | 1:53:A:PHE:H     | 1:53:A:PHE:HD1   | 2        | 0.41          |
| (1,3644) | 1:53:A:PHE:H     | 1:53:A:PHE:HD1   | 8        | 0.41          |
| (1,3612) | 1:120:A:ALA:HB2  | 1:120:A:ALA:HA   | 3        | 0.41          |
| (1,3601) | 1:113:A:ALA:HB2  | 1:111:A:GLU:H    | 6        | 0.41          |
| (1,3601) | 1:113:A:ALA:HB3  | 1:111:A:GLU:H    | 9        | 0.41          |
| (1,3601) | 1:113:A:ALA:HB2  | 1:111:A:GLU:H    | 16       | 0.41          |
| (1,3599) | 1:92:A:ALA:HB1   | 1:113:A:ALA:HB2  | 13       | 0.41          |
| (1,3594) | 1:105:A:LEU:HB2  | 1:110:A:VAL:HG12 | 12       | 0.41          |
| (1,3578) | 1:105:A:LEU:HD13 | 1:109:A:HIS:HA   | 1        | 0.41          |
| (1,3578) | 1:105:A:LEU:HD12 | 1:109:A:HIS:HA   | 8        | 0.41          |
| (1,3578) | 1:105:A:LEU:HD12 | 1:109:A:HIS:HA   | 13       | 0.41          |
| (1,3578) | 1:105:A:LEU:HD11 | 1:109:A:HIS:HA   | 17       | 0.41          |
| (1,3570) | 1:90:A:PRO:HA    | 1:105:A:LEU:HD12 | 17       | 0.41          |
| (1,3554) | 1:66:A:LEU:HB2   | 1:66:A:LEU:HD21  | 14       | 0.41          |
| (1,3482) | 1:71:A:LEU:HB2   | 1:31:A:LEU:HD11  | 4        | 0.41          |
| (1,3482) | 1:71:A:LEU:HB2   | 1:31:A:LEU:HD12  | 5        | 0.41          |
| (1,3482) | 1:71:A:LEU:HB2   | 1:31:A:LEU:HD12  | 9        | 0.41          |
| (1,3482) | 1:71:A:LEU:HB2   | 1:31:A:LEU:HD12  | 11       | 0.41          |
| (1,3482) | 1:71:A:LEU:HB2   | 1:31:A:LEU:HD11  | 13       | 0.41          |
| (1,3464) | 1:86:A:TYR:HE1   | 1:85:A:LEU:HD13  | 10       | 0.41          |
| (1,3464) | 1:86:A:TYR:HE1   | 1:85:A:LEU:HD11  | 15       | 0.41          |
| (1,3463) | 1:35:A:PHE:HE1   | 1:38:A:CYS:HB2   | 12       | 0.41          |
| (1,3463) | 1:35:A:PHE:HE2   | 1:38:A:CYS:HB2   | 17       | 0.41          |
| (1,3418) | 1:117:A:LEU:HB2  | 1:117:A:LEU:HD13 | 2        | 0.41          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3418) | 1:117:A:LEU:HB2 | 1:117:A:LEU:HD13 | 9        | 0.41          |
| (1,3373) | 1:88:A:VAL:HA   | 1:93:A:THR:HG22  | 1        | 0.41          |
| (1,3368) | 1:31:A:LEU:HD12 | 1:31:A:LEU:HA    | 4        | 0.41          |
| (1,3323) | 1:66:A:LEU:HD22 | 1:66:A:LEU:H     | 7        | 0.41          |
| (1,3323) | 1:66:A:LEU:HD23 | 1:66:A:LEU:H     | 12       | 0.41          |
| (1,3323) | 1:66:A:LEU:HD23 | 1:66:A:LEU:H     | 17       | 0.41          |
| (1,3309) | 1:117:A:LEU:HA  | 1:117:A:LEU:HG   | 11       | 0.41          |
| (1,3309) | 1:117:A:LEU:HA  | 1:117:A:LEU:HG   | 15       | 0.41          |
| (1,3286) | 1:116:A:GLN:HG3 | 1:116:A:GLN:HE21 | 1        | 0.41          |
| (1,3266) | 1:85:A:LEU:HD12 | 1:85:A:LEU:HD21  | 10       | 0.41          |
| (1,3266) | 1:85:A:LEU:HD11 | 1:85:A:LEU:HD22  | 14       | 0.41          |
| (1,3266) | 1:85:A:LEU:HD11 | 1:85:A:LEU:HD21  | 16       | 0.41          |
| (1,3231) | 1:27:A:VAL:HG22 | 1:27:A:VAL:HA    | 1        | 0.41          |
| (1,3231) | 1:27:A:VAL:HG23 | 1:27:A:VAL:HA    | 2        | 0.41          |
| (1,3231) | 1:27:A:VAL:HG23 | 1:27:A:VAL:HA    | 10       | 0.41          |
| (1,3231) | 1:27:A:VAL:HG23 | 1:27:A:VAL:HA    | 15       | 0.41          |
| (1,3199) | 1:113:A:ALA:HB1 | 1:112:A:HIS:HB2  | 14       | 0.41          |
| (1,3196) | 1:64:A:MET:HB2  | 1:64:A:MET:HA    | 1        | 0.41          |
| (1,3196) | 1:64:A:MET:HB2  | 1:64:A:MET:HA    | 5        | 0.41          |
| (1,3196) | 1:64:A:MET:HB2  | 1:64:A:MET:HA    | 8        | 0.41          |
| (1,3196) | 1:64:A:MET:HB2  | 1:64:A:MET:HA    | 15       | 0.41          |
| (1,3103) | 1:56:A:LEU:HD11 | 1:60:A:VAL:HB    | 8        | 0.41          |
| (1,3103) | 1:56:A:LEU:HD11 | 1:60:A:VAL:HB    | 9        | 0.41          |
| (1,3101) | 1:56:A:LEU:HD11 | 1:53:A:PHE:HA    | 13       | 0.41          |
| (1,3101) | 1:56:A:LEU:HD11 | 1:53:A:PHE:HA    | 15       | 0.41          |
| (1,3081) | 1:97:A:LEU:HD11 | 1:55:A:ASP:HA    | 3        | 0.41          |
| (1,3081) | 1:97:A:LEU:HD11 | 1:55:A:ASP:HA    | 4        | 0.41          |
| (1,3078) | 1:54:A:GLN:HB3  | 1:57:A:VAL:HG12  | 8        | 0.41          |
| (1,3078) | 1:54:A:GLN:HB3  | 1:57:A:VAL:HG11  | 13       | 0.41          |
| (1,3077) | 1:54:A:GLN:HB2  | 1:57:A:VAL:HG11  | 16       | 0.41          |
| (1,3070) | 1:55:A:ASP:H    | 1:54:A:GLN:HB2   | 8        | 0.41          |
| (1,3070) | 1:55:A:ASP:H    | 1:54:A:GLN:HB2   | 15       | 0.41          |
| (1,3051) | 1:78:A:TYR:HE1  | 1:28:A:ILE:HG22  | 13       | 0.41          |
| (1,3045) | 1:52:A:ILE:HG13 | 1:54:A:GLN:HE21  | 5        | 0.41          |
| (1,3024) | 1:64:A:MET:HE1  | 1:65:A:ASN:HB3   | 3        | 0.41          |
| (1,3024) | 1:64:A:MET:HE3  | 1:65:A:ASN:HB3   | 11       | 0.41          |
| (1,3022) | 1:64:A:MET:HE1  | 1:30:A:PHE:HA    | 4        | 0.41          |
| (1,3002) | 1:57:A:VAL:HG13 | 1:60:A:VAL:HB    | 5        | 0.41          |
| (1,3002) | 1:57:A:VAL:HG12 | 1:60:A:VAL:HB    | 6        | 0.41          |
| (1,2923) | 1:21:A:LEU:HD22 | 1:30:A:PHE:H     | 4        | 0.41          |
| (1,2923) | 1:21:A:LEU:HD21 | 1:30:A:PHE:H     | 7        | 0.41          |
| (1,2900) | 1:28:A:ILE:HD13 | 1:31:A:LEU:HB3   | 7        | 0.41          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2886) | 1:41:A:ALA:HA    | 1:32:A:ALA:HB1   | 17       | 0.41          |
| (1,2880) | 1:61:A:ALA:HB1   | 1:57:A:VAL:HG11  | 10       | 0.41          |
| (1,2877) | 1:61:A:ALA:HB3   | 1:61:A:ALA:HA    | 2        | 0.41          |
| (1,2877) | 1:61:A:ALA:HB3   | 1:61:A:ALA:HA    | 13       | 0.41          |
| (1,2872) | 1:129:A:ALA:HB2  | 1:129:A:ALA:HA   | 1        | 0.41          |
| (1,2872) | 1:129:A:ALA:HB3  | 1:129:A:ALA:HA   | 5        | 0.41          |
| (1,2854) | 1:85:A:LEU:HD21  | 1:84:A:TYR:HD2   | 12       | 0.41          |
| (1,2841) | 1:110:A:VAL:HG12 | 1:109:A:HIS:H    | 15       | 0.41          |
| (1,2836) | 1:95:A:VAL:HG21  | 1:97:A:LEU:HD21  | 14       | 0.41          |
| (1,2827) | 1:97:A:LEU:HD21  | 1:52:A:ILE:HB    | 8        | 0.41          |
| (1,2785) | 1:50:A:ILE:HG21  | 1:51:A:GLY:HA3   | 7        | 0.41          |
| (1,2785) | 1:50:A:ILE:HG21  | 1:51:A:GLY:HA3   | 15       | 0.41          |
| (1,2678) | 1:53:A:PHE:HB3   | 1:53:A:PHE:HE2   | 1        | 0.41          |
| (1,2678) | 1:53:A:PHE:HB3   | 1:53:A:PHE:HE1   | 7        | 0.41          |
| (1,2678) | 1:53:A:PHE:HB3   | 1:53:A:PHE:HE2   | 8        | 0.41          |
| (1,2678) | 1:53:A:PHE:HB3   | 1:53:A:PHE:HE1   | 12       | 0.41          |
| (1,2678) | 1:53:A:PHE:HB3   | 1:53:A:PHE:HE1   | 13       | 0.41          |
| (1,2678) | 1:53:A:PHE:HB3   | 1:53:A:PHE:HE2   | 15       | 0.41          |
| (1,2664) | 1:97:A:LEU:HD13  | 1:60:A:VAL:HG13  | 14       | 0.41          |
| (1,2614) | 1:30:A:PHE:HD2   | 1:31:A:LEU:HD11  | 3        | 0.41          |
| (1,2614) | 1:30:A:PHE:HD1   | 1:31:A:LEU:HD11  | 7        | 0.41          |
| (1,2614) | 1:30:A:PHE:HD2   | 1:31:A:LEU:HD12  | 11       | 0.41          |
| (1,2614) | 1:30:A:PHE:HD1   | 1:31:A:LEU:HD11  | 14       | 0.41          |
| (1,2577) | 1:60:A:VAL:HG12  | 1:59:A:ARG:HA    | 1        | 0.41          |
| (1,2568) | 1:78:A:TYR:HE2   | 1:28:A:ILE:HD12  | 13       | 0.41          |
| (1,2568) | 1:78:A:TYR:HE1   | 1:28:A:ILE:HD13  | 15       | 0.41          |
| (1,2423) | 1:64:A:MET:HA    | 1:64:A:MET:HE2   | 12       | 0.41          |
| (1,2405) | 1:29:A:ALA:H     | 1:28:A:ILE:HD12  | 2        | 0.41          |
| (1,2405) | 1:29:A:ALA:H     | 1:28:A:ILE:HD12  | 9        | 0.41          |
| (1,2405) | 1:29:A:ALA:H     | 1:28:A:ILE:HD12  | 11       | 0.41          |
| (1,2405) | 1:29:A:ALA:H     | 1:28:A:ILE:HD11  | 13       | 0.41          |
| (1,2405) | 1:29:A:ALA:H     | 1:28:A:ILE:HD13  | 16       | 0.41          |
| (1,2405) | 1:29:A:ALA:H     | 1:28:A:ILE:HD11  | 17       | 0.41          |
| (1,2370) | 1:50:A:ILE:HG13  | 1:50:A:ILE:HG23  | 9        | 0.41          |
| (1,2370) | 1:50:A:ILE:HG13  | 1:50:A:ILE:HG23  | 11       | 0.41          |
| (1,2370) | 1:50:A:ILE:HG13  | 1:50:A:ILE:HG23  | 15       | 0.41          |
| (1,2367) | 1:52:A:ILE:H     | 1:52:A:ILE:HD13  | 9        | 0.41          |
| (1,2271) | 1:113:A:ALA:HB1  | 1:112:A:HIS:HD2  | 3        | 0.41          |
| (1,2256) | 1:101:A:PRO:HB2  | 1:105:A:LEU:HD22 | 5        | 0.41          |
| (1,2256) | 1:101:A:PRO:HB2  | 1:105:A:LEU:HD23 | 11       | 0.41          |
| (1,2230) | 1:28:A:ILE:H     | 1:28:A:ILE:HG23  | 10       | 0.41          |
| (1,2212) | 1:110:A:VAL:HG22 | 1:114:A:ARG:H    | 8        | 0.41          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2212) | 1:110:A:VAL:HG21 | 1:114:A:ARG:H   | 10       | 0.41          |
| (1,2212) | 1:110:A:VAL:HG23 | 1:114:A:ARG:H   | 17       | 0.41          |
| (1,2201) | 1:64:A:MET:HB2   | 1:21:A:LEU:HD23 | 16       | 0.41          |
| (1,2172) | 1:34:A:ARG:HD3   | 1:60:A:VAL:HG11 | 6        | 0.41          |
| (1,2172) | 1:34:A:ARG:HD3   | 1:60:A:VAL:HG11 | 15       | 0.41          |
| (1,2163) | 1:78:A:TYR:HA    | 1:78:A:TYR:HD1  | 3        | 0.41          |
| (1,2163) | 1:78:A:TYR:HA    | 1:78:A:TYR:HD1  | 14       | 0.41          |
| (1,2099) | 1:21:A:LEU:HB2   | 1:21:A:LEU:HD22 | 8        | 0.41          |
| (1,1955) | 1:92:A:ALA:HB2   | 1:113:A:ALA:HB2 | 8        | 0.41          |
| (1,1881) | 1:113:A:ALA:HB3  | 1:88:A:VAL:HA   | 2        | 0.41          |
| (1,1874) | 1:70:A:GLN:HE21  | 1:27:A:VAL:HG12 | 16       | 0.41          |
| (1,1866) | 1:83:A:ARG:HD3   | 1:45:A:ALA:HB1  | 1        | 0.41          |
| (1,1866) | 1:83:A:ARG:HD3   | 1:45:A:ALA:HB1  | 4        | 0.41          |
| (1,1866) | 1:83:A:ARG:HD3   | 1:45:A:ALA:HB2  | 8        | 0.41          |
| (1,1735) | 1:66:A:LEU:HD23  | 1:67:A:SER:H    | 9        | 0.41          |
| (1,1684) | 1:48:A:LEU:HD13  | 1:50:A:ILE:HA   | 1        | 0.41          |
| (1,1682) | 1:41:A:ALA:HB2   | 1:33:A:GLU:H    | 17       | 0.41          |
| (1,1675) | 1:88:A:VAL:HG21  | 1:92:A:ALA:HB2  | 1        | 0.41          |
| (1,1656) | 1:31:A:LEU:HB2   | 1:39:A:PHE:HE1  | 12       | 0.41          |
| (1,1516) | 1:31:A:LEU:HD13  | 1:28:A:ILE:HG22 | 3        | 0.41          |
| (1,1516) | 1:31:A:LEU:HD13  | 1:28:A:ILE:HG22 | 6        | 0.41          |
| (1,1516) | 1:31:A:LEU:HD11  | 1:28:A:ILE:HG21 | 11       | 0.41          |
| (1,1490) | 1:78:A:TYR:HH    | 1:45:A:ALA:HB3  | 11       | 0.41          |
| (1,1484) | 1:57:A:VAL:HA    | 1:71:A:LEU:HD12 | 10       | 0.41          |
| (1,1481) | 1:64:A:MET:HE1   | 1:30:A:PHE:HA   | 10       | 0.41          |
| (1,1481) | 1:64:A:MET:HE3   | 1:30:A:PHE:HA   | 13       | 0.41          |
| (1,1481) | 1:64:A:MET:HE1   | 1:30:A:PHE:HA   | 17       | 0.41          |
| (1,1450) | 1:54:A:GLN:HE22  | 1:54:A:GLN:HG2  | 10       | 0.41          |
| (1,1450) | 1:54:A:GLN:HE22  | 1:54:A:GLN:HG2  | 12       | 0.41          |
| (1,1400) | 1:95:A:VAL:HG22  | 1:99:A:GLY:H    | 6        | 0.41          |
| (1,1398) | 1:88:A:VAL:HG23  | 1:85:A:LEU:H    | 17       | 0.41          |
| (1,1331) | 1:78:A:TYR:HE1   | 1:84:A:TYR:HD1  | 4        | 0.41          |
| (1,1322) | 1:28:A:ILE:H     | 1:27:A:VAL:HG13 | 6        | 0.41          |
| (1,1308) | 1:97:A:LEU:HD21  | 1:35:A:PHE:HD2  | 1        | 0.41          |
| (1,1301) | 1:97:A:LEU:HD11  | 1:97:A:LEU:HA   | 1        | 0.41          |
| (1,1273) | 1:45:A:ALA:HB3   | 1:84:A:TYR:HB3  | 11       | 0.41          |
| (1,1076) | 1:30:A:PHE:HD2   | 1:31:A:LEU:HD12 | 9        | 0.41          |
| (1,1043) | 1:78:A:TYR:HE1   | 1:28:A:ILE:HD13 | 2        | 0.41          |
| (1,1043) | 1:78:A:TYR:HE1   | 1:28:A:ILE:HD11 | 16       | 0.41          |
| (1,825)  | 1:45:A:ALA:HB2   | 1:78:A:TYR:HB3  | 11       | 0.41          |
| (1,825)  | 1:45:A:ALA:HB1   | 1:78:A:TYR:HB3  | 12       | 0.41          |
| (1,789)  | 1:50:A:ILE:HG13  | 1:50:A:ILE:HG21 | 14       | 0.41          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,618)  | 1:95:A:VAL:H    | 1:48:A:LEU:HD11  | 8        | 0.41          |
| (1,604)  | 1:32:A:ALA:HB3  | 1:41:A:ALA:H     | 11       | 0.41          |
| (1,575)  | 1:31:A:LEU:H    | 1:28:A:ILE:HD12  | 2        | 0.41          |
| (1,570)  | 1:60:A:VAL:HG11 | 1:34:A:ARG:HE    | 5        | 0.41          |
| (1,564)  | 1:59:A:ARG:HE   | 1:97:A:LEU:HD11  | 16       | 0.41          |
| (1,549)  | 1:97:A:LEU:HD11 | 1:98:A:ASP:H     | 5        | 0.41          |
| (1,528)  | 1:65:A:ASN:HB2  | 1:65:A:ASN:HD21  | 6        | 0.41          |
| (1,442)  | 1:41:A:ALA:HB2  | 1:41:A:ALA:H     | 11       | 0.41          |
| (1,410)  | 1:53:A:PHE:H    | 1:56:A:LEU:HB3   | 3        | 0.41          |
| (1,410)  | 1:53:A:PHE:H    | 1:56:A:LEU:HB3   | 11       | 0.41          |
| (1,228)  | 1:95:A:VAL:HG22 | 1:100:A:ASN:H    | 3        | 0.41          |
| (1,217)  | 1:93:A:THR:HG22 | 1:103:A:GLY:H    | 3        | 0.41          |
| (1,217)  | 1:93:A:THR:HG21 | 1:103:A:GLY:H    | 7        | 0.41          |
| (1,126)  | 1:28:A:ILE:H    | 1:29:A:ALA:HB3   | 12       | 0.41          |
| (1,56)   | 1:84:A:TYR:H    | 1:84:A:TYR:HD1   | 17       | 0.41          |
| (1,32)   | 1:53:A:PHE:H    | 1:53:A:PHE:HD2   | 10       | 0.41          |
| (3,152)  | 1:27:A:VAL:H    | 1:74:A:ALA:HB3   | 4        | 0.4           |
| (3,152)  | 1:27:A:VAL:H    | 1:74:A:ALA:HB1   | 5        | 0.4           |
| (3,148)  | 1:22:A:ASN:H    | 1:22:A:ASN:HB2   | 15       | 0.4           |
| (3,139)  | 1:66:A:LEU:HD23 | 1:70:A:GLN:H     | 13       | 0.4           |
| (3,135)  | 1:123:A:ARG:HB3 | 1:120:A:ALA:HA   | 14       | 0.4           |
| (3,124)  | 1:88:A:VAL:HG22 | 1:88:A:VAL:H     | 3        | 0.4           |
| (3,124)  | 1:88:A:VAL:HG21 | 1:88:A:VAL:H     | 17       | 0.4           |
| (3,123)  | 1:50:A:ILE:HD13 | 1:79:A:THR:HA    | 3        | 0.4           |
| (3,123)  | 1:50:A:ILE:HD11 | 1:79:A:THR:HA    | 12       | 0.4           |
| (3,106)  | 1:68:A:LYS:HD2  | 1:68:A:LYS:HA    | 5        | 0.4           |
| (3,69)   | 1:57:A:VAL:HA   | 1:71:A:LEU:HB2   | 7        | 0.4           |
| (3,64)   | 1:55:A:ASP:HB2  | 1:52:A:ILE:HG23  | 4        | 0.4           |
| (3,50)   | 1:31:A:LEU:HD23 | 1:97:A:LEU:HD22  | 2        | 0.4           |
| (3,50)   | 1:31:A:LEU:HD23 | 1:97:A:LEU:HD21  | 11       | 0.4           |
| (3,36)   | 1:49:A:LYS:HB2  | 1:52:A:ILE:HD11  | 9        | 0.4           |
| (3,22)   | 1:48:A:LEU:H    | 1:48:A:LEU:HD11  | 7        | 0.4           |
| (1,4342) | 1:38:A:CYS:H    | 1:95:A:VAL:HG11  | 3        | 0.4           |
| (1,4300) | 1:92:A:ALA:H    | 1:105:A:LEU:HD23 | 6        | 0.4           |
| (1,4300) | 1:92:A:ALA:H    | 1:105:A:LEU:HD21 | 16       | 0.4           |
| (1,4197) | 1:66:A:LEU:HD22 | 1:67:A:SER:H     | 13       | 0.4           |
| (1,4176) | 1:97:A:LEU:HD12 | 1:97:A:LEU:H     | 6        | 0.4           |
| (1,4138) | 1:31:A:LEU:H    | 1:28:A:ILE:HD13  | 4        | 0.4           |
| (1,4138) | 1:31:A:LEU:H    | 1:28:A:ILE:HD12  | 9        | 0.4           |
| (1,4138) | 1:31:A:LEU:H    | 1:28:A:ILE:HD13  | 16       | 0.4           |
| (1,4132) | 1:60:A:VAL:HG11 | 1:34:A:ARG:HE    | 14       | 0.4           |
| (1,4126) | 1:59:A:ARG:HE   | 1:97:A:LEU:HD11  | 14       | 0.4           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,4119) | 1:66:A:LEU:HB2   | 1:70:A:GLN:HE22  | 5        | 0.4           |
| (1,3923) | 1:71:A:LEU:HD13  | 1:72:A:ARG:H     | 1        | 0.4           |
| (1,3834) | 1:95:A:VAL:HG22  | 1:100:A:ASN:H    | 10       | 0.4           |
| (1,3733) | 1:27:A:VAL:HG12  | 1:26:A:GLU:H     | 10       | 0.4           |
| (1,3644) | 1:53:A:PHE:H     | 1:53:A:PHE:HD1   | 15       | 0.4           |
| (1,3612) | 1:120:A:ALA:HB2  | 1:120:A:ALA:HA   | 7        | 0.4           |
| (1,3612) | 1:120:A:ALA:HB2  | 1:120:A:ALA:HA   | 11       | 0.4           |
| (1,3610) | 1:121:A:LYS:HG3  | 1:117:A:LEU:HD12 | 8        | 0.4           |
| (1,3606) | 1:117:A:LEU:HA   | 1:82:A:TRP:HZ2   | 11       | 0.4           |
| (1,3578) | 1:105:A:LEU:HD11 | 1:109:A:HIS:HA   | 3        | 0.4           |
| (1,3578) | 1:105:A:LEU:HD11 | 1:109:A:HIS:HA   | 4        | 0.4           |
| (1,3578) | 1:105:A:LEU:HD12 | 1:109:A:HIS:HA   | 9        | 0.4           |
| (1,3578) | 1:105:A:LEU:HD13 | 1:109:A:HIS:HA   | 10       | 0.4           |
| (1,3578) | 1:105:A:LEU:HD12 | 1:109:A:HIS:HA   | 16       | 0.4           |
| (1,3570) | 1:90:A:PRO:HA    | 1:105:A:LEU:HD11 | 2        | 0.4           |
| (1,3570) | 1:90:A:PRO:HA    | 1:105:A:LEU:HD13 | 9        | 0.4           |
| (1,3570) | 1:90:A:PRO:HA    | 1:105:A:LEU:HD11 | 12       | 0.4           |
| (1,3498) | 1:70:A:GLN:HE21  | 1:27:A:VAL:HG13  | 14       | 0.4           |
| (1,3482) | 1:71:A:LEU:HB2   | 1:31:A:LEU:HD11  | 7        | 0.4           |
| (1,3482) | 1:71:A:LEU:HB2   | 1:31:A:LEU:HD13  | 8        | 0.4           |
| (1,3464) | 1:86:A:TYR:HE1   | 1:85:A:LEU:HD12  | 8        | 0.4           |
| (1,3464) | 1:86:A:TYR:HE2   | 1:85:A:LEU:HD11  | 16       | 0.4           |
| (1,3463) | 1:35:A:PHE:HE2   | 1:38:A:CYS:HB2   | 14       | 0.4           |
| (1,3452) | 1:95:A:VAL:HA    | 1:93:A:THR:HG21  | 1        | 0.4           |
| (1,3452) | 1:95:A:VAL:HA    | 1:93:A:THR:HG22  | 2        | 0.4           |
| (1,3323) | 1:66:A:LEU:HD22  | 1:66:A:LEU:H     | 15       | 0.4           |
| (1,3319) | 1:66:A:LEU:HD21  | 1:27:A:VAL:HG13  | 10       | 0.4           |
| (1,3309) | 1:117:A:LEU:HA   | 1:117:A:LEU:HG   | 2        | 0.4           |
| (1,3309) | 1:117:A:LEU:HA   | 1:117:A:LEU:HG   | 3        | 0.4           |
| (1,3309) | 1:117:A:LEU:HA   | 1:117:A:LEU:HG   | 9        | 0.4           |
| (1,3309) | 1:117:A:LEU:HA   | 1:117:A:LEU:HG   | 12       | 0.4           |
| (1,3286) | 1:116:A:GLN:HG3  | 1:116:A:GLN:HE21 | 4        | 0.4           |
| (1,3286) | 1:116:A:GLN:HG3  | 1:116:A:GLN:HE21 | 5        | 0.4           |
| (1,3286) | 1:116:A:GLN:HG3  | 1:116:A:GLN:HE21 | 9        | 0.4           |
| (1,3286) | 1:116:A:GLN:HG3  | 1:116:A:GLN:HE21 | 10       | 0.4           |
| (1,3286) | 1:116:A:GLN:HG3  | 1:116:A:GLN:HE21 | 13       | 0.4           |
| (1,3286) | 1:116:A:GLN:HG3  | 1:116:A:GLN:HE21 | 16       | 0.4           |
| (1,3282) | 1:44:A:GLU:HG2   | 1:45:A:ALA:HB1   | 12       | 0.4           |
| (1,3266) | 1:85:A:LEU:HD11  | 1:85:A:LEU:HD23  | 8        | 0.4           |
| (1,3258) | 1:48:A:LEU:HD12  | 1:50:A:ILE:HA    | 16       | 0.4           |
| (1,3256) | 1:41:A:ALA:HB3   | 1:33:A:GLU:H     | 12       | 0.4           |
| (1,3199) | 1:113:A:ALA:HB3  | 1:112:A:HIS:HB2  | 9        | 0.4           |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3196) | 1:64:A:MET:HB2  | 1:64:A:MET:HA    | 6        | 0.4           |
| (1,3161) | 1:82:A:TRP:HH2  | 1:120:A:ALA:HB3  | 7        | 0.4           |
| (1,3101) | 1:56:A:LEU:HD13 | 1:53:A:PHE:HA    | 1        | 0.4           |
| (1,3101) | 1:56:A:LEU:HD13 | 1:53:A:PHE:HA    | 3        | 0.4           |
| (1,3101) | 1:56:A:LEU:HD13 | 1:53:A:PHE:HA    | 9        | 0.4           |
| (1,3101) | 1:56:A:LEU:HD13 | 1:53:A:PHE:HA    | 11       | 0.4           |
| (1,3077) | 1:54:A:GLN:HB2  | 1:57:A:VAL:HG11  | 2        | 0.4           |
| (1,3077) | 1:54:A:GLN:HB2  | 1:57:A:VAL:HG11  | 9        | 0.4           |
| (1,3070) | 1:55:A:ASP:H    | 1:54:A:GLN:HB2   | 10       | 0.4           |
| (1,3070) | 1:55:A:ASP:H    | 1:54:A:GLN:HB2   | 11       | 0.4           |
| (1,3070) | 1:55:A:ASP:H    | 1:54:A:GLN:HB2   | 12       | 0.4           |
| (1,3067) | 1:52:A:ILE:HG23 | 1:53:A:PHE:HB3   | 11       | 0.4           |
| (1,3067) | 1:52:A:ILE:HG22 | 1:53:A:PHE:HB3   | 16       | 0.4           |
| (1,3061) | 1:31:A:LEU:HD13 | 1:28:A:ILE:HG23  | 12       | 0.4           |
| (1,3051) | 1:78:A:TYR:HE2  | 1:28:A:ILE:HG22  | 10       | 0.4           |
| (1,3051) | 1:78:A:TYR:HE2  | 1:28:A:ILE:HG22  | 17       | 0.4           |
| (1,3024) | 1:64:A:MET:HE2  | 1:65:A:ASN:HB3   | 10       | 0.4           |
| (1,3023) | 1:64:A:MET:HE3  | 1:27:A:VAL:HA    | 16       | 0.4           |
| (1,3022) | 1:64:A:MET:HE1  | 1:30:A:PHE:HA    | 5        | 0.4           |
| (1,3021) | 1:64:A:MET:HE2  | 1:63:A:GLU:H     | 15       | 0.4           |
| (1,3002) | 1:57:A:VAL:HG12 | 1:60:A:VAL:HB    | 16       | 0.4           |
| (1,2940) | 1:99:A:GLY:HA3  | 1:95:A:VAL:HG12  | 13       | 0.4           |
| (1,2931) | 1:88:A:VAL:HG21 | 1:85:A:LEU:H     | 16       | 0.4           |
| (1,2923) | 1:21:A:LEU:HD22 | 1:30:A:PHE:H     | 9        | 0.4           |
| (1,2890) | 1:33:A:GLU:HB3  | 1:32:A:ALA:HB3   | 3        | 0.4           |
| (1,2877) | 1:61:A:ALA:HB2  | 1:61:A:ALA:HA    | 6        | 0.4           |
| (1,2873) | 1:126:A:ALA:HA  | 1:126:A:ALA:HB3  | 6        | 0.4           |
| (1,2872) | 1:129:A:ALA:HB1 | 1:129:A:ALA:HA   | 15       | 0.4           |
| (1,2872) | 1:129:A:ALA:HB3 | 1:129:A:ALA:HA   | 16       | 0.4           |
| (1,2865) | 1:78:A:TYR:HE1  | 1:48:A:LEU:HD11  | 11       | 0.4           |
| (1,2865) | 1:78:A:TYR:HE1  | 1:48:A:LEU:HD13  | 17       | 0.4           |
| (1,2851) | 1:50:A:ILE:HG23 | 1:50:A:ILE:HA    | 15       | 0.4           |
| (1,2851) | 1:50:A:ILE:HG22 | 1:50:A:ILE:HA    | 16       | 0.4           |
| (1,2831) | 1:97:A:LEU:HD22 | 1:35:A:PHE:HD2   | 7        | 0.4           |
| (1,2827) | 1:97:A:LEU:HD21 | 1:52:A:ILE:HB    | 13       | 0.4           |
| (1,2827) | 1:97:A:LEU:HD23 | 1:52:A:ILE:HB    | 15       | 0.4           |
| (1,2827) | 1:97:A:LEU:HD23 | 1:52:A:ILE:HB    | 17       | 0.4           |
| (1,2817) | 1:97:A:LEU:HD11 | 1:97:A:LEU:HA    | 14       | 0.4           |
| (1,2785) | 1:50:A:ILE:HG22 | 1:51:A:GLY:HA3   | 2        | 0.4           |
| (1,2753) | 1:97:A:LEU:HD13 | 1:59:A:ARG:HD3   | 2        | 0.4           |
| (1,2753) | 1:97:A:LEU:HD13 | 1:59:A:ARG:HD3   | 7        | 0.4           |
| (1,2720) | 1:86:A:TYR:HB3  | 1:117:A:LEU:HD11 | 8        | 0.4           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2720) | 1:86:A:TYR:HB3   | 1:117:A:LEU:HD11 | 13       | 0.4           |
| (1,2678) | 1:53:A:PHE:HB3   | 1:53:A:PHE:HE1   | 3        | 0.4           |
| (1,2616) | 1:21:A:LEU:HA    | 1:21:A:LEU:HD22  | 7        | 0.4           |
| (1,2614) | 1:30:A:PHE:HD2   | 1:31:A:LEU:HD12  | 2        | 0.4           |
| (1,2614) | 1:30:A:PHE:HD2   | 1:31:A:LEU:HD13  | 8        | 0.4           |
| (1,2614) | 1:30:A:PHE:HD2   | 1:31:A:LEU:HD12  | 10       | 0.4           |
| (1,2597) | 1:21:A:LEU:HD22  | 1:27:A:VAL:HG12  | 7        | 0.4           |
| (1,2569) | 1:82:A:TRP:HZ2   | 1:124:A:VAL:HG21 | 2        | 0.4           |
| (1,2568) | 1:78:A:TYR:HE2   | 1:28:A:ILE:HD13  | 9        | 0.4           |
| (1,2542) | 1:21:A:LEU:HD13  | 1:30:A:PHE:HA    | 10       | 0.4           |
| (1,2542) | 1:21:A:LEU:HD11  | 1:30:A:PHE:HA    | 14       | 0.4           |
| (1,2423) | 1:64:A:MET:HA    | 1:64:A:MET:HE2   | 2        | 0.4           |
| (1,2412) | 1:45:A:ALA:HB2   | 1:78:A:TYR:HB3   | 4        | 0.4           |
| (1,2412) | 1:45:A:ALA:HB3   | 1:78:A:TYR:HB3   | 8        | 0.4           |
| (1,2408) | 1:52:A:ILE:HD12  | 1:96:A:ASP:HA    | 12       | 0.4           |
| (1,2405) | 1:29:A:ALA:H     | 1:28:A:ILE:HD12  | 15       | 0.4           |
| (1,2397) | 1:50:A:ILE:HD13  | 1:50:A:ILE:HA    | 8        | 0.4           |
| (1,2370) | 1:50:A:ILE:HG13  | 1:50:A:ILE:HG23  | 6        | 0.4           |
| (1,2370) | 1:50:A:ILE:HG13  | 1:50:A:ILE:HG22  | 16       | 0.4           |
| (1,2369) | 1:52:A:ILE:HD11  | 1:56:A:LEU:H     | 5        | 0.4           |
| (1,2369) | 1:52:A:ILE:HD11  | 1:56:A:LEU:H     | 6        | 0.4           |
| (1,2271) | 1:113:A:ALA:HB2  | 1:112:A:HIS:HD2  | 16       | 0.4           |
| (1,2268) | 1:110:A:VAL:HG13 | 1:89:A:LYS:H     | 15       | 0.4           |
| (1,2256) | 1:101:A:PRO:HB2  | 1:105:A:LEU:HD21 | 4        | 0.4           |
| (1,2256) | 1:101:A:PRO:HB2  | 1:105:A:LEU:HD23 | 8        | 0.4           |
| (1,2256) | 1:101:A:PRO:HB2  | 1:105:A:LEU:HD22 | 14       | 0.4           |
| (1,2256) | 1:101:A:PRO:HB2  | 1:105:A:LEU:HD21 | 16       | 0.4           |
| (1,2230) | 1:28:A:ILE:H     | 1:28:A:ILE:HG23  | 8        | 0.4           |
| (1,2212) | 1:110:A:VAL:HG22 | 1:114:A:ARG:H    | 6        | 0.4           |
| (1,2212) | 1:110:A:VAL:HG23 | 1:114:A:ARG:H    | 9        | 0.4           |
| (1,2212) | 1:110:A:VAL:HG21 | 1:114:A:ARG:H    | 14       | 0.4           |
| (1,2201) | 1:64:A:MET:HB2   | 1:21:A:LEU:HD21  | 1        | 0.4           |
| (1,2196) | 1:107:A:GLU:HA   | 1:110:A:VAL:HG11 | 14       | 0.4           |
| (1,2194) | 1:50:A:ILE:HD13  | 1:80:A:SER:H     | 9        | 0.4           |
| (1,2172) | 1:34:A:ARG:HD3   | 1:60:A:VAL:HG13  | 1        | 0.4           |
| (1,2172) | 1:34:A:ARG:HD3   | 1:60:A:VAL:HG13  | 7        | 0.4           |
| (1,2163) | 1:78:A:TYR:HA    | 1:78:A:TYR:HD1   | 10       | 0.4           |
| (1,2146) | 1:104:A:GLU:HB3  | 1:93:A:THR:HG22  | 6        | 0.4           |
| (1,2099) | 1:21:A:LEU:HB2   | 1:21:A:LEU:HD21  | 12       | 0.4           |
| (1,2025) | 1:97:A:LEU:HD23  | 1:35:A:PHE:HD2   | 11       | 0.4           |
| (1,1949) | 1:92:A:ALA:HB1   | 1:110:A:VAL:HG12 | 1        | 0.4           |
| (1,1874) | 1:70:A:GLN:HE21  | 1:27:A:VAL:HG12  | 6        | 0.4           |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1866) | 1:83:A:ARG:HD3  | 1:45:A:ALA:HB1   | 11       | 0.4           |
| (1,1811) | 1:86:A:TYR:H    | 1:117:A:LEU:HD11 | 15       | 0.4           |
| (1,1793) | 1:88:A:VAL:HG22 | 1:84:A:TYR:HA    | 2        | 0.4           |
| (1,1684) | 1:48:A:LEU:HD13 | 1:50:A:ILE:HA    | 3        | 0.4           |
| (1,1679) | 1:92:A:ALA:HB2  | 1:91:A:GLY:H     | 5        | 0.4           |
| (1,1656) | 1:31:A:LEU:HB2  | 1:39:A:PHE:HE2   | 17       | 0.4           |
| (1,1545) | 1:56:A:LEU:HD12 | 1:60:A:VAL:HB    | 4        | 0.4           |
| (1,1545) | 1:56:A:LEU:HD12 | 1:60:A:VAL:HB    | 15       | 0.4           |
| (1,1516) | 1:31:A:LEU:HD13 | 1:28:A:ILE:HG22  | 4        | 0.4           |
| (1,1516) | 1:31:A:LEU:HD12 | 1:28:A:ILE:HG22  | 8        | 0.4           |
| (1,1516) | 1:31:A:LEU:HD12 | 1:28:A:ILE:HG22  | 16       | 0.4           |
| (1,1484) | 1:57:A:VAL:HA   | 1:71:A:LEU:HD13  | 8        | 0.4           |
| (1,1484) | 1:57:A:VAL:HA   | 1:71:A:LEU:HD12  | 12       | 0.4           |
| (1,1484) | 1:57:A:VAL:HA   | 1:71:A:LEU:HD13  | 17       | 0.4           |
| (1,1481) | 1:64:A:MET:HE2  | 1:30:A:PHE:HA    | 8        | 0.4           |
| (1,1405) | 1:102:A:CYS:H   | 1:95:A:VAL:HG13  | 9        | 0.4           |
| (1,1405) | 1:102:A:CYS:H   | 1:95:A:VAL:HG13  | 14       | 0.4           |
| (1,1405) | 1:102:A:CYS:H   | 1:95:A:VAL:HG12  | 17       | 0.4           |
| (1,1400) | 1:95:A:VAL:HG21 | 1:99:A:GLY:H     | 5        | 0.4           |
| (1,1398) | 1:88:A:VAL:HG23 | 1:85:A:LEU:H     | 4        | 0.4           |
| (1,1322) | 1:28:A:ILE:H    | 1:27:A:VAL:HG11  | 5        | 0.4           |
| (1,1322) | 1:28:A:ILE:H    | 1:27:A:VAL:HG13  | 12       | 0.4           |
| (1,1322) | 1:28:A:ILE:H    | 1:27:A:VAL:HG12  | 17       | 0.4           |
| (1,1315) | 1:95:A:VAL:HG23 | 1:97:A:LEU:HD21  | 5        | 0.4           |
| (1,1305) | 1:97:A:LEU:HD22 | 1:52:A:ILE:HB    | 16       | 0.4           |
| (1,1124) | 1:97:A:LEU:HD11 | 1:57:A:VAL:H     | 2        | 0.4           |
| (1,1075) | 1:31:A:LEU:HD12 | 1:31:A:LEU:HA    | 4        | 0.4           |
| (1,825)  | 1:45:A:ALA:HB2  | 1:78:A:TYR:HB3   | 1        | 0.4           |
| (1,789)  | 1:50:A:ILE:HG13 | 1:50:A:ILE:HG23  | 7        | 0.4           |
| (1,789)  | 1:50:A:ILE:HG13 | 1:50:A:ILE:HG23  | 10       | 0.4           |
| (1,789)  | 1:50:A:ILE:HG13 | 1:50:A:ILE:HG22  | 13       | 0.4           |
| (1,697)  | 1:57:A:VAL:HG13 | 1:56:A:LEU:H     | 10       | 0.4           |
| (1,570)  | 1:60:A:VAL:HG13 | 1:34:A:ARG:HE    | 10       | 0.4           |
| (1,442)  | 1:41:A:ALA:HB1  | 1:41:A:ALA:H     | 14       | 0.4           |
| (1,442)  | 1:41:A:ALA:HB2  | 1:41:A:ALA:H     | 16       | 0.4           |
| (1,410)  | 1:53:A:PHE:H    | 1:56:A:LEU:HB3   | 6        | 0.4           |
| (1,228)  | 1:95:A:VAL:HG23 | 1:100:A:ASN:H    | 4        | 0.4           |
| (1,217)  | 1:93:A:THR:HG21 | 1:103:A:GLY:H    | 15       | 0.4           |
| (1,169)  | 1:120:A:ALA:HB2 | 1:119:A:GLU:H    | 10       | 0.4           |
| (1,126)  | 1:28:A:ILE:H    | 1:29:A:ALA:HB3   | 3        | 0.4           |
| (1,126)  | 1:28:A:ILE:H    | 1:29:A:ALA:HB2   | 7        | 0.4           |
| (1,126)  | 1:28:A:ILE:H    | 1:29:A:ALA:HB3   | 8        | 0.4           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,126)  | 1:28:A:ILE:H     | 1:29:A:ALA:HB3   | 11       | 0.4           |
| (1,126)  | 1:28:A:ILE:H     | 1:29:A:ALA:HB3   | 15       | 0.4           |
| (1,32)   | 1:53:A:PHE:H     | 1:53:A:PHE:HD2   | 6        | 0.4           |
| (1,32)   | 1:53:A:PHE:H     | 1:53:A:PHE:HD2   | 9        | 0.4           |
| (3,147)  | 1:71:A:LEU:H     | 1:66:A:LEU:HD23  | 10       | 0.39          |
| (3,147)  | 1:71:A:LEU:H     | 1:66:A:LEU:HD22  | 16       | 0.39          |
| (3,139)  | 1:66:A:LEU:HD22  | 1:70:A:GLN:H     | 3        | 0.39          |
| (3,139)  | 1:66:A:LEU:HD23  | 1:70:A:GLN:H     | 6        | 0.39          |
| (3,139)  | 1:66:A:LEU:HD21  | 1:70:A:GLN:H     | 8        | 0.39          |
| (3,126)  | 1:21:A:LEU:HD23  | 1:22:A:ASN:H     | 3        | 0.39          |
| (3,124)  | 1:88:A:VAL:HG23  | 1:88:A:VAL:H     | 6        | 0.39          |
| (3,109)  | 1:92:A:ALA:H     | 1:110:A:VAL:HB   | 5        | 0.39          |
| (3,98)   | 1:64:A:MET:HE2   | 1:63:A:GLU:HG3   | 16       | 0.39          |
| (3,84)   | 1:84:A:TYR:HE1   | 1:84:A:TYR:HA    | 5        | 0.39          |
| (3,69)   | 1:57:A:VAL:HA    | 1:71:A:LEU:HB2   | 1        | 0.39          |
| (3,69)   | 1:57:A:VAL:HA    | 1:71:A:LEU:HB2   | 5        | 0.39          |
| (3,69)   | 1:57:A:VAL:HA    | 1:71:A:LEU:HB2   | 15       | 0.39          |
| (3,50)   | 1:31:A:LEU:HD22  | 1:97:A:LEU:HD21  | 16       | 0.39          |
| (3,18)   | 1:58:A:ASP:HB3   | 1:60:A:VAL:HG12  | 3        | 0.39          |
| (3,18)   | 1:58:A:ASP:HB3   | 1:60:A:VAL:HG11  | 4        | 0.39          |
| (3,18)   | 1:58:A:ASP:HB3   | 1:60:A:VAL:HG11  | 9        | 0.39          |
| (3,16)   | 1:90:A:PRO:HA    | 1:110:A:VAL:HG12 | 5        | 0.39          |
| (1,4180) | 1:95:A:VAL:H     | 1:48:A:LEU:HD11  | 12       | 0.39          |
| (1,4138) | 1:31:A:LEU:H     | 1:28:A:ILE:HD13  | 3        | 0.39          |
| (1,4138) | 1:31:A:LEU:H     | 1:28:A:ILE:HD11  | 5        | 0.39          |
| (1,4114) | 1:65:A:ASN:H     | 1:65:A:ASN:HD21  | 13       | 0.39          |
| (1,4109) | 1:97:A:LEU:HD13  | 1:98:A:ASP:H     | 7        | 0.39          |
| (1,4045) | 1:21:A:LEU:HD11  | 1:23:A:SER:H     | 12       | 0.39          |
| (1,3972) | 1:53:A:PHE:H     | 1:56:A:LEU:HB3   | 2        | 0.39          |
| (1,3834) | 1:95:A:VAL:HG23  | 1:100:A:ASN:H    | 12       | 0.39          |
| (1,3644) | 1:53:A:PHE:H     | 1:53:A:PHE:HD2   | 13       | 0.39          |
| (1,3627) | 1:100:A:ASN:H    | 1:100:A:ASN:HD21 | 10       | 0.39          |
| (1,3612) | 1:120:A:ALA:HB2  | 1:120:A:ALA:HA   | 2        | 0.39          |
| (1,3612) | 1:120:A:ALA:HB2  | 1:120:A:ALA:HA   | 14       | 0.39          |
| (1,3606) | 1:117:A:LEU:HA   | 1:82:A:TRP:HZ2   | 2        | 0.39          |
| (1,3601) | 1:113:A:ALA:HB1  | 1:111:A:GLU:H    | 3        | 0.39          |
| (1,3601) | 1:113:A:ALA:HB1  | 1:111:A:GLU:H    | 14       | 0.39          |
| (1,3578) | 1:105:A:LEU:HD11 | 1:109:A:HIS:HA   | 11       | 0.39          |
| (1,3578) | 1:105:A:LEU:HD12 | 1:109:A:HIS:HA   | 14       | 0.39          |
| (1,3482) | 1:71:A:LEU:HB2   | 1:31:A:LEU:HD12  | 15       | 0.39          |
| (1,3464) | 1:86:A:TYR:HE2   | 1:85:A:LEU:HD11  | 3        | 0.39          |
| (1,3464) | 1:86:A:TYR:HE1   | 1:85:A:LEU:HD11  | 7        | 0.39          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3464) | 1:86:A:TYR:HE2  | 1:85:A:LEU:HD12  | 17       | 0.39          |
| (1,3463) | 1:35:A:PHE:HE1  | 1:38:A:CYS:HB2   | 2        | 0.39          |
| (1,3463) | 1:35:A:PHE:HE1  | 1:38:A:CYS:HB2   | 16       | 0.39          |
| (1,3386) | 1:90:A:PRO:HA   | 1:92:A:ALA:HB2   | 7        | 0.39          |
| (1,3386) | 1:90:A:PRO:HA   | 1:92:A:ALA:HB3   | 9        | 0.39          |
| (1,3386) | 1:90:A:PRO:HA   | 1:92:A:ALA:HB3   | 11       | 0.39          |
| (1,3373) | 1:88:A:VAL:HA   | 1:93:A:THR:HG23  | 7        | 0.39          |
| (1,3342) | 1:92:A:ALA:HB1  | 1:88:A:VAL:H     | 2        | 0.39          |
| (1,3319) | 1:66:A:LEU:HD22 | 1:27:A:VAL:HG11  | 17       | 0.39          |
| (1,3309) | 1:117:A:LEU:HA  | 1:117:A:LEU:HG   | 7        | 0.39          |
| (1,3309) | 1:117:A:LEU:HA  | 1:117:A:LEU:HG   | 17       | 0.39          |
| (1,3286) | 1:116:A:GLN:HG3 | 1:116:A:GLN:HE21 | 6        | 0.39          |
| (1,3286) | 1:116:A:GLN:HG3 | 1:116:A:GLN:HE21 | 8        | 0.39          |
| (1,3286) | 1:116:A:GLN:HG3 | 1:116:A:GLN:HE21 | 14       | 0.39          |
| (1,3199) | 1:113:A:ALA:HB2 | 1:112:A:HIS:HB2  | 6        | 0.39          |
| (1,3199) | 1:113:A:ALA:HB2 | 1:112:A:HIS:HB2  | 17       | 0.39          |
| (1,3196) | 1:64:A:MET:HB2  | 1:64:A:MET:HA    | 3        | 0.39          |
| (1,3101) | 1:56:A:LEU:HD11 | 1:53:A:PHE:HA    | 7        | 0.39          |
| (1,3101) | 1:56:A:LEU:HD13 | 1:53:A:PHE:HA    | 8        | 0.39          |
| (1,3101) | 1:56:A:LEU:HD12 | 1:53:A:PHE:HA    | 12       | 0.39          |
| (1,3101) | 1:56:A:LEU:HD12 | 1:53:A:PHE:HA    | 16       | 0.39          |
| (1,3092) | 1:55:A:ASP:HA   | 1:56:A:LEU:HB3   | 17       | 0.39          |
| (1,3078) | 1:54:A:GLN:HB3  | 1:57:A:VAL:HG11  | 3        | 0.39          |
| (1,3078) | 1:54:A:GLN:HB3  | 1:57:A:VAL:HG11  | 4        | 0.39          |
| (1,3078) | 1:54:A:GLN:HB3  | 1:57:A:VAL:HG11  | 9        | 0.39          |
| (1,3077) | 1:54:A:GLN:HB2  | 1:57:A:VAL:HG11  | 4        | 0.39          |
| (1,3070) | 1:55:A:ASP:H    | 1:54:A:GLN:HB2   | 3        | 0.39          |
| (1,3067) | 1:52:A:ILE:HG23 | 1:53:A:PHE:HB3   | 15       | 0.39          |
| (1,3024) | 1:64:A:MET:HE1  | 1:65:A:ASN:HB3   | 13       | 0.39          |
| (1,3022) | 1:64:A:MET:HE1  | 1:30:A:PHE:HA    | 2        | 0.39          |
| (1,2940) | 1:99:A:GLY:HA3  | 1:95:A:VAL:HG13  | 3        | 0.39          |
| (1,2940) | 1:99:A:GLY:HA3  | 1:95:A:VAL:HG13  | 6        | 0.39          |
| (1,2940) | 1:99:A:GLY:HA3  | 1:95:A:VAL:HG13  | 8        | 0.39          |
| (1,2940) | 1:99:A:GLY:HA3  | 1:95:A:VAL:HG11  | 16       | 0.39          |
| (1,2890) | 1:33:A:GLU:HB3  | 1:32:A:ALA:HB1   | 13       | 0.39          |
| (1,2880) | 1:61:A:ALA:HB1  | 1:57:A:VAL:HG11  | 12       | 0.39          |
| (1,2877) | 1:61:A:ALA:HB3  | 1:61:A:ALA:HA    | 14       | 0.39          |
| (1,2877) | 1:61:A:ALA:HB2  | 1:61:A:ALA:HA    | 15       | 0.39          |
| (1,2877) | 1:61:A:ALA:HB3  | 1:61:A:ALA:HA    | 16       | 0.39          |
| (1,2873) | 1:126:A:ALA:HA  | 1:126:A:ALA:HB1  | 14       | 0.39          |
| (1,2873) | 1:126:A:ALA:HA  | 1:126:A:ALA:HB1  | 16       | 0.39          |
| (1,2872) | 1:129:A:ALA:HB2 | 1:129:A:ALA:HA   | 7        | 0.39          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2863) | 1:78:A:TYR:HE1   | 1:84:A:TYR:HD2  | 15       | 0.39          |
| (1,2861) | 1:84:A:TYR:HE1   | 1:84:A:TYR:HA   | 13       | 0.39          |
| (1,2861) | 1:84:A:TYR:HE2   | 1:84:A:TYR:HA   | 16       | 0.39          |
| (1,2851) | 1:50:A:ILE:HG21  | 1:50:A:ILE:HA   | 1        | 0.39          |
| (1,2851) | 1:50:A:ILE:HG23  | 1:50:A:ILE:HA   | 9        | 0.39          |
| (1,2851) | 1:50:A:ILE:HG23  | 1:50:A:ILE:HA   | 12       | 0.39          |
| (1,2851) | 1:50:A:ILE:HG21  | 1:50:A:ILE:HA   | 14       | 0.39          |
| (1,2841) | 1:110:A:VAL:HG12 | 1:109:A:HIS:H   | 2        | 0.39          |
| (1,2841) | 1:110:A:VAL:HG13 | 1:109:A:HIS:H   | 3        | 0.39          |
| (1,2841) | 1:110:A:VAL:HG11 | 1:109:A:HIS:H   | 5        | 0.39          |
| (1,2841) | 1:110:A:VAL:HG12 | 1:109:A:HIS:H   | 11       | 0.39          |
| (1,2841) | 1:110:A:VAL:HG13 | 1:109:A:HIS:H   | 12       | 0.39          |
| (1,2841) | 1:110:A:VAL:HG13 | 1:109:A:HIS:H   | 13       | 0.39          |
| (1,2841) | 1:110:A:VAL:HG13 | 1:109:A:HIS:H   | 17       | 0.39          |
| (1,2830) | 1:39:A:PHE:HZ    | 1:97:A:LEU:HD23 | 2        | 0.39          |
| (1,2827) | 1:97:A:LEU:HD23  | 1:52:A:ILE:HB   | 2        | 0.39          |
| (1,2817) | 1:97:A:LEU:HD11  | 1:97:A:LEU:HA   | 5        | 0.39          |
| (1,2785) | 1:50:A:ILE:HG23  | 1:51:A:GLY:HA3  | 13       | 0.39          |
| (1,2694) | 1:73:A:SER:HB2   | 1:74:A:ALA:H    | 4        | 0.39          |
| (1,2694) | 1:73:A:SER:HB2   | 1:74:A:ALA:H    | 5        | 0.39          |
| (1,2694) | 1:73:A:SER:HB2   | 1:74:A:ALA:H    | 7        | 0.39          |
| (1,2694) | 1:73:A:SER:HB2   | 1:74:A:ALA:H    | 13       | 0.39          |
| (1,2694) | 1:73:A:SER:HB2   | 1:74:A:ALA:H    | 15       | 0.39          |
| (1,2678) | 1:53:A:PHE:HB3   | 1:53:A:PHE:HE2  | 5        | 0.39          |
| (1,2622) | 1:71:A:LEU:HD12  | 1:57:A:VAL:H    | 6        | 0.39          |
| (1,2614) | 1:30:A:PHE:HD2   | 1:31:A:LEU:HD12 | 5        | 0.39          |
| (1,2614) | 1:30:A:PHE:HD1   | 1:31:A:LEU:HD13 | 17       | 0.39          |
| (1,2608) | 1:48:A:LEU:HD13  | 1:52:A:ILE:HG12 | 11       | 0.39          |
| (1,2581) | 1:71:A:LEU:HD12  | 1:60:A:VAL:HG11 | 1        | 0.39          |
| (1,2578) | 1:57:A:VAL:HA    | 1:60:A:VAL:HG13 | 12       | 0.39          |
| (1,2568) | 1:78:A:TYR:HE2   | 1:28:A:ILE:HD11 | 4        | 0.39          |
| (1,2568) | 1:78:A:TYR:HE2   | 1:28:A:ILE:HD12 | 5        | 0.39          |
| (1,2484) | 1:93:A:THR:HB    | 1:95:A:VAL:HG12 | 2        | 0.39          |
| (1,2484) | 1:93:A:THR:HB    | 1:95:A:VAL:HG12 | 6        | 0.39          |
| (1,2458) | 1:21:A:LEU:HA    | 1:21:A:LEU:HD12 | 1        | 0.39          |
| (1,2458) | 1:21:A:LEU:HA    | 1:21:A:LEU:HD12 | 3        | 0.39          |
| (1,2458) | 1:21:A:LEU:HA    | 1:21:A:LEU:HD12 | 16       | 0.39          |
| (1,2423) | 1:64:A:MET:HA    | 1:64:A:MET:HE3  | 8        | 0.39          |
| (1,2423) | 1:64:A:MET:HA    | 1:64:A:MET:HE1  | 13       | 0.39          |
| (1,2412) | 1:45:A:ALA:HB2   | 1:78:A:TYR:HB3  | 7        | 0.39          |
| (1,2409) | 1:49:A:LYS:H     | 1:52:A:ILE:HD13 | 4        | 0.39          |
| (1,2405) | 1:29:A:ALA:H     | 1:28:A:ILE:HD13 | 3        | 0.39          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2405) | 1:29:A:ALA:H     | 1:28:A:ILE:HD12  | 10       | 0.39          |
| (1,2370) | 1:50:A:ILE:HG13  | 1:50:A:ILE:HG21  | 17       | 0.39          |
| (1,2367) | 1:52:A:ILE:H     | 1:52:A:ILE:HD11  | 3        | 0.39          |
| (1,2367) | 1:52:A:ILE:H     | 1:52:A:ILE:HD13  | 4        | 0.39          |
| (1,2268) | 1:110:A:VAL:HG12 | 1:89:A:LYS:H     | 10       | 0.39          |
| (1,2268) | 1:110:A:VAL:HG11 | 1:89:A:LYS:H     | 17       | 0.39          |
| (1,2256) | 1:101:A:PRO:HB2  | 1:105:A:LEU:HD22 | 7        | 0.39          |
| (1,2256) | 1:101:A:PRO:HB2  | 1:105:A:LEU:HD22 | 13       | 0.39          |
| (1,2256) | 1:101:A:PRO:HB2  | 1:105:A:LEU:HD23 | 17       | 0.39          |
| (1,2201) | 1:64:A:MET:HB2   | 1:21:A:LEU:HD21  | 6        | 0.39          |
| (1,2196) | 1:107:A:GLU:HA   | 1:110:A:VAL:HG13 | 3        | 0.39          |
| (1,2196) | 1:107:A:GLU:HA   | 1:110:A:VAL:HG11 | 7        | 0.39          |
| (1,2196) | 1:107:A:GLU:HA   | 1:110:A:VAL:HG12 | 11       | 0.39          |
| (1,2196) | 1:107:A:GLU:HA   | 1:110:A:VAL:HG13 | 17       | 0.39          |
| (1,2179) | 1:52:A:ILE:HG21  | 1:48:A:LEU:HB3   | 11       | 0.39          |
| (1,2179) | 1:52:A:ILE:HG21  | 1:48:A:LEU:HB3   | 13       | 0.39          |
| (1,2172) | 1:34:A:ARG:HD3   | 1:60:A:VAL:HG12  | 8        | 0.39          |
| (1,2172) | 1:34:A:ARG:HD3   | 1:60:A:VAL:HG12  | 13       | 0.39          |
| (1,2163) | 1:78:A:TYR:HA    | 1:78:A:TYR:HD2   | 9        | 0.39          |
| (1,2146) | 1:104:A:GLU:HB3  | 1:93:A:THR:HG23  | 1        | 0.39          |
| (1,2146) | 1:104:A:GLU:HB3  | 1:93:A:THR:HG22  | 3        | 0.39          |
| (1,2146) | 1:104:A:GLU:HB3  | 1:93:A:THR:HG21  | 9        | 0.39          |
| (1,2146) | 1:104:A:GLU:HB3  | 1:93:A:THR:HG22  | 11       | 0.39          |
| (1,2099) | 1:21:A:LEU:HB2   | 1:21:A:LEU:HD22  | 2        | 0.39          |
| (1,2025) | 1:97:A:LEU:HD23  | 1:35:A:PHE:HD2   | 9        | 0.39          |
| (1,2005) | 1:95:A:VAL:HG21  | 1:48:A:LEU:HD11  | 8        | 0.39          |
| (1,1866) | 1:83:A:ARG:HD3   | 1:45:A:ALA:HB2   | 15       | 0.39          |
| (1,1866) | 1:83:A:ARG:HD3   | 1:45:A:ALA:HB2   | 17       | 0.39          |
| (1,1790) | 1:90:A:PRO:HA    | 1:92:A:ALA:HB1   | 17       | 0.39          |
| (1,1741) | 1:55:A:ASP:HB2   | 1:56:A:LEU:HD22  | 2        | 0.39          |
| (1,1741) | 1:55:A:ASP:HB2   | 1:56:A:LEU:HD22  | 14       | 0.39          |
| (1,1735) | 1:66:A:LEU:HD22  | 1:67:A:SER:H     | 13       | 0.39          |
| (1,1684) | 1:48:A:LEU:HD12  | 1:50:A:ILE:HA    | 13       | 0.39          |
| (1,1545) | 1:56:A:LEU:HD13  | 1:60:A:VAL:HB    | 10       | 0.39          |
| (1,1545) | 1:56:A:LEU:HD11  | 1:60:A:VAL:HB    | 14       | 0.39          |
| (1,1516) | 1:31:A:LEU:HD13  | 1:28:A:ILE:HG23  | 7        | 0.39          |
| (1,1490) | 1:78:A:TYR:HH    | 1:45:A:ALA:HB3   | 3        | 0.39          |
| (1,1484) | 1:57:A:VAL:HA    | 1:71:A:LEU:HD12  | 16       | 0.39          |
| (1,1481) | 1:64:A:MET:HE3   | 1:30:A:PHE:HA    | 3        | 0.39          |
| (1,1481) | 1:64:A:MET:HE1   | 1:30:A:PHE:HA    | 12       | 0.39          |
| (1,1450) | 1:54:A:GLN:HE22  | 1:54:A:GLN:HG2   | 8        | 0.39          |
| (1,1405) | 1:102:A:CYS:H    | 1:95:A:VAL:HG12  | 6        | 0.39          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1405) | 1:102:A:CYS:H    | 1:95:A:VAL:HG13  | 12       | 0.39          |
| (1,1403) | 1:95:A:VAL:HG23  | 1:95:A:VAL:HG13  | 7        | 0.39          |
| (1,1400) | 1:95:A:VAL:HG22  | 1:99:A:GLY:H     | 15       | 0.39          |
| (1,1398) | 1:88:A:VAL:HG22  | 1:85:A:LEU:H     | 14       | 0.39          |
| (1,1322) | 1:28:A:ILE:H     | 1:27:A:VAL:HG11  | 10       | 0.39          |
| (1,1315) | 1:95:A:VAL:HG22  | 1:97:A:LEU:HD21  | 2        | 0.39          |
| (1,1308) | 1:97:A:LEU:HD23  | 1:35:A:PHE:HD1   | 13       | 0.39          |
| (1,1231) | 1:97:A:LEU:HD13  | 1:59:A:ARG:HD3   | 5        | 0.39          |
| (1,1124) | 1:97:A:LEU:HD12  | 1:57:A:VAL:H     | 16       | 0.39          |
| (1,909)  | 1:53:A:PHE:HE2   | 1:72:A:ARG:HG3   | 6        | 0.39          |
| (1,825)  | 1:45:A:ALA:HB2   | 1:78:A:TYR:HB3   | 9        | 0.39          |
| (1,825)  | 1:45:A:ALA:HB2   | 1:78:A:TYR:HB3   | 16       | 0.39          |
| (1,788)  | 1:52:A:ILE:HD11  | 1:56:A:LEU:H     | 17       | 0.39          |
| (1,576)  | 1:50:A:ILE:HD11  | 1:50:A:ILE:H     | 7        | 0.39          |
| (1,575)  | 1:31:A:LEU:H     | 1:28:A:ILE:HD12  | 11       | 0.39          |
| (1,549)  | 1:97:A:LEU:HD13  | 1:98:A:ASP:H     | 2        | 0.39          |
| (1,528)  | 1:65:A:ASN:HB2   | 1:65:A:ASN:HD21  | 3        | 0.39          |
| (1,410)  | 1:53:A:PHE:H     | 1:56:A:LEU:HB3   | 14       | 0.39          |
| (1,389)  | 1:58:A:ASP:H     | 1:57:A:VAL:HG13  | 12       | 0.39          |
| (1,338)  | 1:71:A:LEU:HD12  | 1:72:A:ARG:H     | 2        | 0.39          |
| (1,338)  | 1:71:A:LEU:HD12  | 1:72:A:ARG:H     | 3        | 0.39          |
| (1,338)  | 1:71:A:LEU:HD12  | 1:72:A:ARG:H     | 8        | 0.39          |
| (1,338)  | 1:71:A:LEU:HD11  | 1:72:A:ARG:H     | 9        | 0.39          |
| (1,338)  | 1:71:A:LEU:HD13  | 1:72:A:ARG:H     | 11       | 0.39          |
| (1,338)  | 1:71:A:LEU:HD13  | 1:72:A:ARG:H     | 14       | 0.39          |
| (1,338)  | 1:71:A:LEU:HD11  | 1:72:A:ARG:H     | 16       | 0.39          |
| (1,263)  | 1:110:A:VAL:HG22 | 1:91:A:GLY:H     | 1        | 0.39          |
| (1,263)  | 1:110:A:VAL:HG23 | 1:91:A:GLY:H     | 2        | 0.39          |
| (1,263)  | 1:110:A:VAL:HG22 | 1:91:A:GLY:H     | 9        | 0.39          |
| (1,228)  | 1:95:A:VAL:HG21  | 1:100:A:ASN:H    | 7        | 0.39          |
| (1,228)  | 1:95:A:VAL:HG21  | 1:100:A:ASN:H    | 16       | 0.39          |
| (1,217)  | 1:93:A:THR:HG22  | 1:103:A:GLY:H    | 6        | 0.39          |
| (1,12)   | 1:100:A:ASN:H    | 1:100:A:ASN:HD21 | 9        | 0.39          |
| (1,12)   | 1:100:A:ASN:H    | 1:100:A:ASN:HD21 | 12       | 0.39          |
| (3,147)  | 1:71:A:LEU:H     | 1:66:A:LEU:HD22  | 3        | 0.38          |
| (3,139)  | 1:66:A:LEU:HD22  | 1:70:A:GLN:H     | 14       | 0.38          |
| (3,139)  | 1:66:A:LEU:HD23  | 1:70:A:GLN:H     | 15       | 0.38          |
| (3,139)  | 1:66:A:LEU:HD22  | 1:70:A:GLN:H     | 16       | 0.38          |
| (3,130)  | 1:52:A:ILE:HG21  | 1:50:A:ILE:HA    | 6        | 0.38          |
| (3,124)  | 1:88:A:VAL:HG23  | 1:88:A:VAL:H     | 9        | 0.38          |
| (3,117)  | 1:48:A:LEU:HD22  | 1:39:A:PHE:HD1   | 1        | 0.38          |
| (3,112)  | 1:82:A:TRP:HA    | 1:117:A:LEU:HD11 | 3        | 0.38          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (3,110)  | 1:105:A:LEU:HG   | 1:110:A:VAL:HG21 | 1        | 0.38          |
| (3,110)  | 1:105:A:LEU:HG   | 1:110:A:VAL:HG21 | 4        | 0.38          |
| (3,87)   | 1:117:A:LEU:HD13 | 1:121:A:LYS:H    | 5        | 0.38          |
| (3,84)   | 1:84:A:TYR:HE2   | 1:84:A:TYR:HA    | 7        | 0.38          |
| (3,84)   | 1:84:A:TYR:HE2   | 1:84:A:TYR:HA    | 15       | 0.38          |
| (3,69)   | 1:57:A:VAL:HA    | 1:71:A:LEU:HB2   | 3        | 0.38          |
| (3,64)   | 1:102:A:CYS:HB2  | 1:52:A:ILE:HG21  | 11       | 0.38          |
| (3,62)   | 1:52:A:ILE:HG22  | 1:56:A:LEU:H     | 7        | 0.38          |
| (3,50)   | 1:31:A:LEU:HD22  | 1:97:A:LEU:HD22  | 14       | 0.38          |
| (1,4342) | 1:38:A:CYS:H     | 1:95:A:VAL:HG11  | 5        | 0.38          |
| (1,4259) | 1:57:A:VAL:HG13  | 1:56:A:LEU:H     | 12       | 0.38          |
| (1,4126) | 1:59:A:ARG:HE    | 1:97:A:LEU:HD13  | 7        | 0.38          |
| (1,4114) | 1:65:A:ASN:H     | 1:65:A:ASN:HD21  | 7        | 0.38          |
| (1,4114) | 1:65:A:ASN:H     | 1:65:A:ASN:HD21  | 16       | 0.38          |
| (1,4112) | 1:54:A:GLN:HE22  | 1:57:A:VAL:H     | 1        | 0.38          |
| (1,3834) | 1:95:A:VAL:HG23  | 1:100:A:ASN:H    | 8        | 0.38          |
| (1,3733) | 1:27:A:VAL:HG11  | 1:26:A:GLU:H     | 3        | 0.38          |
| (1,3733) | 1:27:A:VAL:HG13  | 1:26:A:GLU:H     | 12       | 0.38          |
| (1,3678) | 1:95:A:VAL:H     | 1:96:A:ASP:H     | 5        | 0.38          |
| (1,3644) | 1:53:A:PHE:H     | 1:53:A:PHE:HD1   | 1        | 0.38          |
| (1,3644) | 1:53:A:PHE:H     | 1:53:A:PHE:HD1   | 16       | 0.38          |
| (1,3627) | 1:100:A:ASN:H    | 1:100:A:ASN:HD21 | 2        | 0.38          |
| (1,3627) | 1:100:A:ASN:H    | 1:100:A:ASN:HD21 | 14       | 0.38          |
| (1,3606) | 1:117:A:LEU:HA   | 1:82:A:TRP:HZ2   | 3        | 0.38          |
| (1,3606) | 1:117:A:LEU:HA   | 1:82:A:TRP:HZ2   | 17       | 0.38          |
| (1,3599) | 1:92:A:ALA:HB2   | 1:113:A:ALA:HB2  | 8        | 0.38          |
| (1,3578) | 1:105:A:LEU:HD12 | 1:109:A:HIS:HA   | 15       | 0.38          |
| (1,3498) | 1:70:A:GLN:HE21  | 1:27:A:VAL:HG12  | 1        | 0.38          |
| (1,3498) | 1:70:A:GLN:HE21  | 1:27:A:VAL:HG13  | 2        | 0.38          |
| (1,3498) | 1:70:A:GLN:HE21  | 1:27:A:VAL:HG12  | 8        | 0.38          |
| (1,3482) | 1:71:A:LEU:HB2   | 1:31:A:LEU:HD12  | 10       | 0.38          |
| (1,3482) | 1:71:A:LEU:HB2   | 1:31:A:LEU:HD13  | 16       | 0.38          |
| (1,3464) | 1:86:A:TYR:HE2   | 1:85:A:LEU:HD12  | 5        | 0.38          |
| (1,3464) | 1:86:A:TYR:HE1   | 1:85:A:LEU:HD11  | 6        | 0.38          |
| (1,3446) | 1:65:A:ASN:HD22  | 1:20:A:LYS:HG2   | 8        | 0.38          |
| (1,3446) | 1:65:A:ASN:HD22  | 1:20:A:LYS:HG2   | 10       | 0.38          |
| (1,3446) | 1:65:A:ASN:HD22  | 1:20:A:LYS:HG2   | 13       | 0.38          |
| (1,3386) | 1:90:A:PRO:HA    | 1:92:A:ALA:HB2   | 2        | 0.38          |
| (1,3330) | 1:25:A:LYS:HE3   | 1:77:A:LEU:HD11  | 14       | 0.38          |
| (1,3319) | 1:66:A:LEU:HD22  | 1:27:A:VAL:HG12  | 8        | 0.38          |
| (1,3302) | 1:83:A:ARG:HB2   | 1:86:A:TYR:HD1   | 5        | 0.38          |
| (1,3199) | 1:113:A:ALA:HB3  | 1:112:A:HIS:HB2  | 7        | 0.38          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3199) | 1:113:A:ALA:HB1  | 1:112:A:HIS:HB2  | 8        | 0.38          |
| (1,3198) | 1:114:A:ARG:HA   | 1:113:A:ALA:HB1  | 5        | 0.38          |
| (1,3198) | 1:114:A:ARG:HA   | 1:113:A:ALA:HB3  | 13       | 0.38          |
| (1,3196) | 1:64:A:MET:HB2   | 1:64:A:MET:HA    | 14       | 0.38          |
| (1,3161) | 1:82:A:TRP:HH2   | 1:120:A:ALA:HB3  | 5        | 0.38          |
| (1,3115) | 1:58:A:ASP:HA    | 1:57:A:VAL:HG22  | 11       | 0.38          |
| (1,3101) | 1:56:A:LEU:HD11  | 1:53:A:PHE:HA    | 4        | 0.38          |
| (1,3092) | 1:55:A:ASP:HA    | 1:56:A:LEU:HB3   | 6        | 0.38          |
| (1,3092) | 1:55:A:ASP:HA    | 1:56:A:LEU:HB3   | 8        | 0.38          |
| (1,3078) | 1:54:A:GLN:HB3   | 1:57:A:VAL:HG11  | 2        | 0.38          |
| (1,3070) | 1:55:A:ASP:H     | 1:54:A:GLN:HB2   | 1        | 0.38          |
| (1,3070) | 1:55:A:ASP:H     | 1:54:A:GLN:HB2   | 2        | 0.38          |
| (1,3070) | 1:55:A:ASP:H     | 1:54:A:GLN:HB2   | 4        | 0.38          |
| (1,3070) | 1:55:A:ASP:H     | 1:54:A:GLN:HB2   | 9        | 0.38          |
| (1,3067) | 1:52:A:ILE:HG23  | 1:53:A:PHE:HB3   | 4        | 0.38          |
| (1,3067) | 1:52:A:ILE:HG23  | 1:53:A:PHE:HB3   | 8        | 0.38          |
| (1,3027) | 1:57:A:VAL:HA    | 1:71:A:LEU:HD12  | 10       | 0.38          |
| (1,3024) | 1:64:A:MET:HE2   | 1:65:A:ASN:HB3   | 17       | 0.38          |
| (1,2991) | 1:54:A:GLN:HE22  | 1:54:A:GLN:HG2   | 10       | 0.38          |
| (1,2991) | 1:54:A:GLN:HE22  | 1:54:A:GLN:HG2   | 12       | 0.38          |
| (1,2940) | 1:99:A:GLY:HA3   | 1:95:A:VAL:HG11  | 11       | 0.38          |
| (1,2890) | 1:33:A:GLU:HB3   | 1:32:A:ALA:HB1   | 8        | 0.38          |
| (1,2890) | 1:33:A:GLU:HB3   | 1:32:A:ALA:HB2   | 12       | 0.38          |
| (1,2890) | 1:33:A:GLU:HB3   | 1:32:A:ALA:HB1   | 16       | 0.38          |
| (1,2877) | 1:61:A:ALA:HB2   | 1:61:A:ALA:HA    | 17       | 0.38          |
| (1,2873) | 1:126:A:ALA:HA   | 1:126:A:ALA:HB2  | 2        | 0.38          |
| (1,2873) | 1:126:A:ALA:HA   | 1:126:A:ALA:HB1  | 8        | 0.38          |
| (1,2865) | 1:78:A:TYR:HE1   | 1:48:A:LEU:HD13  | 2        | 0.38          |
| (1,2861) | 1:84:A:TYR:HE2   | 1:84:A:TYR:HA    | 3        | 0.38          |
| (1,2861) | 1:84:A:TYR:HE1   | 1:84:A:TYR:HA    | 8        | 0.38          |
| (1,2851) | 1:50:A:ILE:HG21  | 1:50:A:ILE:HA    | 5        | 0.38          |
| (1,2851) | 1:50:A:ILE:HG23  | 1:50:A:ILE:HA    | 6        | 0.38          |
| (1,2841) | 1:110:A:VAL:HG13 | 1:109:A:HIS:H    | 4        | 0.38          |
| (1,2831) | 1:97:A:LEU:HD21  | 1:35:A:PHE:HD2   | 1        | 0.38          |
| (1,2817) | 1:97:A:LEU:HD13  | 1:97:A:LEU:HA    | 2        | 0.38          |
| (1,2785) | 1:50:A:ILE:HG23  | 1:51:A:GLY:HA3   | 8        | 0.38          |
| (1,2785) | 1:50:A:ILE:HG23  | 1:51:A:GLY:HA3   | 16       | 0.38          |
| (1,2720) | 1:86:A:TYR:HB3   | 1:117:A:LEU:HD11 | 10       | 0.38          |
| (1,2694) | 1:73:A:SER:HB2   | 1:74:A:ALA:H     | 3        | 0.38          |
| (1,2694) | 1:73:A:SER:HB2   | 1:74:A:ALA:H     | 10       | 0.38          |
| (1,2694) | 1:73:A:SER:HB2   | 1:74:A:ALA:H     | 12       | 0.38          |
| (1,2694) | 1:73:A:SER:HB2   | 1:74:A:ALA:H     | 16       | 0.38          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2694) | 1:73:A:SER:HB2  | 1:74:A:ALA:H     | 17       | 0.38          |
| (1,2675) | 1:85:A:LEU:HB2  | 1:86:A:TYR:HD1   | 15       | 0.38          |
| (1,2614) | 1:30:A:PHE:HD2  | 1:31:A:LEU:HD11  | 4        | 0.38          |
| (1,2614) | 1:30:A:PHE:HD2  | 1:31:A:LEU:HD11  | 6        | 0.38          |
| (1,2614) | 1:30:A:PHE:HD1  | 1:31:A:LEU:HD11  | 13       | 0.38          |
| (1,2614) | 1:30:A:PHE:HD2  | 1:31:A:LEU:HD12  | 15       | 0.38          |
| (1,2569) | 1:82:A:TRP:HZ2  | 1:124:A:VAL:HG21 | 11       | 0.38          |
| (1,2568) | 1:78:A:TYR:HE1  | 1:28:A:ILE:HD11  | 3        | 0.38          |
| (1,2547) | 1:11:A:SER:HA   | 1:12:A:GLN:HG3   | 15       | 0.38          |
| (1,2542) | 1:21:A:LEU:HD12 | 1:30:A:PHE:HA    | 3        | 0.38          |
| (1,2484) | 1:93:A:THR:HB   | 1:95:A:VAL:HG11  | 7        | 0.38          |
| (1,2412) | 1:45:A:ALA:HB3  | 1:78:A:TYR:HB3   | 15       | 0.38          |
| (1,2408) | 1:52:A:ILE:HD13 | 1:96:A:ASP:HA    | 17       | 0.38          |
| (1,2405) | 1:29:A:ALA:H    | 1:28:A:ILE:HD11  | 14       | 0.38          |
| (1,2367) | 1:52:A:ILE:H    | 1:52:A:ILE:HD13  | 8        | 0.38          |
| (1,2367) | 1:52:A:ILE:H    | 1:52:A:ILE:HD11  | 11       | 0.38          |
| (1,2230) | 1:28:A:ILE:H    | 1:28:A:ILE:HG23  | 4        | 0.38          |
| (1,2201) | 1:64:A:MET:HB2  | 1:21:A:LEU:HD22  | 11       | 0.38          |
| (1,2201) | 1:64:A:MET:HB2  | 1:21:A:LEU:HD22  | 17       | 0.38          |
| (1,2196) | 1:107:A:GLU:HA  | 1:110:A:VAL:HG11 | 1        | 0.38          |
| (1,2196) | 1:107:A:GLU:HA  | 1:110:A:VAL:HG13 | 4        | 0.38          |
| (1,2196) | 1:107:A:GLU:HA  | 1:110:A:VAL:HG13 | 6        | 0.38          |
| (1,2196) | 1:107:A:GLU:HA  | 1:110:A:VAL:HG12 | 8        | 0.38          |
| (1,2196) | 1:107:A:GLU:HA  | 1:110:A:VAL:HG11 | 10       | 0.38          |
| (1,2196) | 1:107:A:GLU:HA  | 1:110:A:VAL:HG12 | 16       | 0.38          |
| (1,2194) | 1:50:A:ILE:HD12 | 1:80:A:SER:H     | 11       | 0.38          |
| (1,2190) | 1:61:A:ALA:HB2  | 1:62:A:GLY:HA2   | 1        | 0.38          |
| (1,2190) | 1:61:A:ALA:HB2  | 1:62:A:GLY:HA2   | 15       | 0.38          |
| (1,2172) | 1:34:A:ARG:HD3  | 1:60:A:VAL:HG12  | 12       | 0.38          |
| (1,2163) | 1:78:A:TYR:HA   | 1:78:A:TYR:HD1   | 2        | 0.38          |
| (1,2163) | 1:78:A:TYR:HA   | 1:78:A:TYR:HD1   | 17       | 0.38          |
| (1,2099) | 1:21:A:LEU:HB2  | 1:21:A:LEU:HD23  | 11       | 0.38          |
| (1,2098) | 1:21:A:LEU:HD22 | 1:27:A:VAL:HG12  | 7        | 0.38          |
| (1,2094) | 1:95:A:VAL:HG21 | 1:97:A:LEU:HD22  | 13       | 0.38          |
| (1,2006) | 1:78:A:TYR:HE1  | 1:48:A:LEU:HD12  | 12       | 0.38          |
| (1,2005) | 1:95:A:VAL:HG23 | 1:48:A:LEU:HD12  | 15       | 0.38          |
| (1,1960) | 1:121:A:LYS:HG3 | 1:117:A:LEU:HD13 | 4        | 0.38          |
| (1,1811) | 1:86:A:TYR:H    | 1:117:A:LEU:HD11 | 7        | 0.38          |
| (1,1741) | 1:55:A:ASP:HB2  | 1:56:A:LEU:HD21  | 3        | 0.38          |
| (1,1741) | 1:55:A:ASP:HB2  | 1:56:A:LEU:HD23  | 4        | 0.38          |
| (1,1741) | 1:55:A:ASP:HB2  | 1:56:A:LEU:HD22  | 5        | 0.38          |
| (1,1741) | 1:55:A:ASP:HB2  | 1:56:A:LEU:HD23  | 6        | 0.38          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1741) | 1:55:A:ASP:HB2  | 1:56:A:LEU:HD22 | 9        | 0.38          |
| (1,1741) | 1:55:A:ASP:HB2  | 1:56:A:LEU:HD21 | 16       | 0.38          |
| (1,1698) | 1:44:A:GLU:HG2  | 1:45:A:ALA:HB2  | 10       | 0.38          |
| (1,1684) | 1:48:A:LEU:HD13 | 1:50:A:ILE:HA   | 10       | 0.38          |
| (1,1516) | 1:31:A:LEU:HD13 | 1:28:A:ILE:HG21 | 14       | 0.38          |
| (1,1513) | 1:52:A:ILE:HG22 | 1:53:A:PHE:HB3  | 10       | 0.38          |
| (1,1502) | 1:52:A:ILE:HG13 | 1:54:A:GLN:HE21 | 14       | 0.38          |
| (1,1490) | 1:78:A:TYR:HH   | 1:45:A:ALA:HB3  | 9        | 0.38          |
| (1,1484) | 1:57:A:VAL:HA   | 1:71:A:LEU:HD12 | 13       | 0.38          |
| (1,1481) | 1:64:A:MET:HE2  | 1:30:A:PHE:HA   | 1        | 0.38          |
| (1,1408) | 1:57:A:VAL:HG21 | 1:57:A:VAL:HB   | 3        | 0.38          |
| (1,1408) | 1:57:A:VAL:HG22 | 1:57:A:VAL:HB   | 5        | 0.38          |
| (1,1405) | 1:102:A:CYS:H   | 1:95:A:VAL:HG12 | 2        | 0.38          |
| (1,1400) | 1:95:A:VAL:HG21 | 1:99:A:GLY:H    | 17       | 0.38          |
| (1,1398) | 1:88:A:VAL:HG23 | 1:85:A:LEU:H    | 12       | 0.38          |
| (1,1343) | 1:78:A:TYR:HE2  | 1:48:A:LEU:HD11 | 4        | 0.38          |
| (1,1322) | 1:28:A:ILE:H    | 1:27:A:VAL:HG11 | 3        | 0.38          |
| (1,1322) | 1:28:A:ILE:H    | 1:27:A:VAL:HG11 | 11       | 0.38          |
| (1,1304) | 1:97:A:LEU:HD22 | 1:56:A:LEU:HA   | 7        | 0.38          |
| (1,1231) | 1:97:A:LEU:HD13 | 1:59:A:ARG:HD3  | 16       | 0.38          |
| (1,1136) | 1:31:A:LEU:HD13 | 1:35:A:PHE:HD1  | 11       | 0.38          |
| (1,1124) | 1:97:A:LEU:HD11 | 1:57:A:VAL:H    | 12       | 0.38          |
| (1,1073) | 1:97:A:LEU:HD12 | 1:97:A:LEU:H    | 10       | 0.38          |
| (1,909)  | 1:53:A:PHE:HE1  | 1:72:A:ARG:HG3  | 2        | 0.38          |
| (1,825)  | 1:45:A:ALA:HB1  | 1:78:A:TYR:HB3  | 6        | 0.38          |
| (1,825)  | 1:45:A:ALA:HB2  | 1:78:A:TYR:HB3  | 13       | 0.38          |
| (1,822)  | 1:49:A:LYS:H    | 1:52:A:ILE:HD11 | 9        | 0.38          |
| (1,822)  | 1:49:A:LYS:H    | 1:52:A:ILE:HD12 | 13       | 0.38          |
| (1,789)  | 1:50:A:ILE:HG13 | 1:50:A:ILE:HG23 | 3        | 0.38          |
| (1,788)  | 1:52:A:ILE:HD12 | 1:56:A:LEU:H    | 8        | 0.38          |
| (1,614)  | 1:97:A:LEU:HD12 | 1:97:A:LEU:H    | 10       | 0.38          |
| (1,614)  | 1:97:A:LEU:HD11 | 1:97:A:LEU:H    | 15       | 0.38          |
| (1,576)  | 1:50:A:ILE:HD12 | 1:50:A:ILE:H    | 5        | 0.38          |
| (1,575)  | 1:31:A:LEU:H    | 1:28:A:ILE:HD12 | 7        | 0.38          |
| (1,575)  | 1:31:A:LEU:H    | 1:28:A:ILE:HD11 | 17       | 0.38          |
| (1,549)  | 1:97:A:LEU:HD11 | 1:98:A:ASP:H    | 14       | 0.38          |
| (1,528)  | 1:65:A:ASN:HB2  | 1:65:A:ASN:HD21 | 15       | 0.38          |
| (1,442)  | 1:41:A:ALA:HB1  | 1:41:A:ALA:H    | 15       | 0.38          |
| (1,338)  | 1:71:A:LEU:HD11 | 1:72:A:ARG:H    | 4        | 0.38          |
| (1,338)  | 1:71:A:LEU:HD12 | 1:72:A:ARG:H    | 5        | 0.38          |
| (1,338)  | 1:71:A:LEU:HD12 | 1:72:A:ARG:H    | 7        | 0.38          |
| (1,338)  | 1:71:A:LEU:HD11 | 1:72:A:ARG:H    | 10       | 0.38          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,338)  | 1:71:A:LEU:HD11  | 1:72:A:ARG:H     | 13       | 0.38          |
| (1,338)  | 1:71:A:LEU:HD13  | 1:72:A:ARG:H     | 15       | 0.38          |
| (1,338)  | 1:71:A:LEU:HD12  | 1:72:A:ARG:H     | 17       | 0.38          |
| (1,228)  | 1:95:A:VAL:HG23  | 1:100:A:ASN:H    | 1        | 0.38          |
| (1,228)  | 1:95:A:VAL:HG22  | 1:100:A:ASN:H    | 6        | 0.38          |
| (1,228)  | 1:95:A:VAL:HG21  | 1:100:A:ASN:H    | 11       | 0.38          |
| (1,228)  | 1:95:A:VAL:HG21  | 1:100:A:ASN:H    | 17       | 0.38          |
| (1,126)  | 1:28:A:ILE:H     | 1:29:A:ALA:HB3   | 9        | 0.38          |
| (1,126)  | 1:28:A:ILE:H     | 1:29:A:ALA:HB2   | 16       | 0.38          |
| (1,117)  | 1:27:A:VAL:HG12  | 1:26:A:GLU:H     | 17       | 0.38          |
| (1,56)   | 1:84:A:TYR:H     | 1:84:A:TYR:HD2   | 4        | 0.38          |
| (1,32)   | 1:53:A:PHE:H     | 1:53:A:PHE:HD2   | 4        | 0.38          |
| (1,32)   | 1:53:A:PHE:H     | 1:53:A:PHE:HD2   | 7        | 0.38          |
| (1,32)   | 1:53:A:PHE:H     | 1:53:A:PHE:HD2   | 11       | 0.38          |
| (1,32)   | 1:53:A:PHE:H     | 1:53:A:PHE:HD2   | 12       | 0.38          |
| (3,152)  | 1:27:A:VAL:H     | 1:74:A:ALA:HB1   | 13       | 0.37          |
| (3,147)  | 1:71:A:LEU:H     | 1:66:A:LEU:HD23  | 4        | 0.37          |
| (3,147)  | 1:71:A:LEU:H     | 1:66:A:LEU:HD23  | 7        | 0.37          |
| (3,147)  | 1:71:A:LEU:H     | 1:66:A:LEU:HD23  | 13       | 0.37          |
| (3,143)  | 1:25:A:LYS:H     | 1:77:A:LEU:HD22  | 14       | 0.37          |
| (3,143)  | 1:25:A:LYS:H     | 1:77:A:LEU:HD22  | 15       | 0.37          |
| (3,139)  | 1:66:A:LEU:HD23  | 1:70:A:GLN:H     | 1        | 0.37          |
| (3,135)  | 1:123:A:ARG:HB3  | 1:120:A:ALA:HA   | 1        | 0.37          |
| (3,135)  | 1:123:A:ARG:HB3  | 1:120:A:ALA:HA   | 2        | 0.37          |
| (3,135)  | 1:123:A:ARG:HB3  | 1:120:A:ALA:HA   | 3        | 0.37          |
| (3,135)  | 1:123:A:ARG:HB3  | 1:120:A:ALA:HA   | 17       | 0.37          |
| (3,124)  | 1:88:A:VAL:HG23  | 1:84:A:TYR:HE2   | 4        | 0.37          |
| (3,112)  | 1:82:A:TRP:HA    | 1:117:A:LEU:HD12 | 7        | 0.37          |
| (3,110)  | 1:105:A:LEU:HG   | 1:110:A:VAL:HG23 | 6        | 0.37          |
| (3,110)  | 1:105:A:LEU:HG   | 1:110:A:VAL:HG21 | 9        | 0.37          |
| (3,110)  | 1:105:A:LEU:HG   | 1:110:A:VAL:HG21 | 16       | 0.37          |
| (3,87)   | 1:117:A:LEU:HD13 | 1:121:A:LYS:H    | 14       | 0.37          |
| (3,86)   | 1:84:A:TYR:HE1   | 1:47:A:PRO:HB3   | 17       | 0.37          |
| (3,83)   | 1:114:A:ARG:HB2  | 1:113:A:ALA:HB1  | 2        | 0.37          |
| (3,50)   | 1:31:A:LEU:HD22  | 1:97:A:LEU:HD23  | 13       | 0.37          |
| (3,22)   | 1:48:A:LEU:H     | 1:48:A:LEU:HD11  | 14       | 0.37          |
| (3,18)   | 1:58:A:ASP:HB3   | 1:60:A:VAL:HG13  | 5        | 0.37          |
| (1,4342) | 1:38:A:CYS:H     | 1:95:A:VAL:HG12  | 11       | 0.37          |
| (1,4247) | 1:54:A:GLN:HE22  | 1:57:A:VAL:HG11  | 13       | 0.37          |
| (1,4247) | 1:54:A:GLN:HE22  | 1:57:A:VAL:HG11  | 16       | 0.37          |
| (1,4197) | 1:66:A:LEU:HD23  | 1:67:A:SER:H     | 1        | 0.37          |
| (1,4197) | 1:66:A:LEU:HD22  | 1:67:A:SER:H     | 16       | 0.37          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,4180) | 1:95:A:VAL:H     | 1:48:A:LEU:HD11  | 16       | 0.37          |
| (1,4091) | 1:65:A:ASN:HD22  | 1:20:A:LYS:HA    | 10       | 0.37          |
| (1,4045) | 1:21:A:LEU:HD11  | 1:23:A:SER:H     | 15       | 0.37          |
| (1,3972) | 1:53:A:PHE:H     | 1:56:A:LEU:HB3   | 8        | 0.37          |
| (1,3972) | 1:53:A:PHE:H     | 1:56:A:LEU:HB3   | 16       | 0.37          |
| (1,3941) | 1:63:A:GLU:H     | 1:61:A:ALA:HB3   | 17       | 0.37          |
| (1,3839) | 1:65:A:ASN:HB3   | 1:65:A:ASN:HD21  | 4        | 0.37          |
| (1,3738) | 1:103:A:GLY:HA3  | 1:104:A:GLU:H    | 7        | 0.37          |
| (1,3678) | 1:95:A:VAL:H     | 1:96:A:ASP:H     | 17       | 0.37          |
| (1,3644) | 1:53:A:PHE:H     | 1:53:A:PHE:HD2   | 17       | 0.37          |
| (1,3606) | 1:117:A:LEU:HA   | 1:82:A:TRP:HZ2   | 7        | 0.37          |
| (1,3606) | 1:117:A:LEU:HA   | 1:82:A:TRP:HZ2   | 9        | 0.37          |
| (1,3593) | 1:92:A:ALA:HB1   | 1:110:A:VAL:HG12 | 1        | 0.37          |
| (1,3590) | 1:110:A:VAL:HG21 | 1:109:A:HIS:HB2  | 4        | 0.37          |
| (1,3578) | 1:105:A:LEU:HD13 | 1:109:A:HIS:HA   | 5        | 0.37          |
| (1,3564) | 1:105:A:LEU:HB3  | 1:104:A:GLU:HG2  | 7        | 0.37          |
| (1,3508) | 1:113:A:ALA:HB2  | 1:88:A:VAL:HA    | 3        | 0.37          |
| (1,3508) | 1:113:A:ALA:HB3  | 1:88:A:VAL:HA    | 5        | 0.37          |
| (1,3501) | 1:27:A:VAL:HG22  | 1:28:A:ILE:HA    | 11       | 0.37          |
| (1,3482) | 1:71:A:LEU:HB2   | 1:31:A:LEU:HD11  | 12       | 0.37          |
| (1,3481) | 1:83:A:ARG:HD3   | 1:45:A:ALA:HB1   | 7        | 0.37          |
| (1,3481) | 1:83:A:ARG:HD3   | 1:45:A:ALA:HB1   | 16       | 0.37          |
| (1,3464) | 1:86:A:TYR:HE2   | 1:85:A:LEU:HD13  | 1        | 0.37          |
| (1,3464) | 1:86:A:TYR:HE1   | 1:85:A:LEU:HD13  | 4        | 0.37          |
| (1,3464) | 1:86:A:TYR:HE1   | 1:85:A:LEU:HD12  | 13       | 0.37          |
| (1,3446) | 1:65:A:ASN:HD22  | 1:20:A:LYS:HG2   | 3        | 0.37          |
| (1,3437) | 1:21:A:LEU:HB2   | 1:21:A:LEU:HD12  | 9        | 0.37          |
| (1,3402) | 1:58:A:ASP:H     | 1:55:A:ASP:HA    | 7        | 0.37          |
| (1,3386) | 1:90:A:PRO:HA    | 1:92:A:ALA:HB2   | 4        | 0.37          |
| (1,3386) | 1:90:A:PRO:HA    | 1:92:A:ALA:HB2   | 5        | 0.37          |
| (1,3319) | 1:66:A:LEU:HD23  | 1:27:A:VAL:HG13  | 3        | 0.37          |
| (1,3319) | 1:66:A:LEU:HD23  | 1:27:A:VAL:HG13  | 14       | 0.37          |
| (1,3258) | 1:48:A:LEU:HD12  | 1:50:A:ILE:HA    | 9        | 0.37          |
| (1,3256) | 1:41:A:ALA:HB2   | 1:33:A:GLU:H     | 14       | 0.37          |
| (1,3253) | 1:92:A:ALA:HB2   | 1:91:A:GLY:H     | 10       | 0.37          |
| (1,3253) | 1:92:A:ALA:HB2   | 1:91:A:GLY:H     | 15       | 0.37          |
| (1,3248) | 1:88:A:VAL:HG21  | 1:92:A:ALA:HB2   | 1        | 0.37          |
| (1,3199) | 1:113:A:ALA:HB2  | 1:112:A:HIS:HB2  | 4        | 0.37          |
| (1,3198) | 1:114:A:ARG:HA   | 1:113:A:ALA:HB1  | 1        | 0.37          |
| (1,3161) | 1:82:A:TRP:HH2   | 1:120:A:ALA:HB3  | 3        | 0.37          |
| (1,3135) | 1:68:A:LYS:HD3   | 1:68:A:LYS:HB2   | 1        | 0.37          |
| (1,3115) | 1:58:A:ASP:HA    | 1:57:A:VAL:HG21  | 3        | 0.37          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3103) | 1:56:A:LEU:HD11  | 1:60:A:VAL:HB    | 1        | 0.37          |
| (1,3092) | 1:55:A:ASP:HA    | 1:56:A:LEU:HB3   | 10       | 0.37          |
| (1,3092) | 1:55:A:ASP:HA    | 1:56:A:LEU:HB3   | 15       | 0.37          |
| (1,3078) | 1:54:A:GLN:HB3   | 1:57:A:VAL:HG11  | 15       | 0.37          |
| (1,3067) | 1:52:A:ILE:HG21  | 1:53:A:PHE:HB3   | 2        | 0.37          |
| (1,3061) | 1:31:A:LEU:HD13  | 1:28:A:ILE:HG22  | 3        | 0.37          |
| (1,3061) | 1:31:A:LEU:HD13  | 1:28:A:ILE:HG22  | 6        | 0.37          |
| (1,3027) | 1:57:A:VAL:HA    | 1:71:A:LEU:HD13  | 8        | 0.37          |
| (1,3027) | 1:57:A:VAL:HA    | 1:71:A:LEU:HD13  | 17       | 0.37          |
| (1,3024) | 1:64:A:MET:HE3   | 1:65:A:ASN:HB3   | 1        | 0.37          |
| (1,3024) | 1:64:A:MET:HE3   | 1:65:A:ASN:HB3   | 14       | 0.37          |
| (1,3002) | 1:57:A:VAL:HG12  | 1:60:A:VAL:HB    | 3        | 0.37          |
| (1,2940) | 1:99:A:GLY:HA3   | 1:95:A:VAL:HG11  | 9        | 0.37          |
| (1,2933) | 1:95:A:VAL:HG23  | 1:99:A:GLY:H     | 1        | 0.37          |
| (1,2931) | 1:88:A:VAL:HG21  | 1:85:A:LEU:H     | 3        | 0.37          |
| (1,2890) | 1:33:A:GLU:HB3   | 1:32:A:ALA:HB1   | 9        | 0.37          |
| (1,2890) | 1:33:A:GLU:HB3   | 1:32:A:ALA:HB1   | 17       | 0.37          |
| (1,2886) | 1:41:A:ALA:HA    | 1:32:A:ALA:HB3   | 15       | 0.37          |
| (1,2873) | 1:126:A:ALA:HA   | 1:126:A:ALA:HB1  | 9        | 0.37          |
| (1,2873) | 1:126:A:ALA:HA   | 1:126:A:ALA:HB1  | 17       | 0.37          |
| (1,2872) | 1:129:A:ALA:HB2  | 1:129:A:ALA:HA   | 13       | 0.37          |
| (1,2870) | 1:133:A:ALA:HA   | 1:133:A:ALA:HB1  | 1        | 0.37          |
| (1,2863) | 1:78:A:TYR:HE2   | 1:84:A:TYR:HD1   | 5        | 0.37          |
| (1,2851) | 1:50:A:ILE:HG23  | 1:50:A:ILE:HA    | 3        | 0.37          |
| (1,2851) | 1:50:A:ILE:HG23  | 1:50:A:ILE:HA    | 10       | 0.37          |
| (1,2851) | 1:50:A:ILE:HG22  | 1:50:A:ILE:HA    | 13       | 0.37          |
| (1,2842) | 1:28:A:ILE:H     | 1:27:A:VAL:HG13  | 6        | 0.37          |
| (1,2841) | 1:110:A:VAL:HG13 | 1:109:A:HIS:H    | 6        | 0.37          |
| (1,2841) | 1:110:A:VAL:HG11 | 1:109:A:HIS:H    | 9        | 0.37          |
| (1,2841) | 1:110:A:VAL:HG12 | 1:109:A:HIS:H    | 16       | 0.37          |
| (1,2827) | 1:97:A:LEU:HD22  | 1:52:A:ILE:HB    | 1        | 0.37          |
| (1,2827) | 1:97:A:LEU:HD23  | 1:52:A:ILE:HB    | 12       | 0.37          |
| (1,2817) | 1:97:A:LEU:HD11  | 1:97:A:LEU:HA    | 1        | 0.37          |
| (1,2720) | 1:86:A:TYR:HB3   | 1:117:A:LEU:HD13 | 2        | 0.37          |
| (1,2720) | 1:86:A:TYR:HB3   | 1:117:A:LEU:HD11 | 4        | 0.37          |
| (1,2720) | 1:86:A:TYR:HB3   | 1:117:A:LEU:HD12 | 5        | 0.37          |
| (1,2720) | 1:86:A:TYR:HB3   | 1:117:A:LEU:HD11 | 6        | 0.37          |
| (1,2720) | 1:86:A:TYR:HB3   | 1:117:A:LEU:HD11 | 16       | 0.37          |
| (1,2614) | 1:30:A:PHE:HD1   | 1:31:A:LEU:HD12  | 1        | 0.37          |
| (1,2614) | 1:30:A:PHE:HD2   | 1:31:A:LEU:HD12  | 9        | 0.37          |
| (1,2569) | 1:82:A:TRP:HZ2   | 1:124:A:VAL:HG21 | 12       | 0.37          |
| (1,2569) | 1:82:A:TRP:HZ2   | 1:124:A:VAL:HG21 | 13       | 0.37          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2569) | 1:82:A:TRP:HZ2  | 1:124:A:VAL:HG22 | 17       | 0.37          |
| (1,2568) | 1:78:A:TYR:HE1  | 1:28:A:ILE:HD13  | 2        | 0.37          |
| (1,2568) | 1:78:A:TYR:HE1  | 1:28:A:ILE:HD11  | 16       | 0.37          |
| (1,2547) | 1:11:A:SER:HA   | 1:12:A:GLN:HG3   | 2        | 0.37          |
| (1,2480) | 1:71:A:LEU:HB2  | 1:27:A:VAL:HG13  | 5        | 0.37          |
| (1,2418) | 1:113:A:ALA:HB2 | 1:110:A:VAL:HG11 | 6        | 0.37          |
| (1,2412) | 1:45:A:ALA:HB3  | 1:78:A:TYR:HB3   | 17       | 0.37          |
| (1,2409) | 1:49:A:LYS:H    | 1:52:A:ILE:HD11  | 16       | 0.37          |
| (1,2405) | 1:29:A:ALA:H    | 1:28:A:ILE:HD12  | 1        | 0.37          |
| (1,2370) | 1:50:A:ILE:HG13 | 1:50:A:ILE:HG21  | 14       | 0.37          |
| (1,2367) | 1:52:A:ILE:H    | 1:52:A:ILE:HD13  | 1        | 0.37          |
| (1,2344) | 1:104:A:GLU:HG2 | 1:105:A:LEU:HD22 | 7        | 0.37          |
| (1,2344) | 1:104:A:GLU:HG2 | 1:105:A:LEU:HD23 | 9        | 0.37          |
| (1,2271) | 1:113:A:ALA:HB3 | 1:112:A:HIS:HD2  | 12       | 0.37          |
| (1,2271) | 1:113:A:ALA:HB1 | 1:112:A:HIS:HD2  | 14       | 0.37          |
| (1,2256) | 1:101:A:PRO:HB2 | 1:105:A:LEU:HD23 | 6        | 0.37          |
| (1,2256) | 1:101:A:PRO:HB2 | 1:105:A:LEU:HD23 | 9        | 0.37          |
| (1,2256) | 1:101:A:PRO:HB2 | 1:105:A:LEU:HD21 | 12       | 0.37          |
| (1,2196) | 1:107:A:GLU:HA  | 1:110:A:VAL:HG11 | 9        | 0.37          |
| (1,2196) | 1:107:A:GLU:HA  | 1:110:A:VAL:HG13 | 12       | 0.37          |
| (1,2190) | 1:61:A:ALA:HB2  | 1:62:A:GLY:HA2   | 7        | 0.37          |
| (1,2190) | 1:61:A:ALA:HB1  | 1:62:A:GLY:HA2   | 13       | 0.37          |
| (1,2190) | 1:61:A:ALA:HB2  | 1:62:A:GLY:HA2   | 17       | 0.37          |
| (1,2179) | 1:52:A:ILE:HG22 | 1:48:A:LEU:HB3   | 15       | 0.37          |
| (1,2178) | 1:48:A:LEU:HB2  | 1:52:A:ILE:HG22  | 1        | 0.37          |
| (1,2172) | 1:34:A:ARG:HD3  | 1:60:A:VAL:HG12  | 4        | 0.37          |
| (1,1912) | 1:64:A:MET:HE3  | 1:65:A:ASN:HB2   | 14       | 0.37          |
| (1,1811) | 1:86:A:TYR:H    | 1:117:A:LEU:HD11 | 11       | 0.37          |
| (1,1686) | 1:85:A:LEU:HD12 | 1:85:A:LEU:HD23  | 13       | 0.37          |
| (1,1679) | 1:92:A:ALA:HB3  | 1:91:A:GLY:H     | 1        | 0.37          |
| (1,1656) | 1:31:A:LEU:HB2  | 1:39:A:PHE:HE2   | 2        | 0.37          |
| (1,1656) | 1:31:A:LEU:HB2  | 1:39:A:PHE:HE2   | 4        | 0.37          |
| (1,1553) | 1:57:A:VAL:HG13 | 1:61:A:ALA:H     | 12       | 0.37          |
| (1,1507) | 1:78:A:TYR:HE1  | 1:28:A:ILE:HG22  | 6        | 0.37          |
| (1,1507) | 1:78:A:TYR:HE2  | 1:28:A:ILE:HG23  | 12       | 0.37          |
| (1,1490) | 1:78:A:TYR:HH   | 1:45:A:ALA:HB1   | 14       | 0.37          |
| (1,1484) | 1:57:A:VAL:HA   | 1:71:A:LEU:HD13  | 7        | 0.37          |
| (1,1483) | 1:21:A:LEU:HG   | 1:64:A:MET:HE2   | 7        | 0.37          |
| (1,1481) | 1:64:A:MET:HE2  | 1:30:A:PHE:HA    | 14       | 0.37          |
| (1,1481) | 1:64:A:MET:HE3  | 1:30:A:PHE:HA    | 15       | 0.37          |
| (1,1450) | 1:54:A:GLN:HE22 | 1:54:A:GLN:HG2   | 15       | 0.37          |
| (1,1450) | 1:54:A:GLN:HE22 | 1:54:A:GLN:HG2   | 17       | 0.37          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1408) | 1:57:A:VAL:HG22  | 1:57:A:VAL:HB   | 11       | 0.37          |
| (1,1405) | 1:102:A:CYS:H    | 1:95:A:VAL:HG12 | 3        | 0.37          |
| (1,1405) | 1:102:A:CYS:H    | 1:95:A:VAL:HG12 | 5        | 0.37          |
| (1,1398) | 1:88:A:VAL:HG22  | 1:85:A:LEU:H    | 6        | 0.37          |
| (1,1398) | 1:88:A:VAL:HG22  | 1:85:A:LEU:H    | 9        | 0.37          |
| (1,1322) | 1:28:A:ILE:H     | 1:27:A:VAL:HG11 | 2        | 0.37          |
| (1,1322) | 1:28:A:ILE:H     | 1:27:A:VAL:HG11 | 13       | 0.37          |
| (1,1322) | 1:28:A:ILE:H     | 1:27:A:VAL:HG11 | 14       | 0.37          |
| (1,1308) | 1:97:A:LEU:HD22  | 1:35:A:PHE:HD2  | 10       | 0.37          |
| (1,1308) | 1:97:A:LEU:HD22  | 1:35:A:PHE:HD2  | 17       | 0.37          |
| (1,1231) | 1:97:A:LEU:HD13  | 1:59:A:ARG:HD3  | 14       | 0.37          |
| (1,1073) | 1:97:A:LEU:HD11  | 1:97:A:LEU:H    | 15       | 0.37          |
| (1,1061) | 1:21:A:LEU:HD23  | 1:27:A:VAL:HG11 | 6        | 0.37          |
| (1,1061) | 1:21:A:LEU:HD23  | 1:27:A:VAL:HG13 | 15       | 0.37          |
| (1,979)  | 1:122:A:ALA:HA   | 1:122:A:ALA:HB1 | 3        | 0.37          |
| (1,979)  | 1:122:A:ALA:HA   | 1:122:A:ALA:HB1 | 7        | 0.37          |
| (1,909)  | 1:53:A:PHE:HE2   | 1:72:A:ARG:HG3  | 9        | 0.37          |
| (1,825)  | 1:45:A:ALA:HB1   | 1:78:A:TYR:HB3  | 2        | 0.37          |
| (1,789)  | 1:50:A:ILE:HG13  | 1:50:A:ILE:HG21 | 1        | 0.37          |
| (1,789)  | 1:50:A:ILE:HG13  | 1:50:A:ILE:HG21 | 5        | 0.37          |
| (1,788)  | 1:52:A:ILE:HD13  | 1:56:A:LEU:H    | 12       | 0.37          |
| (1,575)  | 1:31:A:LEU:H     | 1:28:A:ILE:HD12 | 1        | 0.37          |
| (1,575)  | 1:31:A:LEU:H     | 1:28:A:ILE:HD11 | 8        | 0.37          |
| (1,575)  | 1:31:A:LEU:H     | 1:28:A:ILE:HD12 | 10       | 0.37          |
| (1,575)  | 1:31:A:LEU:H     | 1:28:A:ILE:HD12 | 12       | 0.37          |
| (1,575)  | 1:31:A:LEU:H     | 1:28:A:ILE:HD11 | 14       | 0.37          |
| (1,575)  | 1:31:A:LEU:H     | 1:28:A:ILE:HD12 | 15       | 0.37          |
| (1,570)  | 1:60:A:VAL:HG11  | 1:34:A:ARG:HE   | 2        | 0.37          |
| (1,528)  | 1:65:A:ASN:HB2   | 1:65:A:ASN:HD21 | 1        | 0.37          |
| (1,528)  | 1:65:A:ASN:HB2   | 1:65:A:ASN:HD21 | 5        | 0.37          |
| (1,528)  | 1:65:A:ASN:HB2   | 1:65:A:ASN:HD21 | 14       | 0.37          |
| (1,410)  | 1:53:A:PHE:H     | 1:56:A:LEU:HB3  | 9        | 0.37          |
| (1,338)  | 1:71:A:LEU:HD13  | 1:72:A:ARG:H    | 6        | 0.37          |
| (1,338)  | 1:71:A:LEU:HD11  | 1:72:A:ARG:H    | 12       | 0.37          |
| (1,263)  | 1:110:A:VAL:HG22 | 1:91:A:GLY:H    | 3        | 0.37          |
| (1,228)  | 1:95:A:VAL:HG22  | 1:100:A:ASN:H   | 13       | 0.37          |
| (1,228)  | 1:95:A:VAL:HG22  | 1:100:A:ASN:H   | 15       | 0.37          |
| (1,217)  | 1:93:A:THR:HG22  | 1:103:A:GLY:H   | 11       | 0.37          |
| (1,217)  | 1:93:A:THR:HG21  | 1:103:A:GLY:H   | 13       | 0.37          |
| (1,32)   | 1:53:A:PHE:H     | 1:53:A:PHE:HD1  | 2        | 0.37          |
| (1,32)   | 1:53:A:PHE:H     | 1:53:A:PHE:HD1  | 8        | 0.37          |
| (3,143)  | 1:25:A:LYS:H     | 1:77:A:LEU:HD22 | 17       | 0.36          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (3,139)  | 1:66:A:LEU:HD23  | 1:70:A:GLN:H     | 10       | 0.36          |
| (3,124)  | 1:88:A:VAL:HG23  | 1:88:A:VAL:H     | 8        | 0.36          |
| (3,124)  | 1:88:A:VAL:HG23  | 1:88:A:VAL:H     | 15       | 0.36          |
| (3,112)  | 1:82:A:TRP:HA    | 1:117:A:LEU:HD11 | 12       | 0.36          |
| (3,111)  | 1:111:A:GLU:HG2  | 1:112:A:HIS:HA   | 5        | 0.36          |
| (3,110)  | 1:105:A:LEU:HG   | 1:110:A:VAL:HG22 | 2        | 0.36          |
| (3,110)  | 1:105:A:LEU:HG   | 1:110:A:VAL:HG21 | 3        | 0.36          |
| (3,110)  | 1:105:A:LEU:HG   | 1:110:A:VAL:HG23 | 8        | 0.36          |
| (3,110)  | 1:105:A:LEU:HG   | 1:110:A:VAL:HG21 | 12       | 0.36          |
| (3,110)  | 1:105:A:LEU:HG   | 1:110:A:VAL:HG22 | 14       | 0.36          |
| (3,110)  | 1:105:A:LEU:HG   | 1:110:A:VAL:HG22 | 15       | 0.36          |
| (3,110)  | 1:105:A:LEU:HG   | 1:110:A:VAL:HG21 | 17       | 0.36          |
| (3,106)  | 1:68:A:LYS:HD2   | 1:68:A:LYS:HA    | 3        | 0.36          |
| (3,84)   | 1:84:A:TYR:HE2   | 1:84:A:TYR:HA    | 1        | 0.36          |
| (3,69)   | 1:57:A:VAL:HA    | 1:71:A:LEU:HB2   | 6        | 0.36          |
| (3,69)   | 1:57:A:VAL:HA    | 1:71:A:LEU:HB2   | 9        | 0.36          |
| (3,64)   | 1:55:A:ASP:HB2   | 1:52:A:ILE:HG21  | 9        | 0.36          |
| (3,36)   | 1:49:A:LYS:HB2   | 1:52:A:ILE:HD11  | 11       | 0.36          |
| (3,16)   | 1:90:A:PRO:HA    | 1:110:A:VAL:HG13 | 11       | 0.36          |
| (3,16)   | 1:90:A:PRO:HA    | 1:110:A:VAL:HG12 | 14       | 0.36          |
| (1,4323) | 1:62:A:GLY:H     | 1:68:A:LYS:HD2   | 3        | 0.36          |
| (1,4300) | 1:92:A:ALA:H     | 1:105:A:LEU:HD22 | 14       | 0.36          |
| (1,4197) | 1:66:A:LEU:HD23  | 1:67:A:SER:H     | 12       | 0.36          |
| (1,4153) | 1:18:A:GLN:HB3   | 1:18:A:GLN:H     | 10       | 0.36          |
| (1,4138) | 1:31:A:LEU:H     | 1:28:A:ILE:HD13  | 6        | 0.36          |
| (1,4138) | 1:31:A:LEU:H     | 1:28:A:ILE:HD11  | 13       | 0.36          |
| (1,4126) | 1:59:A:ARG:HE    | 1:97:A:LEU:HD13  | 2        | 0.36          |
| (1,4114) | 1:65:A:ASN:H     | 1:65:A:ASN:HD21  | 9        | 0.36          |
| (1,4087) | 1:65:A:ASN:HB2   | 1:65:A:ASN:HD21  | 11       | 0.36          |
| (1,4084) | 1:20:A:LYS:HB3   | 1:22:A:ASN:HD22  | 15       | 0.36          |
| (1,4045) | 1:21:A:LEU:HD13  | 1:23:A:SER:H     | 1        | 0.36          |
| (1,3839) | 1:65:A:ASN:HB3   | 1:65:A:ASN:HD21  | 13       | 0.36          |
| (1,3839) | 1:65:A:ASN:HB3   | 1:65:A:ASN:HD21  | 16       | 0.36          |
| (1,3732) | 1:21:A:LEU:HD11  | 1:30:A:PHE:H     | 8        | 0.36          |
| (1,3678) | 1:95:A:VAL:H     | 1:96:A:ASP:H     | 6        | 0.36          |
| (1,3612) | 1:120:A:ALA:HB3  | 1:120:A:ALA:HA   | 10       | 0.36          |
| (1,3606) | 1:117:A:LEU:HA   | 1:82:A:TRP:HZ2   | 15       | 0.36          |
| (1,3590) | 1:110:A:VAL:HG21 | 1:109:A:HIS:HB2  | 17       | 0.36          |
| (1,3570) | 1:90:A:PRO:HA    | 1:105:A:LEU:HD11 | 1        | 0.36          |
| (1,3570) | 1:90:A:PRO:HA    | 1:105:A:LEU:HD13 | 15       | 0.36          |
| (1,3564) | 1:105:A:LEU:HB3  | 1:104:A:GLU:HG2  | 9        | 0.36          |
| (1,3564) | 1:105:A:LEU:HB3  | 1:104:A:GLU:HG2  | 11       | 0.36          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3508) | 1:113:A:ALA:HB3 | 1:88:A:VAL:HA   | 2        | 0.36          |
| (1,3498) | 1:70:A:GLN:HE21 | 1:27:A:VAL:HG12 | 6        | 0.36          |
| (1,3498) | 1:70:A:GLN:HE21 | 1:27:A:VAL:HG12 | 16       | 0.36          |
| (1,3482) | 1:71:A:LEU:HB2  | 1:31:A:LEU:HD13 | 17       | 0.36          |
| (1,3481) | 1:83:A:ARG:HD3  | 1:45:A:ALA:HB3  | 12       | 0.36          |
| (1,3464) | 1:86:A:TYR:HE1  | 1:85:A:LEU:HD11 | 14       | 0.36          |
| (1,3463) | 1:35:A:PHE:HE2  | 1:38:A:CYS:HB2  | 11       | 0.36          |
| (1,3437) | 1:21:A:LEU:HB2  | 1:21:A:LEU:HD12 | 4        | 0.36          |
| (1,3402) | 1:58:A:ASP:H    | 1:55:A:ASP:HA   | 1        | 0.36          |
| (1,3373) | 1:88:A:VAL:HA   | 1:93:A:THR:HG22 | 5        | 0.36          |
| (1,3323) | 1:66:A:LEU:HD22 | 1:66:A:LEU:H    | 11       | 0.36          |
| (1,3302) | 1:83:A:ARG:HB2  | 1:86:A:TYR:HD2  | 14       | 0.36          |
| (1,3256) | 1:41:A:ALA:HB2  | 1:33:A:GLU:H    | 17       | 0.36          |
| (1,3223) | 1:84:A:TYR:HE1  | 1:79:A:THR:HA   | 4        | 0.36          |
| (1,3198) | 1:114:A:ARG:HA  | 1:113:A:ALA:HB1 | 4        | 0.36          |
| (1,3161) | 1:82:A:TRP:HH2  | 1:120:A:ALA:HB3 | 1        | 0.36          |
| (1,3135) | 1:68:A:LYS:HD3  | 1:68:A:LYS:HB2  | 8        | 0.36          |
| (1,3135) | 1:68:A:LYS:HD3  | 1:68:A:LYS:HB2  | 10       | 0.36          |
| (1,3135) | 1:68:A:LYS:HD3  | 1:68:A:LYS:HB2  | 15       | 0.36          |
| (1,3132) | 1:68:A:LYS:HB2  | 1:53:A:PHE:HE1  | 11       | 0.36          |
| (1,3115) | 1:58:A:ASP:HA   | 1:57:A:VAL:HG21 | 10       | 0.36          |
| (1,3115) | 1:58:A:ASP:HA   | 1:57:A:VAL:HG23 | 15       | 0.36          |
| (1,3101) | 1:56:A:LEU:HD13 | 1:53:A:PHE:HA   | 2        | 0.36          |
| (1,3101) | 1:56:A:LEU:HD13 | 1:53:A:PHE:HA   | 5        | 0.36          |
| (1,3101) | 1:56:A:LEU:HD12 | 1:53:A:PHE:HA   | 10       | 0.36          |
| (1,3101) | 1:56:A:LEU:HD12 | 1:53:A:PHE:HA   | 17       | 0.36          |
| (1,3092) | 1:55:A:ASP:HA   | 1:56:A:LEU:HB3  | 5        | 0.36          |
| (1,3078) | 1:54:A:GLN:HB3  | 1:57:A:VAL:HG12 | 11       | 0.36          |
| (1,3077) | 1:54:A:GLN:HB2  | 1:57:A:VAL:HG11 | 3        | 0.36          |
| (1,3061) | 1:31:A:LEU:HD12 | 1:28:A:ILE:HG22 | 8        | 0.36          |
| (1,3061) | 1:31:A:LEU:HD11 | 1:28:A:ILE:HG21 | 11       | 0.36          |
| (1,3061) | 1:31:A:LEU:HD12 | 1:28:A:ILE:HG22 | 16       | 0.36          |
| (1,3036) | 1:78:A:TYR:HH   | 1:45:A:ALA:HB3  | 5        | 0.36          |
| (1,3036) | 1:78:A:TYR:HH   | 1:45:A:ALA:HB3  | 11       | 0.36          |
| (1,3027) | 1:57:A:VAL:HA   | 1:71:A:LEU:HD12 | 12       | 0.36          |
| (1,3027) | 1:57:A:VAL:HA   | 1:71:A:LEU:HD12 | 16       | 0.36          |
| (1,3022) | 1:64:A:MET:HE1  | 1:30:A:PHE:HA   | 10       | 0.36          |
| (1,3022) | 1:64:A:MET:HE3  | 1:30:A:PHE:HA   | 13       | 0.36          |
| (1,3022) | 1:64:A:MET:HE1  | 1:30:A:PHE:HA   | 17       | 0.36          |
| (1,3002) | 1:57:A:VAL:HG12 | 1:60:A:VAL:HB   | 4        | 0.36          |
| (1,3002) | 1:57:A:VAL:HG12 | 1:60:A:VAL:HB   | 9        | 0.36          |
| (1,3002) | 1:57:A:VAL:HG12 | 1:60:A:VAL:HB   | 13       | 0.36          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2991) | 1:54:A:GLN:HE22  | 1:54:A:GLN:HG2   | 8        | 0.36          |
| (1,2942) | 1:57:A:VAL:HG21  | 1:57:A:VAL:HB    | 3        | 0.36          |
| (1,2942) | 1:57:A:VAL:HG22  | 1:57:A:VAL:HB    | 5        | 0.36          |
| (1,2940) | 1:99:A:GLY:HA3   | 1:95:A:VAL:HG13  | 5        | 0.36          |
| (1,2937) | 1:95:A:VAL:HG23  | 1:95:A:VAL:HG13  | 7        | 0.36          |
| (1,2933) | 1:95:A:VAL:HG22  | 1:99:A:GLY:H     | 6        | 0.36          |
| (1,2931) | 1:88:A:VAL:HG23  | 1:85:A:LEU:H     | 17       | 0.36          |
| (1,2877) | 1:61:A:ALA:HB2   | 1:61:A:ALA:HA    | 1        | 0.36          |
| (1,2877) | 1:61:A:ALA:HB2   | 1:61:A:ALA:HA    | 8        | 0.36          |
| (1,2877) | 1:61:A:ALA:HB2   | 1:61:A:ALA:HA    | 10       | 0.36          |
| (1,2877) | 1:61:A:ALA:HB2   | 1:61:A:ALA:HA    | 12       | 0.36          |
| (1,2873) | 1:126:A:ALA:HA   | 1:126:A:ALA:HB1  | 10       | 0.36          |
| (1,2872) | 1:129:A:ALA:HB1  | 1:129:A:ALA:HA   | 10       | 0.36          |
| (1,2870) | 1:133:A:ALA:HA   | 1:133:A:ALA:HB1  | 5        | 0.36          |
| (1,2870) | 1:133:A:ALA:HA   | 1:133:A:ALA:HB1  | 10       | 0.36          |
| (1,2861) | 1:84:A:TYR:HE1   | 1:84:A:TYR:HA    | 6        | 0.36          |
| (1,2861) | 1:84:A:TYR:HE1   | 1:84:A:TYR:HA    | 9        | 0.36          |
| (1,2861) | 1:84:A:TYR:HE1   | 1:84:A:TYR:HA    | 11       | 0.36          |
| (1,2851) | 1:50:A:ILE:HG23  | 1:50:A:ILE:HA    | 7        | 0.36          |
| (1,2842) | 1:28:A:ILE:H     | 1:27:A:VAL:HG13  | 12       | 0.36          |
| (1,2842) | 1:28:A:ILE:H     | 1:27:A:VAL:HG12  | 17       | 0.36          |
| (1,2841) | 1:110:A:VAL:HG11 | 1:109:A:HIS:H    | 1        | 0.36          |
| (1,2841) | 1:110:A:VAL:HG12 | 1:109:A:HIS:H    | 8        | 0.36          |
| (1,2836) | 1:95:A:VAL:HG23  | 1:97:A:LEU:HD21  | 5        | 0.36          |
| (1,2831) | 1:97:A:LEU:HD23  | 1:35:A:PHE:HD1   | 13       | 0.36          |
| (1,2830) | 1:39:A:PHE:HZ    | 1:97:A:LEU:HD23  | 5        | 0.36          |
| (1,2830) | 1:39:A:PHE:HZ    | 1:97:A:LEU:HD23  | 7        | 0.36          |
| (1,2830) | 1:39:A:PHE:HZ    | 1:97:A:LEU:HD23  | 14       | 0.36          |
| (1,2785) | 1:50:A:ILE:HG23  | 1:51:A:GLY:HA3   | 4        | 0.36          |
| (1,2753) | 1:97:A:LEU:HD13  | 1:59:A:ARG:HD3   | 5        | 0.36          |
| (1,2569) | 1:82:A:TRP:HZ2   | 1:124:A:VAL:HG21 | 7        | 0.36          |
| (1,2547) | 1:11:A:SER:HA    | 1:12:A:GLN:HG3   | 14       | 0.36          |
| (1,2484) | 1:93:A:THR:HB    | 1:95:A:VAL:HG12  | 8        | 0.36          |
| (1,2484) | 1:93:A:THR:HB    | 1:95:A:VAL:HG11  | 13       | 0.36          |
| (1,2484) | 1:93:A:THR:HB    | 1:95:A:VAL:HG13  | 14       | 0.36          |
| (1,2484) | 1:93:A:THR:HB    | 1:95:A:VAL:HG12  | 17       | 0.36          |
| (1,2423) | 1:64:A:MET:HA    | 1:64:A:MET:HE2   | 5        | 0.36          |
| (1,2418) | 1:113:A:ALA:HB2  | 1:110:A:VAL:HG11 | 17       | 0.36          |
| (1,2412) | 1:45:A:ALA:HB1   | 1:78:A:TYR:HB3   | 12       | 0.36          |
| (1,2370) | 1:50:A:ILE:HG13  | 1:50:A:ILE:HG23  | 7        | 0.36          |
| (1,2370) | 1:50:A:ILE:HG13  | 1:50:A:ILE:HG23  | 10       | 0.36          |
| (1,2370) | 1:50:A:ILE:HG13  | 1:50:A:ILE:HG22  | 13       | 0.36          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2367) | 1:52:A:ILE:H     | 1:52:A:ILE:HD11  | 15       | 0.36          |
| (1,2336) | 1:64:A:MET:HE2   | 1:31:A:LEU:HA    | 6        | 0.36          |
| (1,2256) | 1:101:A:PRO:HB2  | 1:105:A:LEU:HD23 | 2        | 0.36          |
| (1,2256) | 1:101:A:PRO:HB2  | 1:105:A:LEU:HD21 | 15       | 0.36          |
| (1,2230) | 1:28:A:ILE:H     | 1:28:A:ILE:HG21  | 2        | 0.36          |
| (1,2230) | 1:28:A:ILE:H     | 1:28:A:ILE:HG23  | 3        | 0.36          |
| (1,2230) | 1:28:A:ILE:H     | 1:28:A:ILE:HG22  | 11       | 0.36          |
| (1,2230) | 1:28:A:ILE:H     | 1:28:A:ILE:HG23  | 16       | 0.36          |
| (1,2201) | 1:64:A:MET:HB2   | 1:21:A:LEU:HD21  | 15       | 0.36          |
| (1,2196) | 1:107:A:GLU:HA   | 1:110:A:VAL:HG12 | 15       | 0.36          |
| (1,2190) | 1:61:A:ALA:HB2   | 1:62:A:GLY:HA2   | 8        | 0.36          |
| (1,2178) | 1:48:A:LEU:HB2   | 1:52:A:ILE:HG23  | 3        | 0.36          |
| (1,2163) | 1:78:A:TYR:HA    | 1:78:A:TYR:HD2   | 4        | 0.36          |
| (1,2163) | 1:78:A:TYR:HA    | 1:78:A:TYR:HD1   | 15       | 0.36          |
| (1,2036) | 1:97:A:LEU:HD23  | 1:97:A:LEU:HB2   | 8        | 0.36          |
| (1,2006) | 1:78:A:TYR:HE1   | 1:48:A:LEU:HD11  | 11       | 0.36          |
| (1,2005) | 1:95:A:VAL:HG22  | 1:48:A:LEU:HD12  | 11       | 0.36          |
| (1,1879) | 1:124:A:VAL:HG11 | 1:124:A:VAL:HG23 | 9        | 0.36          |
| (1,1870) | 1:86:A:TYR:HE1   | 1:85:A:LEU:HD22  | 14       | 0.36          |
| (1,1866) | 1:83:A:ARG:HD3   | 1:45:A:ALA:HB3   | 2        | 0.36          |
| (1,1811) | 1:86:A:TYR:H     | 1:117:A:LEU:HD13 | 3        | 0.36          |
| (1,1811) | 1:86:A:TYR:H     | 1:117:A:LEU:HD12 | 17       | 0.36          |
| (1,1752) | 1:41:A:ALA:HB2   | 1:28:A:ILE:HG23  | 17       | 0.36          |
| (1,1741) | 1:55:A:ASP:HB2   | 1:56:A:LEU:HD23  | 7        | 0.36          |
| (1,1741) | 1:55:A:ASP:HB2   | 1:56:A:LEU:HD23  | 11       | 0.36          |
| (1,1741) | 1:55:A:ASP:HB2   | 1:56:A:LEU:HD22  | 13       | 0.36          |
| (1,1735) | 1:66:A:LEU:HD22  | 1:67:A:SER:H     | 16       | 0.36          |
| (1,1698) | 1:44:A:GLU:HG2   | 1:45:A:ALA:HB3   | 14       | 0.36          |
| (1,1656) | 1:31:A:LEU:HB2   | 1:39:A:PHE:HE1   | 16       | 0.36          |
| (1,1628) | 1:87:A:GLY:HA3   | 1:113:A:ALA:HB1  | 1        | 0.36          |
| (1,1545) | 1:56:A:LEU:HD11  | 1:60:A:VAL:HB    | 2        | 0.36          |
| (1,1545) | 1:56:A:LEU:HD13  | 1:60:A:VAL:HB    | 17       | 0.36          |
| (1,1516) | 1:31:A:LEU:HD11  | 1:28:A:ILE:HG23  | 2        | 0.36          |
| (1,1516) | 1:31:A:LEU:HD11  | 1:28:A:ILE:HG22  | 10       | 0.36          |
| (1,1512) | 1:52:A:ILE:HG23  | 1:53:A:PHE:HB2   | 17       | 0.36          |
| (1,1490) | 1:78:A:TYR:HH    | 1:45:A:ALA:HB3   | 1        | 0.36          |
| (1,1490) | 1:78:A:TYR:HH    | 1:45:A:ALA:HB3   | 4        | 0.36          |
| (1,1490) | 1:78:A:TYR:HH    | 1:45:A:ALA:HB3   | 13       | 0.36          |
| (1,1484) | 1:57:A:VAL:HA    | 1:71:A:LEU:HD13  | 3        | 0.36          |
| (1,1484) | 1:57:A:VAL:HA    | 1:71:A:LEU:HD13  | 5        | 0.36          |
| (1,1484) | 1:57:A:VAL:HA    | 1:71:A:LEU:HD12  | 9        | 0.36          |
| (1,1484) | 1:57:A:VAL:HA    | 1:71:A:LEU:HD11  | 11       | 0.36          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1484) | 1:57:A:VAL:HA   | 1:71:A:LEU:HD11 | 15       | 0.36          |
| (1,1482) | 1:64:A:MET:HE3  | 1:27:A:VAL:HA   | 9        | 0.36          |
| (1,1481) | 1:64:A:MET:HE3  | 1:30:A:PHE:HA   | 6        | 0.36          |
| (1,1408) | 1:57:A:VAL:HG21 | 1:57:A:VAL:HB   | 1        | 0.36          |
| (1,1408) | 1:57:A:VAL:HG21 | 1:57:A:VAL:HB   | 13       | 0.36          |
| (1,1405) | 1:102:A:CYS:H   | 1:95:A:VAL:HG13 | 16       | 0.36          |
| (1,1403) | 1:95:A:VAL:HG23 | 1:95:A:VAL:HG12 | 14       | 0.36          |
| (1,1400) | 1:95:A:VAL:HG22 | 1:99:A:GLY:H    | 3        | 0.36          |
| (1,1398) | 1:88:A:VAL:HG22 | 1:85:A:LEU:H    | 2        | 0.36          |
| (1,1398) | 1:88:A:VAL:HG22 | 1:85:A:LEU:H    | 10       | 0.36          |
| (1,1334) | 1:81:A:SER:HB3  | 1:84:A:TYR:HD2  | 2        | 0.36          |
| (1,1322) | 1:28:A:ILE:H    | 1:27:A:VAL:HG13 | 1        | 0.36          |
| (1,1322) | 1:28:A:ILE:H    | 1:27:A:VAL:HG11 | 4        | 0.36          |
| (1,1322) | 1:28:A:ILE:H    | 1:27:A:VAL:HG13 | 16       | 0.36          |
| (1,1231) | 1:97:A:LEU:HD11 | 1:59:A:ARG:HD3  | 17       | 0.36          |
| (1,1124) | 1:97:A:LEU:HD12 | 1:57:A:VAL:H    | 1        | 0.36          |
| (1,1124) | 1:97:A:LEU:HD13 | 1:57:A:VAL:H    | 6        | 0.36          |
| (1,1124) | 1:97:A:LEU:HD12 | 1:57:A:VAL:H    | 14       | 0.36          |
| (1,1124) | 1:97:A:LEU:HD13 | 1:57:A:VAL:H    | 17       | 0.36          |
| (1,1073) | 1:97:A:LEU:HD12 | 1:97:A:LEU:H    | 6        | 0.36          |
| (1,1061) | 1:21:A:LEU:HD21 | 1:27:A:VAL:HG12 | 3        | 0.36          |
| (1,1061) | 1:21:A:LEU:HD22 | 1:27:A:VAL:HG12 | 5        | 0.36          |
| (1,979)  | 1:122:A:ALA:HA  | 1:122:A:ALA:HB1 | 1        | 0.36          |
| (1,979)  | 1:122:A:ALA:HA  | 1:122:A:ALA:HB3 | 8        | 0.36          |
| (1,979)  | 1:122:A:ALA:HA  | 1:122:A:ALA:HB1 | 13       | 0.36          |
| (1,979)  | 1:122:A:ALA:HA  | 1:122:A:ALA:HB3 | 16       | 0.36          |
| (1,942)  | 1:93:A:THR:HB   | 1:95:A:VAL:HG13 | 12       | 0.36          |
| (1,909)  | 1:53:A:PHE:HE2  | 1:72:A:ARG:HG3  | 4        | 0.36          |
| (1,830)  | 1:129:A:ALA:HB1 | 1:127:A:GLN:HB3 | 7        | 0.36          |
| (1,825)  | 1:45:A:ALA:HB2  | 1:78:A:TYR:HB3  | 10       | 0.36          |
| (1,825)  | 1:45:A:ALA:HB3  | 1:78:A:TYR:HB3  | 14       | 0.36          |
| (1,788)  | 1:52:A:ILE:HD13 | 1:56:A:LEU:H    | 7        | 0.36          |
| (1,614)  | 1:97:A:LEU:HD12 | 1:97:A:LEU:H    | 6        | 0.36          |
| (1,575)  | 1:31:A:LEU:H    | 1:28:A:ILE:HD13 | 4        | 0.36          |
| (1,410)  | 1:53:A:PHE:H    | 1:56:A:LEU:HB3  | 4        | 0.36          |
| (1,410)  | 1:53:A:PHE:H    | 1:56:A:LEU:HB3  | 7        | 0.36          |
| (1,338)  | 1:71:A:LEU:HD13 | 1:72:A:ARG:H    | 1        | 0.36          |
| (1,228)  | 1:95:A:VAL:HG21 | 1:100:A:ASN:H   | 5        | 0.36          |
| (1,222)  | 1:102:A:CYS:H   | 1:95:A:VAL:HG11 | 4        | 0.36          |
| (1,117)  | 1:27:A:VAL:HG12 | 1:26:A:GLU:H    | 10       | 0.36          |
| (1,32)   | 1:53:A:PHE:H    | 1:53:A:PHE:HD1  | 15       | 0.36          |
| (3,152)  | 1:27:A:VAL:H    | 1:74:A:ALA:HB3  | 15       | 0.35          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (3,143)  | 1:25:A:LYS:H     | 1:77:A:LEU:HD22  | 5        | 0.35          |
| (3,112)  | 1:82:A:TRP:HA    | 1:117:A:LEU:HD11 | 2        | 0.35          |
| (3,112)  | 1:82:A:TRP:HA    | 1:117:A:LEU:HD11 | 9        | 0.35          |
| (3,112)  | 1:82:A:TRP:HA    | 1:117:A:LEU:HD13 | 17       | 0.35          |
| (3,110)  | 1:105:A:LEU:HG   | 1:110:A:VAL:HG23 | 7        | 0.35          |
| (3,110)  | 1:105:A:LEU:HG   | 1:110:A:VAL:HG22 | 10       | 0.35          |
| (3,69)   | 1:57:A:VAL:HA    | 1:71:A:LEU:HB2   | 2        | 0.35          |
| (3,69)   | 1:57:A:VAL:HA    | 1:71:A:LEU:HB2   | 4        | 0.35          |
| (3,34)   | 1:97:A:LEU:HD23  | 1:31:A:LEU:HD13  | 2        | 0.35          |
| (3,16)   | 1:90:A:PRO:HA    | 1:110:A:VAL:HG13 | 15       | 0.35          |
| (1,4342) | 1:38:A:CYS:H     | 1:95:A:VAL:HG11  | 2        | 0.35          |
| (1,4342) | 1:38:A:CYS:H     | 1:95:A:VAL:HG13  | 7        | 0.35          |
| (1,4230) | 1:128:A:ARG:HA   | 1:128:A:ARG:H    | 6        | 0.35          |
| (1,4197) | 1:66:A:LEU:HD23  | 1:67:A:SER:H     | 8        | 0.35          |
| (1,4197) | 1:66:A:LEU:HD23  | 1:67:A:SER:H     | 17       | 0.35          |
| (1,4180) | 1:95:A:VAL:H     | 1:48:A:LEU:HD11  | 7        | 0.35          |
| (1,4180) | 1:95:A:VAL:H     | 1:48:A:LEU:HD12  | 15       | 0.35          |
| (1,4132) | 1:60:A:VAL:HG11  | 1:34:A:ARG:HE    | 16       | 0.35          |
| (1,4114) | 1:65:A:ASN:H     | 1:65:A:ASN:HD21  | 8        | 0.35          |
| (1,4017) | 1:32:A:ALA:HB2   | 1:35:A:PHE:H     | 9        | 0.35          |
| (1,3972) | 1:53:A:PHE:H     | 1:56:A:LEU:HB3   | 1        | 0.35          |
| (1,3972) | 1:53:A:PHE:H     | 1:56:A:LEU:HB3   | 10       | 0.35          |
| (1,3972) | 1:53:A:PHE:H     | 1:56:A:LEU:HB3   | 13       | 0.35          |
| (1,3972) | 1:53:A:PHE:H     | 1:56:A:LEU:HB3   | 15       | 0.35          |
| (1,3738) | 1:103:A:GLY:HA3  | 1:104:A:GLU:H    | 5        | 0.35          |
| (1,3738) | 1:103:A:GLY:HA3  | 1:104:A:GLU:H    | 6        | 0.35          |
| (1,3738) | 1:103:A:GLY:HA3  | 1:104:A:GLU:H    | 14       | 0.35          |
| (1,3732) | 1:21:A:LEU:HD12  | 1:30:A:PHE:H     | 1        | 0.35          |
| (1,3612) | 1:120:A:ALA:HB3  | 1:120:A:ALA:HA   | 8        | 0.35          |
| (1,3590) | 1:110:A:VAL:HG23 | 1:109:A:HIS:HB2  | 6        | 0.35          |
| (1,3590) | 1:110:A:VAL:HG23 | 1:109:A:HIS:HB2  | 8        | 0.35          |
| (1,3590) | 1:110:A:VAL:HG21 | 1:109:A:HIS:HB2  | 9        | 0.35          |
| (1,3590) | 1:110:A:VAL:HG21 | 1:109:A:HIS:HB2  | 12       | 0.35          |
| (1,3590) | 1:110:A:VAL:HG22 | 1:109:A:HIS:HB2  | 13       | 0.35          |
| (1,3590) | 1:110:A:VAL:HG22 | 1:109:A:HIS:HB2  | 15       | 0.35          |
| (1,3590) | 1:110:A:VAL:HG21 | 1:109:A:HIS:HB2  | 16       | 0.35          |
| (1,3570) | 1:90:A:PRO:HA    | 1:105:A:LEU:HD12 | 3        | 0.35          |
| (1,3570) | 1:90:A:PRO:HA    | 1:105:A:LEU:HD11 | 7        | 0.35          |
| (1,3481) | 1:83:A:ARG:HD3   | 1:45:A:ALA:HB1   | 1        | 0.35          |
| (1,3481) | 1:83:A:ARG:HD3   | 1:45:A:ALA:HB1   | 4        | 0.35          |
| (1,3481) | 1:83:A:ARG:HD3   | 1:45:A:ALA:HB2   | 8        | 0.35          |
| (1,3446) | 1:65:A:ASN:HD22  | 1:20:A:LYS:HG2   | 14       | 0.35          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3427) | 1:117:A:LEU:HA  | 1:117:A:LEU:H    | 5        | 0.35          |
| (1,3414) | 1:86:A:TYR:H    | 1:117:A:LEU:HD11 | 15       | 0.35          |
| (1,3405) | 1:55:A:ASP:HB2  | 1:56:A:LEU:HD21  | 15       | 0.35          |
| (1,3401) | 1:86:A:TYR:HE1  | 1:86:A:TYR:HA    | 7        | 0.35          |
| (1,3390) | 1:88:A:VAL:HG22 | 1:84:A:TYR:HA    | 2        | 0.35          |
| (1,3345) | 1:29:A:ALA:HA   | 1:29:A:ALA:HB3   | 1        | 0.35          |
| (1,3342) | 1:92:A:ALA:HB1  | 1:88:A:VAL:H     | 5        | 0.35          |
| (1,3319) | 1:66:A:LEU:HD21 | 1:27:A:VAL:HG13  | 7        | 0.35          |
| (1,3264) | 1:121:A:LYS:HG2 | 1:121:A:LYS:H    | 15       | 0.35          |
| (1,3258) | 1:48:A:LEU:HD13 | 1:50:A:ILE:HA    | 1        | 0.35          |
| (1,3258) | 1:48:A:LEU:HD13 | 1:50:A:ILE:HA    | 3        | 0.35          |
| (1,3253) | 1:92:A:ALA:HB2  | 1:91:A:GLY:H     | 5        | 0.35          |
| (1,3228) | 1:31:A:LEU:HB2  | 1:39:A:PHE:HE1   | 12       | 0.35          |
| (1,3216) | 1:48:A:LEU:HG   | 1:84:A:TYR:HD1   | 8        | 0.35          |
| (1,3216) | 1:48:A:LEU:HG   | 1:84:A:TYR:HD1   | 9        | 0.35          |
| (1,3216) | 1:48:A:LEU:HG   | 1:84:A:TYR:HD2   | 15       | 0.35          |
| (1,3199) | 1:113:A:ALA:HB3 | 1:112:A:HIS:HB2  | 12       | 0.35          |
| (1,3161) | 1:82:A:TRP:HH2  | 1:120:A:ALA:HB3  | 6        | 0.35          |
| (1,3161) | 1:82:A:TRP:HH2  | 1:120:A:ALA:HB3  | 13       | 0.35          |
| (1,3161) | 1:82:A:TRP:HH2  | 1:120:A:ALA:HB3  | 16       | 0.35          |
| (1,3135) | 1:68:A:LYS:HD3  | 1:68:A:LYS:HB2   | 12       | 0.35          |
| (1,3135) | 1:68:A:LYS:HD3  | 1:68:A:LYS:HB2   | 13       | 0.35          |
| (1,3135) | 1:68:A:LYS:HD3  | 1:68:A:LYS:HB2   | 16       | 0.35          |
| (1,3115) | 1:58:A:ASP:HA   | 1:57:A:VAL:HG22  | 5        | 0.35          |
| (1,3115) | 1:58:A:ASP:HA   | 1:57:A:VAL:HG21  | 7        | 0.35          |
| (1,3115) | 1:58:A:ASP:HA   | 1:57:A:VAL:HG23  | 12       | 0.35          |
| (1,3115) | 1:58:A:ASP:HA   | 1:57:A:VAL:HG21  | 13       | 0.35          |
| (1,3115) | 1:58:A:ASP:HA   | 1:57:A:VAL:HG21  | 17       | 0.35          |
| (1,3114) | 1:57:A:VAL:HG23 | 1:57:A:VAL:HG11  | 4        | 0.35          |
| (1,3114) | 1:57:A:VAL:HG23 | 1:57:A:VAL:HG11  | 9        | 0.35          |
| (1,3103) | 1:56:A:LEU:HD12 | 1:60:A:VAL:HB    | 15       | 0.35          |
| (1,3101) | 1:56:A:LEU:HD13 | 1:53:A:PHE:HA    | 6        | 0.35          |
| (1,3101) | 1:56:A:LEU:HD13 | 1:53:A:PHE:HA    | 14       | 0.35          |
| (1,3092) | 1:55:A:ASP:HA   | 1:56:A:LEU:HB3   | 4        | 0.35          |
| (1,3092) | 1:55:A:ASP:HA   | 1:56:A:LEU:HB3   | 9        | 0.35          |
| (1,3092) | 1:55:A:ASP:HA   | 1:56:A:LEU:HB3   | 14       | 0.35          |
| (1,3078) | 1:54:A:GLN:HB3  | 1:57:A:VAL:HG11  | 1        | 0.35          |
| (1,3077) | 1:54:A:GLN:HB2  | 1:57:A:VAL:HG11  | 6        | 0.35          |
| (1,3077) | 1:54:A:GLN:HB2  | 1:57:A:VAL:HG11  | 13       | 0.35          |
| (1,3067) | 1:52:A:ILE:HG21 | 1:53:A:PHE:HB3   | 3        | 0.35          |
| (1,3067) | 1:52:A:ILE:HG21 | 1:53:A:PHE:HB3   | 9        | 0.35          |
| (1,3061) | 1:31:A:LEU:HD13 | 1:28:A:ILE:HG22  | 4        | 0.35          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3061) | 1:31:A:LEU:HD13  | 1:28:A:ILE:HG23  | 7        | 0.35          |
| (1,3027) | 1:57:A:VAL:HA    | 1:71:A:LEU:HD12  | 13       | 0.35          |
| (1,3022) | 1:64:A:MET:HE2   | 1:30:A:PHE:HA    | 8        | 0.35          |
| (1,3002) | 1:57:A:VAL:HG13  | 1:60:A:VAL:HB    | 11       | 0.35          |
| (1,2942) | 1:57:A:VAL:HG22  | 1:57:A:VAL:HB    | 11       | 0.35          |
| (1,2940) | 1:99:A:GLY:HA3   | 1:95:A:VAL:HG13  | 1        | 0.35          |
| (1,2940) | 1:99:A:GLY:HA3   | 1:95:A:VAL:HG12  | 7        | 0.35          |
| (1,2940) | 1:99:A:GLY:HA3   | 1:95:A:VAL:HG12  | 15       | 0.35          |
| (1,2933) | 1:95:A:VAL:HG21  | 1:99:A:GLY:H     | 5        | 0.35          |
| (1,2931) | 1:88:A:VAL:HG23  | 1:85:A:LEU:H     | 4        | 0.35          |
| (1,2890) | 1:33:A:GLU:HB3   | 1:32:A:ALA:HB2   | 14       | 0.35          |
| (1,2870) | 1:133:A:ALA:HA   | 1:133:A:ALA:HB3  | 2        | 0.35          |
| (1,2870) | 1:133:A:ALA:HA   | 1:133:A:ALA:HB3  | 3        | 0.35          |
| (1,2870) | 1:133:A:ALA:HA   | 1:133:A:ALA:HB1  | 4        | 0.35          |
| (1,2870) | 1:133:A:ALA:HA   | 1:133:A:ALA:HB3  | 6        | 0.35          |
| (1,2870) | 1:133:A:ALA:HA   | 1:133:A:ALA:HB2  | 7        | 0.35          |
| (1,2870) | 1:133:A:ALA:HA   | 1:133:A:ALA:HB1  | 8        | 0.35          |
| (1,2870) | 1:133:A:ALA:HA   | 1:133:A:ALA:HB3  | 9        | 0.35          |
| (1,2870) | 1:133:A:ALA:HA   | 1:133:A:ALA:HB1  | 11       | 0.35          |
| (1,2870) | 1:133:A:ALA:HA   | 1:133:A:ALA:HB3  | 12       | 0.35          |
| (1,2870) | 1:133:A:ALA:HA   | 1:133:A:ALA:HB1  | 13       | 0.35          |
| (1,2870) | 1:133:A:ALA:HA   | 1:133:A:ALA:HB3  | 15       | 0.35          |
| (1,2870) | 1:133:A:ALA:HA   | 1:133:A:ALA:HB3  | 16       | 0.35          |
| (1,2870) | 1:133:A:ALA:HA   | 1:133:A:ALA:HB2  | 17       | 0.35          |
| (1,2842) | 1:28:A:ILE:H     | 1:27:A:VAL:HG11  | 5        | 0.35          |
| (1,2842) | 1:28:A:ILE:H     | 1:27:A:VAL:HG11  | 10       | 0.35          |
| (1,2841) | 1:110:A:VAL:HG11 | 1:109:A:HIS:H    | 7        | 0.35          |
| (1,2841) | 1:110:A:VAL:HG11 | 1:109:A:HIS:H    | 14       | 0.35          |
| (1,2836) | 1:95:A:VAL:HG22  | 1:97:A:LEU:HD21  | 2        | 0.35          |
| (1,2830) | 1:39:A:PHE:HZ    | 1:97:A:LEU:HD21  | 4        | 0.35          |
| (1,2827) | 1:97:A:LEU:HD22  | 1:52:A:ILE:HB    | 16       | 0.35          |
| (1,2761) | 1:76:A:ARG:HA    | 1:76:A:ARG:HD2   | 11       | 0.35          |
| (1,2753) | 1:97:A:LEU:HD13  | 1:59:A:ARG:HD3   | 16       | 0.35          |
| (1,2662) | 1:97:A:LEU:HD11  | 1:57:A:VAL:H     | 2        | 0.35          |
| (1,2583) | 1:60:A:VAL:HG13  | 1:34:A:ARG:HG2   | 3        | 0.35          |
| (1,2542) | 1:21:A:LEU:HD13  | 1:30:A:PHE:HA    | 2        | 0.35          |
| (1,2502) | 1:42:A:GLU:HA    | 1:43:A:GLY:H     | 17       | 0.35          |
| (1,2484) | 1:93:A:THR:HB    | 1:95:A:VAL:HG13  | 10       | 0.35          |
| (1,2480) | 1:71:A:LEU:HB2   | 1:27:A:VAL:HG13  | 2        | 0.35          |
| (1,2458) | 1:21:A:LEU:HA    | 1:21:A:LEU:HD11  | 14       | 0.35          |
| (1,2423) | 1:64:A:MET:HA    | 1:64:A:MET:HE3   | 14       | 0.35          |
| (1,2418) | 1:113:A:ALA:HB1  | 1:110:A:VAL:HG12 | 10       | 0.35          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2412) | 1:45:A:ALA:HB2   | 1:78:A:TYR:HB3   | 1        | 0.35          |
| (1,2412) | 1:45:A:ALA:HB2   | 1:78:A:TYR:HB3   | 11       | 0.35          |
| (1,2346) | 1:105:A:LEU:HD12 | 1:107:A:GLU:HA   | 14       | 0.35          |
| (1,2334) | 1:60:A:VAL:HG12  | 1:63:A:GLU:HG3   | 3        | 0.35          |
| (1,2256) | 1:101:A:PRO:HB2  | 1:105:A:LEU:HD21 | 1        | 0.35          |
| (1,2256) | 1:101:A:PRO:HB2  | 1:105:A:LEU:HD22 | 3        | 0.35          |
| (1,2230) | 1:28:A:ILE:H     | 1:28:A:ILE:HG22  | 9        | 0.35          |
| (1,2230) | 1:28:A:ILE:H     | 1:28:A:ILE:HG23  | 17       | 0.35          |
| (1,2212) | 1:110:A:VAL:HG23 | 1:114:A:ARG:H    | 12       | 0.35          |
| (1,2196) | 1:107:A:GLU:HA   | 1:110:A:VAL:HG13 | 13       | 0.35          |
| (1,2179) | 1:52:A:ILE:HG22  | 1:48:A:LEU:HB3   | 1        | 0.35          |
| (1,2178) | 1:48:A:LEU:HB2   | 1:52:A:ILE:HG23  | 9        | 0.35          |
| (1,2172) | 1:34:A:ARG:HD3   | 1:60:A:VAL:HG12  | 9        | 0.35          |
| (1,2149) | 1:21:A:LEU:HD21  | 1:30:A:PHE:HD2   | 2        | 0.35          |
| (1,2099) | 1:21:A:LEU:HB2   | 1:21:A:LEU:HD23  | 3        | 0.35          |
| (1,2099) | 1:21:A:LEU:HB2   | 1:21:A:LEU:HD21  | 13       | 0.35          |
| (1,2099) | 1:21:A:LEU:HB2   | 1:21:A:LEU:HD23  | 17       | 0.35          |
| (1,2094) | 1:95:A:VAL:HG23  | 1:97:A:LEU:HD22  | 11       | 0.35          |
| (1,2088) | 1:82:A:TRP:HZ2   | 1:124:A:VAL:HG21 | 2        | 0.35          |
| (1,2025) | 1:97:A:LEU:HD22  | 1:35:A:PHE:HD1   | 6        | 0.35          |
| (1,2006) | 1:78:A:TYR:HE1   | 1:48:A:LEU:HD13  | 17       | 0.35          |
| (1,1903) | 1:122:A:ALA:HB1  | 1:121:A:LYS:HE3  | 15       | 0.35          |
| (1,1879) | 1:124:A:VAL:HG13 | 1:124:A:VAL:HG23 | 8        | 0.35          |
| (1,1866) | 1:83:A:ARG:HD3   | 1:45:A:ALA:HB3   | 6        | 0.35          |
| (1,1839) | 1:95:A:VAL:HA    | 1:93:A:THR:HG21  | 5        | 0.35          |
| (1,1813) | 1:117:A:LEU:HD13 | 1:117:A:LEU:HB3  | 1        | 0.35          |
| (1,1811) | 1:86:A:TYR:H     | 1:117:A:LEU:HD13 | 9        | 0.35          |
| (1,1811) | 1:86:A:TYR:H     | 1:117:A:LEU:HD13 | 12       | 0.35          |
| (1,1799) | 1:71:A:LEU:HA    | 1:74:A:ALA:HB2   | 17       | 0.35          |
| (1,1790) | 1:90:A:PRO:HA    | 1:92:A:ALA:HB3   | 1        | 0.35          |
| (1,1746) | 1:71:A:LEU:HD22  | 1:74:A:ALA:H     | 17       | 0.35          |
| (1,1735) | 1:66:A:LEU:HD23  | 1:67:A:SER:H     | 1        | 0.35          |
| (1,1735) | 1:66:A:LEU:HD23  | 1:67:A:SER:H     | 12       | 0.35          |
| (1,1686) | 1:85:A:LEU:HD11  | 1:85:A:LEU:HD21  | 6        | 0.35          |
| (1,1684) | 1:48:A:LEU:HD12  | 1:50:A:ILE:HA    | 14       | 0.35          |
| (1,1545) | 1:56:A:LEU:HD12  | 1:60:A:VAL:HB    | 13       | 0.35          |
| (1,1516) | 1:31:A:LEU:HD11  | 1:28:A:ILE:HG21  | 1        | 0.35          |
| (1,1514) | 1:52:A:ILE:HG21  | 1:48:A:LEU:HG    | 17       | 0.35          |
| (1,1484) | 1:57:A:VAL:HA    | 1:71:A:LEU:HD11  | 1        | 0.35          |
| (1,1484) | 1:57:A:VAL:HA    | 1:71:A:LEU:HD12  | 4        | 0.35          |
| (1,1480) | 1:64:A:MET:HE2   | 1:63:A:GLU:H     | 2        | 0.35          |
| (1,1478) | 1:64:A:MET:HE3   | 1:66:A:LEU:H     | 7        | 0.35          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1450) | 1:54:A:GLN:HE22  | 1:54:A:GLN:HG2  | 13       | 0.35          |
| (1,1408) | 1:57:A:VAL:HG21  | 1:57:A:VAL:HB   | 7        | 0.35          |
| (1,1408) | 1:57:A:VAL:HG21  | 1:57:A:VAL:HB   | 10       | 0.35          |
| (1,1405) | 1:102:A:CYS:H    | 1:95:A:VAL:HG12 | 1        | 0.35          |
| (1,1403) | 1:95:A:VAL:HG21  | 1:95:A:VAL:HG11 | 2        | 0.35          |
| (1,1400) | 1:95:A:VAL:HG23  | 1:99:A:GLY:H    | 8        | 0.35          |
| (1,1400) | 1:95:A:VAL:HG21  | 1:99:A:GLY:H    | 9        | 0.35          |
| (1,1398) | 1:88:A:VAL:HG22  | 1:85:A:LEU:H    | 8        | 0.35          |
| (1,1398) | 1:88:A:VAL:HG22  | 1:85:A:LEU:H    | 13       | 0.35          |
| (1,1398) | 1:88:A:VAL:HG22  | 1:85:A:LEU:H    | 15       | 0.35          |
| (1,1365) | 1:32:A:ALA:HB1   | 1:28:A:ILE:HG21 | 2        | 0.35          |
| (1,1365) | 1:32:A:ALA:HB3   | 1:28:A:ILE:HG22 | 14       | 0.35          |
| (1,1331) | 1:78:A:TYR:HE2   | 1:84:A:TYR:HD2  | 2        | 0.35          |
| (1,1331) | 1:78:A:TYR:HE2   | 1:84:A:TYR:HD2  | 17       | 0.35          |
| (1,1322) | 1:28:A:ILE:H     | 1:27:A:VAL:HG13 | 8        | 0.35          |
| (1,1322) | 1:28:A:ILE:H     | 1:27:A:VAL:HG13 | 9        | 0.35          |
| (1,1322) | 1:28:A:ILE:H     | 1:27:A:VAL:HG12 | 15       | 0.35          |
| (1,1304) | 1:97:A:LEU:HD22  | 1:56:A:LEU:HA   | 5        | 0.35          |
| (1,1304) | 1:97:A:LEU:HD22  | 1:56:A:LEU:HA   | 6        | 0.35          |
| (1,1273) | 1:45:A:ALA:HB2   | 1:84:A:TYR:HB3  | 2        | 0.35          |
| (1,1124) | 1:97:A:LEU:HD13  | 1:57:A:VAL:H    | 10       | 0.35          |
| (1,1124) | 1:97:A:LEU:HD12  | 1:57:A:VAL:H    | 13       | 0.35          |
| (1,1061) | 1:21:A:LEU:HD23  | 1:27:A:VAL:HG11 | 1        | 0.35          |
| (1,1061) | 1:21:A:LEU:HD23  | 1:27:A:VAL:HG11 | 9        | 0.35          |
| (1,1061) | 1:21:A:LEU:HD22  | 1:27:A:VAL:HG11 | 12       | 0.35          |
| (1,1061) | 1:21:A:LEU:HD22  | 1:27:A:VAL:HG12 | 13       | 0.35          |
| (1,1061) | 1:21:A:LEU:HD21  | 1:27:A:VAL:HG13 | 17       | 0.35          |
| (1,1048) | 1:124:A:VAL:HG22 | 1:120:A:ALA:HA  | 13       | 0.35          |
| (1,979)  | 1:122:A:ALA:HA   | 1:122:A:ALA:HB2 | 4        | 0.35          |
| (1,979)  | 1:122:A:ALA:HA   | 1:122:A:ALA:HB1 | 5        | 0.35          |
| (1,979)  | 1:122:A:ALA:HA   | 1:122:A:ALA:HB2 | 6        | 0.35          |
| (1,979)  | 1:122:A:ALA:HA   | 1:122:A:ALA:HB2 | 9        | 0.35          |
| (1,979)  | 1:122:A:ALA:HA   | 1:122:A:ALA:HB2 | 10       | 0.35          |
| (1,979)  | 1:122:A:ALA:HA   | 1:122:A:ALA:HB2 | 12       | 0.35          |
| (1,979)  | 1:122:A:ALA:HA   | 1:122:A:ALA:HB1 | 14       | 0.35          |
| (1,979)  | 1:122:A:ALA:HA   | 1:122:A:ALA:HB1 | 15       | 0.35          |
| (1,979)  | 1:122:A:ALA:HA   | 1:122:A:ALA:HB1 | 17       | 0.35          |
| (1,942)  | 1:93:A:THR:HB    | 1:95:A:VAL:HG13 | 16       | 0.35          |
| (1,909)  | 1:53:A:PHE:HE2   | 1:72:A:ARG:HG3  | 11       | 0.35          |
| (1,909)  | 1:53:A:PHE:HE1   | 1:72:A:ARG:HG3  | 14       | 0.35          |
| (1,825)  | 1:45:A:ALA:HB2   | 1:78:A:TYR:HB3  | 3        | 0.35          |
| (1,822)  | 1:49:A:LYS:H     | 1:52:A:ILE:HD13 | 2        | 0.35          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,788)  | 1:52:A:ILE:HD12  | 1:56:A:LEU:H     | 2        | 0.35          |
| (1,788)  | 1:52:A:ILE:HD11  | 1:56:A:LEU:H     | 13       | 0.35          |
| (1,788)  | 1:52:A:ILE:HD13  | 1:56:A:LEU:H     | 15       | 0.35          |
| (1,575)  | 1:31:A:LEU:H     | 1:28:A:ILE:HD13  | 3        | 0.35          |
| (1,575)  | 1:31:A:LEU:H     | 1:28:A:ILE:HD12  | 9        | 0.35          |
| (1,575)  | 1:31:A:LEU:H     | 1:28:A:ILE:HD13  | 16       | 0.35          |
| (1,564)  | 1:59:A:ARG:HE    | 1:97:A:LEU:HD11  | 14       | 0.35          |
| (1,557)  | 1:66:A:LEU:HB2   | 1:70:A:GLN:HE22  | 5        | 0.35          |
| (1,552)  | 1:65:A:ASN:H     | 1:65:A:ASN:HD21  | 13       | 0.35          |
| (1,228)  | 1:95:A:VAL:HG22  | 1:100:A:ASN:H    | 10       | 0.35          |
| (1,228)  | 1:95:A:VAL:HG23  | 1:100:A:ASN:H    | 12       | 0.35          |
| (1,32)   | 1:53:A:PHE:H     | 1:53:A:PHE:HD2   | 13       | 0.35          |
| (1,12)   | 1:100:A:ASN:H    | 1:100:A:ASN:HD21 | 10       | 0.35          |
| (3,147)  | 1:71:A:LEU:H     | 1:66:A:LEU:HD22  | 14       | 0.34          |
| (3,147)  | 1:71:A:LEU:H     | 1:66:A:LEU:HD23  | 15       | 0.34          |
| (3,139)  | 1:66:A:LEU:HD21  | 1:70:A:GLN:H     | 12       | 0.34          |
| (3,135)  | 1:123:A:ARG:HB3  | 1:120:A:ALA:HA   | 9        | 0.34          |
| (3,135)  | 1:123:A:ARG:HB3  | 1:120:A:ALA:HA   | 10       | 0.34          |
| (3,123)  | 1:50:A:ILE:HD13  | 1:79:A:THR:HA    | 5        | 0.34          |
| (3,112)  | 1:82:A:TRP:HA    | 1:117:A:LEU:HD12 | 15       | 0.34          |
| (3,110)  | 1:105:A:LEU:HG   | 1:110:A:VAL:HG22 | 13       | 0.34          |
| (3,95)   | 1:75:A:LEU:HD13  | 1:50:A:ILE:H     | 2        | 0.34          |
| (3,87)   | 1:117:A:LEU:HD12 | 1:121:A:LYS:H    | 16       | 0.34          |
| (3,83)   | 1:114:A:ARG:HB2  | 1:113:A:ALA:HB3  | 13       | 0.34          |
| (3,83)   | 1:114:A:ARG:HB2  | 1:113:A:ALA:HB1  | 15       | 0.34          |
| (3,69)   | 1:57:A:VAL:HA    | 1:71:A:LEU:HB2   | 11       | 0.34          |
| (3,64)   | 1:55:A:ASP:HB2   | 1:52:A:ILE:HG21  | 2        | 0.34          |
| (3,59)   | 1:117:A:LEU:HA   | 1:85:A:LEU:HD21  | 1        | 0.34          |
| (3,36)   | 1:49:A:LYS:HB2   | 1:52:A:ILE:HD11  | 1        | 0.34          |
| (3,22)   | 1:48:A:LEU:H     | 1:48:A:LEU:HD12  | 5        | 0.34          |
| (3,18)   | 1:58:A:ASP:HB3   | 1:60:A:VAL:HG13  | 15       | 0.34          |
| (1,4342) | 1:38:A:CYS:H     | 1:95:A:VAL:HG11  | 8        | 0.34          |
| (1,4300) | 1:92:A:ALA:H     | 1:105:A:LEU:HD23 | 9        | 0.34          |
| (1,4255) | 1:75:A:LEU:HD23  | 1:54:A:GLN:H     | 1        | 0.34          |
| (1,4255) | 1:75:A:LEU:HD21  | 1:54:A:GLN:H     | 11       | 0.34          |
| (1,4210) | 1:110:A:VAL:HG11 | 1:113:A:ALA:H    | 6        | 0.34          |
| (1,4114) | 1:65:A:ASN:H     | 1:65:A:ASN:HD21  | 2        | 0.34          |
| (1,4045) | 1:21:A:LEU:HD12  | 1:23:A:SER:H     | 8        | 0.34          |
| (1,3889) | 1:100:A:ASN:HB3  | 1:100:A:ASN:HD21 | 11       | 0.34          |
| (1,3845) | 1:95:A:VAL:HG11  | 1:96:A:ASP:H     | 14       | 0.34          |
| (1,3839) | 1:65:A:ASN:HB3   | 1:65:A:ASN:HD21  | 9        | 0.34          |
| (1,3769) | 1:130:A:GLU:H    | 1:129:A:ALA:HB1  | 9        | 0.34          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3769) | 1:130:A:GLU:H    | 1:129:A:ALA:HB1  | 10       | 0.34          |
| (1,3769) | 1:130:A:GLU:H    | 1:129:A:ALA:HB3  | 17       | 0.34          |
| (1,3744) | 1:35:A:PHE:HD1   | 1:39:A:PHE:H     | 8        | 0.34          |
| (1,3738) | 1:103:A:GLY:HA3  | 1:104:A:GLU:H    | 2        | 0.34          |
| (1,3732) | 1:21:A:LEU:HD13  | 1:30:A:PHE:H     | 2        | 0.34          |
| (1,3732) | 1:21:A:LEU:HD12  | 1:30:A:PHE:H     | 3        | 0.34          |
| (1,3732) | 1:21:A:LEU:HD13  | 1:30:A:PHE:H     | 5        | 0.34          |
| (1,3732) | 1:21:A:LEU:HD11  | 1:30:A:PHE:H     | 6        | 0.34          |
| (1,3732) | 1:21:A:LEU:HD13  | 1:30:A:PHE:H     | 13       | 0.34          |
| (1,3732) | 1:21:A:LEU:HD11  | 1:30:A:PHE:H     | 14       | 0.34          |
| (1,3732) | 1:21:A:LEU:HD13  | 1:30:A:PHE:H     | 15       | 0.34          |
| (1,3678) | 1:95:A:VAL:H     | 1:96:A:ASP:H     | 4        | 0.34          |
| (1,3678) | 1:95:A:VAL:H     | 1:96:A:ASP:H     | 10       | 0.34          |
| (1,3678) | 1:95:A:VAL:H     | 1:96:A:ASP:H     | 13       | 0.34          |
| (1,3627) | 1:100:A:ASN:H    | 1:100:A:ASN:HD21 | 3        | 0.34          |
| (1,3612) | 1:120:A:ALA:HB2  | 1:120:A:ALA:HA   | 1        | 0.34          |
| (1,3612) | 1:120:A:ALA:HB2  | 1:120:A:ALA:HA   | 6        | 0.34          |
| (1,3610) | 1:121:A:LYS:HG3  | 1:117:A:LEU:HD13 | 4        | 0.34          |
| (1,3606) | 1:117:A:LEU:HA   | 1:82:A:TRP:HZ2   | 12       | 0.34          |
| (1,3600) | 1:113:A:ALA:HB1  | 1:92:A:ALA:HA    | 11       | 0.34          |
| (1,3590) | 1:110:A:VAL:HG22 | 1:109:A:HIS:HB2  | 2        | 0.34          |
| (1,3590) | 1:110:A:VAL:HG21 | 1:109:A:HIS:HB2  | 3        | 0.34          |
| (1,3590) | 1:110:A:VAL:HG21 | 1:109:A:HIS:HB2  | 5        | 0.34          |
| (1,3590) | 1:110:A:VAL:HG22 | 1:109:A:HIS:HB2  | 11       | 0.34          |
| (1,3584) | 1:110:A:VAL:HA   | 1:105:A:LEU:HD21 | 10       | 0.34          |
| (1,3564) | 1:105:A:LEU:HB3  | 1:104:A:GLU:HG2  | 1        | 0.34          |
| (1,3564) | 1:105:A:LEU:HB3  | 1:104:A:GLU:HG2  | 3        | 0.34          |
| (1,3513) | 1:72:A:ARG:HG3   | 1:73:A:SER:HB3   | 12       | 0.34          |
| (1,3481) | 1:83:A:ARG:HD3   | 1:45:A:ALA:HB1   | 11       | 0.34          |
| (1,3427) | 1:117:A:LEU:HA   | 1:117:A:LEU:H    | 1        | 0.34          |
| (1,3427) | 1:117:A:LEU:HA   | 1:117:A:LEU:H    | 4        | 0.34          |
| (1,3427) | 1:117:A:LEU:HA   | 1:117:A:LEU:H    | 6        | 0.34          |
| (1,3427) | 1:117:A:LEU:HA   | 1:117:A:LEU:H    | 10       | 0.34          |
| (1,3427) | 1:117:A:LEU:HA   | 1:117:A:LEU:H    | 13       | 0.34          |
| (1,3427) | 1:117:A:LEU:HA   | 1:117:A:LEU:H    | 16       | 0.34          |
| (1,3417) | 1:117:A:LEU:HG   | 1:117:A:LEU:HD11 | 7        | 0.34          |
| (1,3405) | 1:55:A:ASP:HB2   | 1:56:A:LEU:HD21  | 8        | 0.34          |
| (1,3405) | 1:55:A:ASP:HB2   | 1:56:A:LEU:HD23  | 17       | 0.34          |
| (1,3402) | 1:58:A:ASP:H     | 1:55:A:ASP:HA    | 8        | 0.34          |
| (1,3402) | 1:58:A:ASP:H     | 1:55:A:ASP:HA    | 12       | 0.34          |
| (1,3402) | 1:58:A:ASP:H     | 1:55:A:ASP:HA    | 16       | 0.34          |
| (1,3386) | 1:90:A:PRO:HA    | 1:92:A:ALA:HB1   | 17       | 0.34          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3345) | 1:29:A:ALA:HA   | 1:29:A:ALA:HB3  | 5        | 0.34          |
| (1,3345) | 1:29:A:ALA:HA   | 1:29:A:ALA:HB2  | 14       | 0.34          |
| (1,3319) | 1:66:A:LEU:HD21 | 1:27:A:VAL:HG12 | 1        | 0.34          |
| (1,3319) | 1:66:A:LEU:HD23 | 1:27:A:VAL:HG13 | 5        | 0.34          |
| (1,3319) | 1:66:A:LEU:HD21 | 1:27:A:VAL:HG11 | 15       | 0.34          |
| (1,3266) | 1:85:A:LEU:HD12 | 1:85:A:LEU:HD23 | 13       | 0.34          |
| (1,3228) | 1:31:A:LEU:HB2  | 1:39:A:PHE:HE2  | 17       | 0.34          |
| (1,3216) | 1:48:A:LEU:HG   | 1:84:A:TYR:HD1  | 10       | 0.34          |
| (1,3198) | 1:114:A:ARG:HA  | 1:113:A:ALA:HB1 | 2        | 0.34          |
| (1,3161) | 1:82:A:TRP:HH2  | 1:120:A:ALA:HB3 | 4        | 0.34          |
| (1,3161) | 1:82:A:TRP:HH2  | 1:120:A:ALA:HB1 | 10       | 0.34          |
| (1,3161) | 1:82:A:TRP:HH2  | 1:120:A:ALA:HB3 | 14       | 0.34          |
| (1,3135) | 1:68:A:LYS:HD3  | 1:68:A:LYS:HB2  | 2        | 0.34          |
| (1,3135) | 1:68:A:LYS:HD3  | 1:68:A:LYS:HB2  | 4        | 0.34          |
| (1,3135) | 1:68:A:LYS:HD3  | 1:68:A:LYS:HB2  | 7        | 0.34          |
| (1,3135) | 1:68:A:LYS:HD3  | 1:68:A:LYS:HB2  | 9        | 0.34          |
| (1,3115) | 1:58:A:ASP:HA   | 1:57:A:VAL:HG23 | 8        | 0.34          |
| (1,3114) | 1:57:A:VAL:HG22 | 1:57:A:VAL:HG11 | 3        | 0.34          |
| (1,3114) | 1:57:A:VAL:HG22 | 1:57:A:VAL:HG11 | 13       | 0.34          |
| (1,3103) | 1:56:A:LEU:HD12 | 1:60:A:VAL:HB   | 4        | 0.34          |
| (1,3103) | 1:56:A:LEU:HD13 | 1:60:A:VAL:HB   | 10       | 0.34          |
| (1,3092) | 1:55:A:ASP:HA   | 1:56:A:LEU:HB3  | 3        | 0.34          |
| (1,3092) | 1:55:A:ASP:HA   | 1:56:A:LEU:HB3  | 12       | 0.34          |
| (1,3081) | 1:97:A:LEU:HD13 | 1:55:A:ASP:HA   | 2        | 0.34          |
| (1,3077) | 1:54:A:GLN:HB2  | 1:57:A:VAL:HG11 | 1        | 0.34          |
| (1,3077) | 1:54:A:GLN:HB2  | 1:57:A:VAL:HG13 | 14       | 0.34          |
| (1,3077) | 1:54:A:GLN:HB2  | 1:57:A:VAL:HG11 | 15       | 0.34          |
| (1,3067) | 1:52:A:ILE:HG23 | 1:53:A:PHE:HB3  | 1        | 0.34          |
| (1,3051) | 1:78:A:TYR:HE1  | 1:28:A:ILE:HG22 | 6        | 0.34          |
| (1,3036) | 1:78:A:TYR:HH   | 1:45:A:ALA:HB3  | 3        | 0.34          |
| (1,3024) | 1:64:A:MET:HE2  | 1:65:A:ASN:HB3  | 2        | 0.34          |
| (1,3024) | 1:64:A:MET:HE3  | 1:65:A:ASN:HB3  | 8        | 0.34          |
| (1,3022) | 1:64:A:MET:HE3  | 1:30:A:PHE:HA   | 3        | 0.34          |
| (1,3022) | 1:64:A:MET:HE1  | 1:30:A:PHE:HA   | 12       | 0.34          |
| (1,3002) | 1:57:A:VAL:HG12 | 1:60:A:VAL:HB   | 1        | 0.34          |
| (1,3002) | 1:57:A:VAL:HG12 | 1:60:A:VAL:HB   | 2        | 0.34          |
| (1,3002) | 1:57:A:VAL:HG12 | 1:60:A:VAL:HB   | 15       | 0.34          |
| (1,2991) | 1:54:A:GLN:HE22 | 1:54:A:GLN:HG2  | 15       | 0.34          |
| (1,2991) | 1:54:A:GLN:HE22 | 1:54:A:GLN:HG2  | 17       | 0.34          |
| (1,2942) | 1:57:A:VAL:HG21 | 1:57:A:VAL:HB   | 1        | 0.34          |
| (1,2942) | 1:57:A:VAL:HG21 | 1:57:A:VAL:HB   | 13       | 0.34          |
| (1,2933) | 1:95:A:VAL:HG22 | 1:99:A:GLY:H    | 15       | 0.34          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2931) | 1:88:A:VAL:HG22 | 1:85:A:LEU:H     | 14       | 0.34          |
| (1,2873) | 1:126:A:ALA:HA  | 1:126:A:ALA:HB2  | 12       | 0.34          |
| (1,2873) | 1:126:A:ALA:HA  | 1:126:A:ALA:HB2  | 15       | 0.34          |
| (1,2870) | 1:133:A:ALA:HA  | 1:133:A:ALA:HB3  | 14       | 0.34          |
| (1,2865) | 1:78:A:TYR:HE2  | 1:48:A:LEU:HD11  | 4        | 0.34          |
| (1,2863) | 1:78:A:TYR:HE1  | 1:84:A:TYR:HD2   | 7        | 0.34          |
| (1,2863) | 1:78:A:TYR:HE1  | 1:84:A:TYR:HD1   | 10       | 0.34          |
| (1,2861) | 1:84:A:TYR:HE1  | 1:84:A:TYR:HA    | 5        | 0.34          |
| (1,2851) | 1:50:A:ILE:HG23 | 1:50:A:ILE:HA    | 11       | 0.34          |
| (1,2845) | 1:22:A:ASN:H    | 1:27:A:VAL:HG12  | 7        | 0.34          |
| (1,2830) | 1:39:A:PHE:HZ   | 1:97:A:LEU:HD21  | 8        | 0.34          |
| (1,2830) | 1:39:A:PHE:HZ   | 1:97:A:LEU:HD23  | 10       | 0.34          |
| (1,2824) | 1:97:A:LEU:HD22 | 1:56:A:LEU:HA    | 7        | 0.34          |
| (1,2782) | 1:61:A:ALA:HB2  | 1:62:A:GLY:HA2   | 11       | 0.34          |
| (1,2753) | 1:97:A:LEU:HD13 | 1:59:A:ARG:HD3   | 14       | 0.34          |
| (1,2720) | 1:86:A:TYR:HB3  | 1:117:A:LEU:HD13 | 1        | 0.34          |
| (1,2675) | 1:85:A:LEU:HB2  | 1:86:A:TYR:HD1   | 7        | 0.34          |
| (1,2597) | 1:21:A:LEU:HD23 | 1:27:A:VAL:HG11  | 6        | 0.34          |
| (1,2597) | 1:21:A:LEU:HD23 | 1:27:A:VAL:HG13  | 15       | 0.34          |
| (1,2569) | 1:82:A:TRP:HZ2  | 1:124:A:VAL:HG21 | 6        | 0.34          |
| (1,2569) | 1:82:A:TRP:HZ2  | 1:124:A:VAL:HG23 | 9        | 0.34          |
| (1,2513) | 1:122:A:ALA:HA  | 1:122:A:ALA:HB1  | 3        | 0.34          |
| (1,2513) | 1:122:A:ALA:HA  | 1:122:A:ALA:HB1  | 7        | 0.34          |
| (1,2513) | 1:122:A:ALA:HA  | 1:122:A:ALA:HB1  | 13       | 0.34          |
| (1,2468) | 1:53:A:PHE:HE2  | 1:72:A:ARG:HG3   | 6        | 0.34          |
| (1,2418) | 1:113:A:ALA:HB2 | 1:110:A:VAL:HG13 | 15       | 0.34          |
| (1,2412) | 1:45:A:ALA:HB2  | 1:78:A:TYR:HB3   | 16       | 0.34          |
| (1,2370) | 1:50:A:ILE:HG13 | 1:50:A:ILE:HG23  | 3        | 0.34          |
| (1,2369) | 1:52:A:ILE:HD11 | 1:56:A:LEU:H     | 17       | 0.34          |
| (1,2367) | 1:52:A:ILE:H    | 1:52:A:ILE:HD13  | 2        | 0.34          |
| (1,2344) | 1:104:A:GLU:HG2 | 1:105:A:LEU:HD21 | 1        | 0.34          |
| (1,2344) | 1:104:A:GLU:HG2 | 1:105:A:LEU:HD22 | 3        | 0.34          |
| (1,2344) | 1:104:A:GLU:HG2 | 1:105:A:LEU:HD23 | 11       | 0.34          |
| (1,2336) | 1:64:A:MET:HE2  | 1:31:A:LEU:HA    | 9        | 0.34          |
| (1,2331) | 1:54:A:GLN:HG2  | 1:55:A:ASP:HA    | 8        | 0.34          |
| (1,2331) | 1:54:A:GLN:HG2  | 1:55:A:ASP:HA    | 12       | 0.34          |
| (1,2230) | 1:28:A:ILE:H    | 1:28:A:ILE:HG23  | 5        | 0.34          |
| (1,2230) | 1:28:A:ILE:H    | 1:28:A:ILE:HG23  | 6        | 0.34          |
| (1,2230) | 1:28:A:ILE:H    | 1:28:A:ILE:HG21  | 12       | 0.34          |
| (1,2201) | 1:64:A:MET:HB2  | 1:21:A:LEU:HD23  | 5        | 0.34          |
| (1,2196) | 1:107:A:GLU:HA  | 1:110:A:VAL:HG12 | 2        | 0.34          |
| (1,2190) | 1:61:A:ALA:HB3  | 1:62:A:GLY:HA2   | 2        | 0.34          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2190) | 1:61:A:ALA:HB3   | 1:62:A:GLY:HA2   | 4        | 0.34          |
| (1,2190) | 1:61:A:ALA:HB1   | 1:62:A:GLY:HA2   | 9        | 0.34          |
| (1,2178) | 1:48:A:LEU:HB2   | 1:52:A:ILE:HG21  | 7        | 0.34          |
| (1,2178) | 1:48:A:LEU:HB2   | 1:52:A:ILE:HG21  | 11       | 0.34          |
| (1,2163) | 1:78:A:TYR:HA    | 1:78:A:TYR:HD2   | 6        | 0.34          |
| (1,2163) | 1:78:A:TYR:HA    | 1:78:A:TYR:HD2   | 8        | 0.34          |
| (1,2163) | 1:78:A:TYR:HA    | 1:78:A:TYR:HD1   | 12       | 0.34          |
| (1,2036) | 1:97:A:LEU:HD22  | 1:97:A:LEU:HB2   | 6        | 0.34          |
| (1,2036) | 1:97:A:LEU:HD23  | 1:97:A:LEU:HB2   | 11       | 0.34          |
| (1,2005) | 1:95:A:VAL:HG23  | 1:48:A:LEU:HD12  | 2        | 0.34          |
| (1,1960) | 1:121:A:LYS:HG3  | 1:117:A:LEU:HD13 | 10       | 0.34          |
| (1,1955) | 1:92:A:ALA:HB3   | 1:113:A:ALA:HB3  | 2        | 0.34          |
| (1,1955) | 1:92:A:ALA:HB2   | 1:113:A:ALA:HB2  | 12       | 0.34          |
| (1,1912) | 1:64:A:MET:HE1   | 1:65:A:ASN:HB2   | 3        | 0.34          |
| (1,1879) | 1:124:A:VAL:HG13 | 1:124:A:VAL:HG23 | 1        | 0.34          |
| (1,1879) | 1:124:A:VAL:HG11 | 1:124:A:VAL:HG22 | 3        | 0.34          |
| (1,1879) | 1:124:A:VAL:HG13 | 1:124:A:VAL:HG21 | 4        | 0.34          |
| (1,1879) | 1:124:A:VAL:HG12 | 1:124:A:VAL:HG22 | 17       | 0.34          |
| (1,1870) | 1:86:A:TYR:HE2   | 1:85:A:LEU:HD22  | 1        | 0.34          |
| (1,1813) | 1:117:A:LEU:HD12 | 1:117:A:LEU:HB3  | 5        | 0.34          |
| (1,1813) | 1:117:A:LEU:HD11 | 1:117:A:LEU:HB3  | 6        | 0.34          |
| (1,1813) | 1:117:A:LEU:HD12 | 1:117:A:LEU:HB3  | 14       | 0.34          |
| (1,1741) | 1:55:A:ASP:HB2   | 1:56:A:LEU:HD22  | 1        | 0.34          |
| (1,1735) | 1:66:A:LEU:HD23  | 1:67:A:SER:H     | 17       | 0.34          |
| (1,1656) | 1:31:A:LEU:HB2   | 1:39:A:PHE:HE1   | 10       | 0.34          |
| (1,1629) | 1:116:A:GLN:HG3  | 1:113:A:ALA:HB1  | 12       | 0.34          |
| (1,1521) | 1:30:A:PHE:HB3   | 1:29:A:ALA:HB3   | 11       | 0.34          |
| (1,1516) | 1:31:A:LEU:HD13  | 1:28:A:ILE:HG22  | 13       | 0.34          |
| (1,1490) | 1:78:A:TYR:HH    | 1:45:A:ALA:HB3   | 7        | 0.34          |
| (1,1490) | 1:78:A:TYR:HH    | 1:45:A:ALA:HB1   | 15       | 0.34          |
| (1,1450) | 1:54:A:GLN:HE22  | 1:54:A:GLN:HG2   | 5        | 0.34          |
| (1,1450) | 1:54:A:GLN:HE22  | 1:54:A:GLN:HG2   | 7        | 0.34          |
| (1,1408) | 1:57:A:VAL:HG23  | 1:57:A:VAL:HB    | 2        | 0.34          |
| (1,1408) | 1:57:A:VAL:HG23  | 1:57:A:VAL:HB    | 15       | 0.34          |
| (1,1408) | 1:57:A:VAL:HG21  | 1:57:A:VAL:HB    | 17       | 0.34          |
| (1,1400) | 1:95:A:VAL:HG21  | 1:99:A:GLY:H     | 7        | 0.34          |
| (1,1398) | 1:88:A:VAL:HG23  | 1:85:A:LEU:H     | 7        | 0.34          |
| (1,1375) | 1:110:A:VAL:HG11 | 1:91:A:GLY:HA2   | 8        | 0.34          |
| (1,1375) | 1:110:A:VAL:HG11 | 1:91:A:GLY:HA2   | 15       | 0.34          |
| (1,1375) | 1:110:A:VAL:HG12 | 1:91:A:GLY:HA2   | 17       | 0.34          |
| (1,1308) | 1:97:A:LEU:HD22  | 1:35:A:PHE:HD1   | 12       | 0.34          |
| (1,1307) | 1:97:A:LEU:HD23  | 1:97:A:LEU:HB2   | 8        | 0.34          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1232) | 1:60:A:VAL:HG12  | 1:59:A:ARG:HD3   | 7        | 0.34          |
| (1,1231) | 1:97:A:LEU:HD13  | 1:59:A:ARG:HD3   | 4        | 0.34          |
| (1,1231) | 1:97:A:LEU:HD12  | 1:59:A:ARG:HD3   | 12       | 0.34          |
| (1,1110) | 1:77:A:LEU:HD23  | 1:77:A:LEU:HB2   | 4        | 0.34          |
| (1,1110) | 1:77:A:LEU:HD23  | 1:77:A:LEU:HB2   | 6        | 0.34          |
| (1,1081) | 1:71:A:LEU:HD11  | 1:57:A:VAL:H     | 8        | 0.34          |
| (1,1062) | 1:27:A:VAL:HG21  | 1:27:A:VAL:HG11  | 7        | 0.34          |
| (1,1061) | 1:21:A:LEU:HD23  | 1:27:A:VAL:HG11  | 8        | 0.34          |
| (1,1061) | 1:21:A:LEU:HD23  | 1:27:A:VAL:HG12  | 10       | 0.34          |
| (1,1060) | 1:74:A:ALA:HB1   | 1:27:A:VAL:HG11  | 13       | 0.34          |
| (1,1048) | 1:124:A:VAL:HG21 | 1:120:A:ALA:HA   | 8        | 0.34          |
| (1,909)  | 1:53:A:PHE:HE1   | 1:72:A:ARG:HG3   | 8        | 0.34          |
| (1,909)  | 1:53:A:PHE:HE2   | 1:72:A:ARG:HG3   | 10       | 0.34          |
| (1,909)  | 1:53:A:PHE:HE2   | 1:72:A:ARG:HG3   | 17       | 0.34          |
| (1,825)  | 1:45:A:ALA:HB2   | 1:78:A:TYR:HB3   | 5        | 0.34          |
| (1,697)  | 1:57:A:VAL:HG13  | 1:56:A:LEU:H     | 12       | 0.34          |
| (1,575)  | 1:31:A:LEU:H     | 1:28:A:ILE:HD11  | 5        | 0.34          |
| (1,570)  | 1:60:A:VAL:HG11  | 1:34:A:ARG:HE    | 14       | 0.34          |
| (1,552)  | 1:65:A:ASN:H     | 1:65:A:ASN:HD21  | 7        | 0.34          |
| (1,552)  | 1:65:A:ASN:H     | 1:65:A:ASN:HD21  | 16       | 0.34          |
| (1,549)  | 1:97:A:LEU:HD13  | 1:98:A:ASP:H     | 7        | 0.34          |
| (1,488)  | 1:21:A:LEU:HD11  | 1:23:A:SER:H     | 12       | 0.34          |
| (1,410)  | 1:53:A:PHE:H     | 1:56:A:LEU:HB3   | 2        | 0.34          |
| (1,228)  | 1:95:A:VAL:HG23  | 1:100:A:ASN:H    | 8        | 0.34          |
| (1,117)  | 1:27:A:VAL:HG11  | 1:26:A:GLU:H     | 3        | 0.34          |
| (1,32)   | 1:53:A:PHE:H     | 1:53:A:PHE:HD1   | 1        | 0.34          |
| (1,32)   | 1:53:A:PHE:H     | 1:53:A:PHE:HD1   | 16       | 0.34          |
| (3,143)  | 1:25:A:LYS:H     | 1:77:A:LEU:HD23  | 4        | 0.33          |
| (3,122)  | 1:27:A:VAL:HG21  | 1:28:A:ILE:HD13  | 6        | 0.33          |
| (3,119)  | 1:98:A:ASP:HB3   | 1:99:A:GLY:HA2   | 9        | 0.33          |
| (3,117)  | 1:48:A:LEU:HD21  | 1:39:A:PHE:HD1   | 17       | 0.33          |
| (3,110)  | 1:105:A:LEU:HG   | 1:110:A:VAL:HG21 | 5        | 0.33          |
| (3,110)  | 1:105:A:LEU:HG   | 1:110:A:VAL:HG22 | 11       | 0.33          |
| (3,109)  | 1:92:A:ALA:H     | 1:110:A:VAL:HB   | 11       | 0.33          |
| (3,87)   | 1:117:A:LEU:HD12 | 1:121:A:LYS:H    | 10       | 0.33          |
| (3,86)   | 1:84:A:TYR:HE1   | 1:47:A:PRO:HB3   | 2        | 0.33          |
| (3,72)   | 1:117:A:LEU:HG   | 1:117:A:LEU:H    | 2        | 0.33          |
| (3,36)   | 1:50:A:ILE:HG23  | 1:49:A:LYS:HB2   | 17       | 0.33          |
| (3,22)   | 1:48:A:LEU:HD12  | 1:97:A:LEU:H     | 17       | 0.33          |
| (3,18)   | 1:58:A:ASP:HB3   | 1:60:A:VAL:HG12  | 7        | 0.33          |
| (3,15)   | 1:85:A:LEU:HB3   | 1:82:A:TRP:HA    | 4        | 0.33          |
| (1,4342) | 1:38:A:CYS:H     | 1:95:A:VAL:HG12  | 14       | 0.33          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,4323) | 1:62:A:GLY:H     | 1:68:A:LYS:HD2   | 5        | 0.33          |
| (1,4300) | 1:92:A:ALA:H     | 1:105:A:LEU:HD22 | 5        | 0.33          |
| (1,4255) | 1:75:A:LEU:HD23  | 1:54:A:GLN:H     | 5        | 0.33          |
| (1,4255) | 1:75:A:LEU:HD23  | 1:54:A:GLN:H     | 6        | 0.33          |
| (1,4255) | 1:75:A:LEU:HD23  | 1:54:A:GLN:H     | 14       | 0.33          |
| (1,4230) | 1:128:A:ARG:HA   | 1:128:A:ARG:H    | 11       | 0.33          |
| (1,4210) | 1:110:A:VAL:HG11 | 1:113:A:ALA:H    | 3        | 0.33          |
| (1,4210) | 1:110:A:VAL:HG12 | 1:113:A:ALA:H    | 5        | 0.33          |
| (1,4210) | 1:110:A:VAL:HG12 | 1:113:A:ALA:H    | 10       | 0.33          |
| (1,4210) | 1:110:A:VAL:HG13 | 1:113:A:ALA:H    | 15       | 0.33          |
| (1,4210) | 1:110:A:VAL:HG11 | 1:113:A:ALA:H    | 17       | 0.33          |
| (1,4197) | 1:66:A:LEU:HD23  | 1:67:A:SER:H     | 6        | 0.33          |
| (1,4109) | 1:97:A:LEU:HD11  | 1:98:A:ASP:H     | 16       | 0.33          |
| (1,4083) | 1:21:A:LEU:HA    | 1:22:A:ASN:HD22  | 15       | 0.33          |
| (1,3845) | 1:95:A:VAL:HG13  | 1:96:A:ASP:H     | 6        | 0.33          |
| (1,3839) | 1:65:A:ASN:HB3   | 1:65:A:ASN:HD21  | 7        | 0.33          |
| (1,3786) | 1:27:A:VAL:HG11  | 1:21:A:LEU:H     | 6        | 0.33          |
| (1,3738) | 1:103:A:GLY:HA3  | 1:104:A:GLU:H    | 1        | 0.33          |
| (1,3738) | 1:103:A:GLY:HA3  | 1:104:A:GLU:H    | 10       | 0.33          |
| (1,3738) | 1:103:A:GLY:HA3  | 1:104:A:GLU:H    | 16       | 0.33          |
| (1,3738) | 1:103:A:GLY:HA3  | 1:104:A:GLU:H    | 17       | 0.33          |
| (1,3732) | 1:21:A:LEU:HD11  | 1:30:A:PHE:H     | 11       | 0.33          |
| (1,3732) | 1:21:A:LEU:HD12  | 1:30:A:PHE:H     | 16       | 0.33          |
| (1,3678) | 1:95:A:VAL:H     | 1:96:A:ASP:H     | 7        | 0.33          |
| (1,3612) | 1:120:A:ALA:HB2  | 1:120:A:ALA:HA   | 4        | 0.33          |
| (1,3612) | 1:120:A:ALA:HB2  | 1:120:A:ALA:HA   | 5        | 0.33          |
| (1,3612) | 1:120:A:ALA:HB2  | 1:120:A:ALA:HA   | 16       | 0.33          |
| (1,3590) | 1:110:A:VAL:HG21 | 1:109:A:HIS:HB2  | 1        | 0.33          |
| (1,3590) | 1:110:A:VAL:HG23 | 1:109:A:HIS:HB2  | 7        | 0.33          |
| (1,3590) | 1:110:A:VAL:HG22 | 1:109:A:HIS:HB2  | 10       | 0.33          |
| (1,3590) | 1:110:A:VAL:HG22 | 1:109:A:HIS:HB2  | 14       | 0.33          |
| (1,3584) | 1:110:A:VAL:HA   | 1:105:A:LEU:HD21 | 2        | 0.33          |
| (1,3584) | 1:110:A:VAL:HA   | 1:105:A:LEU:HD22 | 16       | 0.33          |
| (1,3570) | 1:90:A:PRO:HA    | 1:105:A:LEU:HD12 | 4        | 0.33          |
| (1,3564) | 1:105:A:LEU:HB3  | 1:104:A:GLU:HG2  | 5        | 0.33          |
| (1,3505) | 1:124:A:VAL:HG11 | 1:124:A:VAL:HG23 | 9        | 0.33          |
| (1,3481) | 1:83:A:ARG:HD3   | 1:45:A:ALA:HB2   | 15       | 0.33          |
| (1,3481) | 1:83:A:ARG:HD3   | 1:45:A:ALA:HB2   | 17       | 0.33          |
| (1,3446) | 1:65:A:ASN:HD22  | 1:20:A:LYS:HG2   | 12       | 0.33          |
| (1,3446) | 1:65:A:ASN:HD22  | 1:20:A:LYS:HG2   | 17       | 0.33          |
| (1,3427) | 1:117:A:LEU:HA   | 1:117:A:LEU:H    | 8        | 0.33          |
| (1,3427) | 1:117:A:LEU:HA   | 1:117:A:LEU:H    | 14       | 0.33          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3414) | 1:86:A:TYR:H    | 1:117:A:LEU:HD11 | 7        | 0.33          |
| (1,3414) | 1:86:A:TYR:H    | 1:117:A:LEU:HD11 | 11       | 0.33          |
| (1,3405) | 1:55:A:ASP:HB2  | 1:56:A:LEU:HD23  | 10       | 0.33          |
| (1,3405) | 1:55:A:ASP:HB2  | 1:56:A:LEU:HD21  | 12       | 0.33          |
| (1,3402) | 1:58:A:ASP:H    | 1:55:A:ASP:HA    | 2        | 0.33          |
| (1,3402) | 1:58:A:ASP:H    | 1:55:A:ASP:HA    | 10       | 0.33          |
| (1,3402) | 1:58:A:ASP:H    | 1:55:A:ASP:HA    | 15       | 0.33          |
| (1,3377) | 1:40:A:SER:HB2  | 1:41:A:ALA:HB2   | 17       | 0.33          |
| (1,3341) | 1:41:A:ALA:HB2  | 1:28:A:ILE:HG23  | 17       | 0.33          |
| (1,3319) | 1:66:A:LEU:HD21 | 1:27:A:VAL:HG13  | 4        | 0.33          |
| (1,3319) | 1:66:A:LEU:HD21 | 1:27:A:VAL:HG13  | 11       | 0.33          |
| (1,3282) | 1:44:A:GLU:HG2  | 1:45:A:ALA:HB2   | 10       | 0.33          |
| (1,3266) | 1:85:A:LEU:HD11 | 1:85:A:LEU:HD21  | 6        | 0.33          |
| (1,3264) | 1:121:A:LYS:HG2 | 1:121:A:LYS:H    | 12       | 0.33          |
| (1,3258) | 1:48:A:LEU:HD13 | 1:50:A:ILE:HA    | 10       | 0.33          |
| (1,3258) | 1:48:A:LEU:HD12 | 1:50:A:ILE:HA    | 13       | 0.33          |
| (1,3216) | 1:48:A:LEU:HG   | 1:84:A:TYR:HD2   | 7        | 0.33          |
| (1,3216) | 1:48:A:LEU:HG   | 1:84:A:TYR:HD1   | 11       | 0.33          |
| (1,3216) | 1:48:A:LEU:HG   | 1:84:A:TYR:HD1   | 13       | 0.33          |
| (1,3216) | 1:48:A:LEU:HG   | 1:84:A:TYR:HD2   | 16       | 0.33          |
| (1,3198) | 1:114:A:ARG:HA  | 1:113:A:ALA:HB2  | 7        | 0.33          |
| (1,3198) | 1:114:A:ARG:HA  | 1:113:A:ALA:HB3  | 8        | 0.33          |
| (1,3198) | 1:114:A:ARG:HA  | 1:113:A:ALA:HB3  | 10       | 0.33          |
| (1,3198) | 1:114:A:ARG:HA  | 1:113:A:ALA:HB1  | 15       | 0.33          |
| (1,3189) | 1:110:A:VAL:HA  | 1:105:A:LEU:HD13 | 6        | 0.33          |
| (1,3161) | 1:82:A:TRP:HH2  | 1:120:A:ALA:HB2  | 12       | 0.33          |
| (1,3161) | 1:82:A:TRP:HH2  | 1:120:A:ALA:HB1  | 15       | 0.33          |
| (1,3135) | 1:68:A:LYS:HD3  | 1:68:A:LYS:HB2   | 6        | 0.33          |
| (1,3132) | 1:68:A:LYS:HB2  | 1:53:A:PHE:HE1   | 17       | 0.33          |
| (1,3114) | 1:57:A:VAL:HG22 | 1:57:A:VAL:HG11  | 1        | 0.33          |
| (1,3103) | 1:56:A:LEU:HD11 | 1:60:A:VAL:HB    | 14       | 0.33          |
| (1,3092) | 1:55:A:ASP:HA   | 1:56:A:LEU:HB3   | 2        | 0.33          |
| (1,3092) | 1:55:A:ASP:HA   | 1:56:A:LEU:HB3   | 13       | 0.33          |
| (1,3077) | 1:54:A:GLN:HB2  | 1:57:A:VAL:HG13  | 7        | 0.33          |
| (1,3077) | 1:54:A:GLN:HB2  | 1:57:A:VAL:HG12  | 12       | 0.33          |
| (1,3061) | 1:31:A:LEU:HD13 | 1:28:A:ILE:HG21  | 14       | 0.33          |
| (1,3051) | 1:78:A:TYR:HE2  | 1:28:A:ILE:HG23  | 12       | 0.33          |
| (1,3045) | 1:52:A:ILE:HG13 | 1:54:A:GLN:HE21  | 14       | 0.33          |
| (1,3036) | 1:78:A:TYR:HH   | 1:45:A:ALA:HB3   | 9        | 0.33          |
| (1,3027) | 1:57:A:VAL:HA   | 1:71:A:LEU:HD13  | 3        | 0.33          |
| (1,3027) | 1:57:A:VAL:HA   | 1:71:A:LEU:HD13  | 7        | 0.33          |
| (1,3027) | 1:57:A:VAL:HA   | 1:71:A:LEU:HD12  | 9        | 0.33          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3027) | 1:57:A:VAL:HA   | 1:71:A:LEU:HD11  | 11       | 0.33          |
| (1,3022) | 1:64:A:MET:HE2  | 1:30:A:PHE:HA    | 1        | 0.33          |
| (1,2942) | 1:57:A:VAL:HG21 | 1:57:A:VAL:HB    | 7        | 0.33          |
| (1,2937) | 1:95:A:VAL:HG21 | 1:95:A:VAL:HG11  | 2        | 0.33          |
| (1,2937) | 1:95:A:VAL:HG23 | 1:95:A:VAL:HG12  | 14       | 0.33          |
| (1,2933) | 1:95:A:VAL:HG21 | 1:99:A:GLY:H     | 17       | 0.33          |
| (1,2931) | 1:88:A:VAL:HG22 | 1:85:A:LEU:H     | 6        | 0.33          |
| (1,2931) | 1:88:A:VAL:HG22 | 1:85:A:LEU:H     | 9        | 0.33          |
| (1,2931) | 1:88:A:VAL:HG23 | 1:85:A:LEU:H     | 12       | 0.33          |
| (1,2873) | 1:126:A:ALA:HA  | 1:126:A:ALA:HB2  | 7        | 0.33          |
| (1,2872) | 1:129:A:ALA:HB3 | 1:129:A:ALA:HA   | 11       | 0.33          |
| (1,2861) | 1:84:A:TYR:HE2  | 1:84:A:TYR:HA    | 7        | 0.33          |
| (1,2861) | 1:84:A:TYR:HE2  | 1:84:A:TYR:HA    | 15       | 0.33          |
| (1,2842) | 1:28:A:ILE:H    | 1:27:A:VAL:HG11  | 2        | 0.33          |
| (1,2842) | 1:28:A:ILE:H    | 1:27:A:VAL:HG11  | 3        | 0.33          |
| (1,2842) | 1:28:A:ILE:H    | 1:27:A:VAL:HG11  | 11       | 0.33          |
| (1,2842) | 1:28:A:ILE:H    | 1:27:A:VAL:HG11  | 13       | 0.33          |
| (1,2842) | 1:28:A:ILE:H    | 1:27:A:VAL:HG11  | 14       | 0.33          |
| (1,2831) | 1:97:A:LEU:HD22 | 1:35:A:PHE:HD2   | 10       | 0.33          |
| (1,2831) | 1:97:A:LEU:HD22 | 1:35:A:PHE:HD2   | 17       | 0.33          |
| (1,2830) | 1:39:A:PHE:HZ   | 1:97:A:LEU:HD22  | 1        | 0.33          |
| (1,2830) | 1:39:A:PHE:HZ   | 1:97:A:LEU:HD23  | 3        | 0.33          |
| (1,2830) | 1:39:A:PHE:HZ   | 1:97:A:LEU:HD21  | 13       | 0.33          |
| (1,2830) | 1:39:A:PHE:HZ   | 1:97:A:LEU:HD22  | 16       | 0.33          |
| (1,2830) | 1:39:A:PHE:HZ   | 1:97:A:LEU:HD23  | 17       | 0.33          |
| (1,2753) | 1:97:A:LEU:HD11 | 1:59:A:ARG:HD3   | 17       | 0.33          |
| (1,2675) | 1:85:A:LEU:HB2  | 1:86:A:TYR:HD2   | 3        | 0.33          |
| (1,2672) | 1:31:A:LEU:HD13 | 1:35:A:PHE:HD1   | 11       | 0.33          |
| (1,2662) | 1:97:A:LEU:HD12 | 1:57:A:VAL:H     | 16       | 0.33          |
| (1,2597) | 1:21:A:LEU:HD21 | 1:27:A:VAL:HG12  | 3        | 0.33          |
| (1,2597) | 1:21:A:LEU:HD22 | 1:27:A:VAL:HG12  | 5        | 0.33          |
| (1,2583) | 1:60:A:VAL:HG13 | 1:34:A:ARG:HG2   | 1        | 0.33          |
| (1,2569) | 1:82:A:TRP:HZ2  | 1:124:A:VAL:HG22 | 3        | 0.33          |
| (1,2569) | 1:82:A:TRP:HZ2  | 1:124:A:VAL:HG22 | 5        | 0.33          |
| (1,2542) | 1:21:A:LEU:HD11 | 1:30:A:PHE:HA    | 8        | 0.33          |
| (1,2513) | 1:122:A:ALA:HA  | 1:122:A:ALA:HB1  | 1        | 0.33          |
| (1,2513) | 1:122:A:ALA:HA  | 1:122:A:ALA:HB2  | 4        | 0.33          |
| (1,2513) | 1:122:A:ALA:HA  | 1:122:A:ALA:HB1  | 5        | 0.33          |
| (1,2513) | 1:122:A:ALA:HA  | 1:122:A:ALA:HB2  | 6        | 0.33          |
| (1,2513) | 1:122:A:ALA:HA  | 1:122:A:ALA:HB3  | 8        | 0.33          |
| (1,2513) | 1:122:A:ALA:HA  | 1:122:A:ALA:HB2  | 9        | 0.33          |
| (1,2513) | 1:122:A:ALA:HA  | 1:122:A:ALA:HB2  | 12       | 0.33          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2513) | 1:122:A:ALA:HA   | 1:122:A:ALA:HB3  | 16       | 0.33          |
| (1,2513) | 1:122:A:ALA:HA   | 1:122:A:ALA:HB1  | 17       | 0.33          |
| (1,2468) | 1:53:A:PHE:HE1   | 1:72:A:ARG:HG3   | 2        | 0.33          |
| (1,2468) | 1:53:A:PHE:HE2   | 1:72:A:ARG:HG3   | 9        | 0.33          |
| (1,2418) | 1:113:A:ALA:HB2  | 1:110:A:VAL:HG13 | 2        | 0.33          |
| (1,2418) | 1:113:A:ALA:HB2  | 1:110:A:VAL:HG12 | 5        | 0.33          |
| (1,2418) | 1:113:A:ALA:HB1  | 1:110:A:VAL:HG13 | 8        | 0.33          |
| (1,2417) | 1:129:A:ALA:HB1  | 1:127:A:GLN:HB3  | 7        | 0.33          |
| (1,2415) | 1:45:A:ALA:HB1   | 1:84:A:TYR:HD1   | 8        | 0.33          |
| (1,2412) | 1:45:A:ALA:HB2   | 1:78:A:TYR:HB3   | 9        | 0.33          |
| (1,2409) | 1:49:A:LYS:H     | 1:52:A:ILE:HD11  | 9        | 0.33          |
| (1,2409) | 1:49:A:LYS:H     | 1:52:A:ILE:HD12  | 13       | 0.33          |
| (1,2370) | 1:50:A:ILE:HG13  | 1:50:A:ILE:HG21  | 1        | 0.33          |
| (1,2370) | 1:50:A:ILE:HG13  | 1:50:A:ILE:HG21  | 5        | 0.33          |
| (1,2369) | 1:52:A:ILE:HD12  | 1:56:A:LEU:H     | 8        | 0.33          |
| (1,2367) | 1:52:A:ILE:H     | 1:52:A:ILE:HD11  | 16       | 0.33          |
| (1,2363) | 1:48:A:LEU:HD13  | 1:84:A:TYR:HE2   | 17       | 0.33          |
| (1,2350) | 1:110:A:VAL:HG21 | 1:110:A:VAL:HA   | 1        | 0.33          |
| (1,2350) | 1:110:A:VAL:HG21 | 1:110:A:VAL:HA   | 3        | 0.33          |
| (1,2350) | 1:110:A:VAL:HG21 | 1:110:A:VAL:HA   | 5        | 0.33          |
| (1,2350) | 1:110:A:VAL:HG23 | 1:110:A:VAL:HA   | 7        | 0.33          |
| (1,2350) | 1:110:A:VAL:HG23 | 1:110:A:VAL:HA   | 8        | 0.33          |
| (1,2350) | 1:110:A:VAL:HG22 | 1:110:A:VAL:HA   | 11       | 0.33          |
| (1,2350) | 1:110:A:VAL:HG22 | 1:110:A:VAL:HA   | 15       | 0.33          |
| (1,2350) | 1:110:A:VAL:HG21 | 1:110:A:VAL:HA   | 17       | 0.33          |
| (1,2346) | 1:105:A:LEU:HD13 | 1:107:A:GLU:HA   | 1        | 0.33          |
| (1,2344) | 1:104:A:GLU:HG2  | 1:105:A:LEU:HD21 | 15       | 0.33          |
| (1,2331) | 1:54:A:GLN:HG2   | 1:55:A:ASP:HA    | 10       | 0.33          |
| (1,2268) | 1:110:A:VAL:HG11 | 1:89:A:LYS:H     | 3        | 0.33          |
| (1,2268) | 1:110:A:VAL:HG12 | 1:89:A:LYS:H     | 9        | 0.33          |
| (1,2230) | 1:28:A:ILE:H     | 1:28:A:ILE:HG23  | 13       | 0.33          |
| (1,2230) | 1:28:A:ILE:H     | 1:28:A:ILE:HG22  | 14       | 0.33          |
| (1,2230) | 1:28:A:ILE:H     | 1:28:A:ILE:HG23  | 15       | 0.33          |
| (1,2179) | 1:52:A:ILE:HG21  | 1:48:A:LEU:HB3   | 7        | 0.33          |
| (1,2179) | 1:52:A:ILE:HG21  | 1:48:A:LEU:HB3   | 10       | 0.33          |
| (1,2163) | 1:78:A:TYR:HA    | 1:78:A:TYR:HD1   | 7        | 0.33          |
| (1,2149) | 1:21:A:LEU:HD21  | 1:30:A:PHE:HD2   | 11       | 0.33          |
| (1,2088) | 1:82:A:TRP:HZ2   | 1:124:A:VAL:HG21 | 11       | 0.33          |
| (1,2088) | 1:82:A:TRP:HZ2   | 1:124:A:VAL:HG21 | 13       | 0.33          |
| (1,2036) | 1:97:A:LEU:HD23  | 1:97:A:LEU:HB2   | 9        | 0.33          |
| (1,2036) | 1:97:A:LEU:HD22  | 1:97:A:LEU:HB2   | 12       | 0.33          |
| (1,2025) | 1:97:A:LEU:HD22  | 1:35:A:PHE:HD2   | 3        | 0.33          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2025) | 1:97:A:LEU:HD22  | 1:35:A:PHE:HD2   | 15       | 0.33          |
| (1,2006) | 1:78:A:TYR:HE1   | 1:48:A:LEU:HD13  | 2        | 0.33          |
| (1,1960) | 1:121:A:LYS:HG3  | 1:117:A:LEU:HD12 | 1        | 0.33          |
| (1,1960) | 1:121:A:LYS:HG3  | 1:117:A:LEU:HD13 | 16       | 0.33          |
| (1,1955) | 1:92:A:ALA:HB2   | 1:113:A:ALA:HB1  | 6        | 0.33          |
| (1,1955) | 1:92:A:ALA:HB2   | 1:113:A:ALA:HB1  | 17       | 0.33          |
| (1,1947) | 1:93:A:THR:HB    | 1:88:A:VAL:HG11  | 4        | 0.33          |
| (1,1903) | 1:122:A:ALA:HB3  | 1:121:A:LYS:HE3  | 16       | 0.33          |
| (1,1879) | 1:124:A:VAL:HG12 | 1:124:A:VAL:HG21 | 11       | 0.33          |
| (1,1879) | 1:124:A:VAL:HG11 | 1:124:A:VAL:HG21 | 12       | 0.33          |
| (1,1870) | 1:86:A:TYR:HE1   | 1:85:A:LEU:HD22  | 8        | 0.33          |
| (1,1811) | 1:86:A:TYR:H     | 1:117:A:LEU:HD13 | 2        | 0.33          |
| (1,1799) | 1:71:A:LEU:HA    | 1:74:A:ALA:HB2   | 3        | 0.33          |
| (1,1735) | 1:66:A:LEU:HD23  | 1:67:A:SER:H     | 8        | 0.33          |
| (1,1686) | 1:85:A:LEU:HD13  | 1:85:A:LEU:HD22  | 1        | 0.33          |
| (1,1683) | 1:48:A:LEU:HD12  | 1:38:A:CYS:HA    | 4        | 0.33          |
| (1,1679) | 1:92:A:ALA:HB2   | 1:91:A:GLY:H     | 6        | 0.33          |
| (1,1679) | 1:92:A:ALA:HB1   | 1:91:A:GLY:H     | 11       | 0.33          |
| (1,1656) | 1:31:A:LEU:HB2   | 1:39:A:PHE:HE2   | 6        | 0.33          |
| (1,1656) | 1:31:A:LEU:HB2   | 1:39:A:PHE:HE2   | 7        | 0.33          |
| (1,1514) | 1:52:A:ILE:HG23  | 1:48:A:LEU:HG    | 2        | 0.33          |
| (1,1514) | 1:52:A:ILE:HG22  | 1:48:A:LEU:HG    | 4        | 0.33          |
| (1,1490) | 1:78:A:TYR:HH    | 1:45:A:ALA:HB3   | 10       | 0.33          |
| (1,1490) | 1:78:A:TYR:HH    | 1:45:A:ALA:HB3   | 16       | 0.33          |
| (1,1484) | 1:57:A:VAL:HA    | 1:71:A:LEU:HD13  | 2        | 0.33          |
| (1,1483) | 1:21:A:LEU:HG    | 1:64:A:MET:HE3   | 9        | 0.33          |
| (1,1480) | 1:64:A:MET:HE3   | 1:63:A:GLU:H     | 8        | 0.33          |
| (1,1408) | 1:57:A:VAL:HG23  | 1:57:A:VAL:HB    | 8        | 0.33          |
| (1,1408) | 1:57:A:VAL:HG23  | 1:57:A:VAL:HB    | 12       | 0.33          |
| (1,1405) | 1:102:A:CYS:H    | 1:95:A:VAL:HG13  | 11       | 0.33          |
| (1,1400) | 1:95:A:VAL:HG23  | 1:99:A:GLY:H     | 4        | 0.33          |
| (1,1375) | 1:110:A:VAL:HG13 | 1:91:A:GLY:HA2   | 10       | 0.33          |
| (1,1375) | 1:110:A:VAL:HG12 | 1:91:A:GLY:HA2   | 12       | 0.33          |
| (1,1375) | 1:110:A:VAL:HG11 | 1:91:A:GLY:HA2   | 16       | 0.33          |
| (1,1322) | 1:28:A:ILE:H     | 1:27:A:VAL:HG11  | 7        | 0.33          |
| (1,1307) | 1:97:A:LEU:HD22  | 1:97:A:LEU:HB2   | 6        | 0.33          |
| (1,1307) | 1:97:A:LEU:HD23  | 1:97:A:LEU:HB2   | 11       | 0.33          |
| (1,1304) | 1:97:A:LEU:HD22  | 1:56:A:LEU:HA    | 3        | 0.33          |
| (1,1304) | 1:97:A:LEU:HD23  | 1:56:A:LEU:HA    | 11       | 0.33          |
| (1,1304) | 1:97:A:LEU:HD22  | 1:56:A:LEU:HA    | 15       | 0.33          |
| (1,1304) | 1:97:A:LEU:HD21  | 1:56:A:LEU:HA    | 16       | 0.33          |
| (1,1231) | 1:97:A:LEU:HD13  | 1:59:A:ARG:HD3   | 3        | 0.33          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1231) | 1:97:A:LEU:HD12 | 1:59:A:ARG:HD3   | 9        | 0.33          |
| (1,1231) | 1:97:A:LEU:HD13 | 1:59:A:ARG:HD3   | 15       | 0.33          |
| (1,1124) | 1:97:A:LEU:HD11 | 1:57:A:VAL:H     | 8        | 0.33          |
| (1,1110) | 1:77:A:LEU:HD21 | 1:77:A:LEU:HB2   | 9        | 0.33          |
| (1,1110) | 1:77:A:LEU:HD21 | 1:77:A:LEU:HB2   | 12       | 0.33          |
| (1,1081) | 1:71:A:LEU:HD12 | 1:57:A:VAL:H     | 14       | 0.33          |
| (1,1061) | 1:21:A:LEU:HD23 | 1:27:A:VAL:HG12  | 2        | 0.33          |
| (1,1061) | 1:21:A:LEU:HD21 | 1:27:A:VAL:HG12  | 11       | 0.33          |
| (1,1061) | 1:21:A:LEU:HD22 | 1:27:A:VAL:HG12  | 14       | 0.33          |
| (1,1061) | 1:21:A:LEU:HD22 | 1:27:A:VAL:HG11  | 16       | 0.33          |
| (1,1060) | 1:74:A:ALA:HB3  | 1:27:A:VAL:HG11  | 7        | 0.33          |
| (1,1030) | 1:86:A:TYR:HE1  | 1:86:A:TYR:HB2   | 8        | 0.33          |
| (1,909)  | 1:53:A:PHE:HE1  | 1:72:A:ARG:HG3   | 5        | 0.33          |
| (1,909)  | 1:53:A:PHE:HE1  | 1:72:A:ARG:HG3   | 15       | 0.33          |
| (1,909)  | 1:53:A:PHE:HE1  | 1:72:A:ARG:HG3   | 16       | 0.33          |
| (1,895)  | 1:129:A:ALA:HB1 | 1:129:A:ALA:HA   | 6        | 0.33          |
| (1,852)  | 1:65:A:ASN:HB3  | 1:65:A:ASN:HD21  | 2        | 0.33          |
| (1,818)  | 1:28:A:ILE:HD11 | 1:78:A:TYR:HB3   | 2        | 0.33          |
| (1,788)  | 1:52:A:ILE:HD12 | 1:56:A:LEU:H     | 1        | 0.33          |
| (1,788)  | 1:52:A:ILE:HD12 | 1:56:A:LEU:H     | 4        | 0.33          |
| (1,618)  | 1:95:A:VAL:H    | 1:48:A:LEU:HD11  | 12       | 0.33          |
| (1,564)  | 1:59:A:ARG:HE   | 1:97:A:LEU:HD13  | 7        | 0.33          |
| (1,528)  | 1:65:A:ASN:HB2  | 1:65:A:ASN:HD21  | 11       | 0.33          |
| (1,488)  | 1:21:A:LEU:HD11 | 1:23:A:SER:H     | 15       | 0.33          |
| (1,117)  | 1:27:A:VAL:HG13 | 1:26:A:GLU:H     | 12       | 0.33          |
| (1,116)  | 1:21:A:LEU:HD11 | 1:30:A:PHE:H     | 8        | 0.33          |
| (1,32)   | 1:53:A:PHE:H    | 1:53:A:PHE:HD2   | 17       | 0.33          |
| (1,12)   | 1:100:A:ASN:H   | 1:100:A:ASN:HD21 | 2        | 0.33          |
| (1,12)   | 1:100:A:ASN:H   | 1:100:A:ASN:HD21 | 14       | 0.33          |
| (3,152)  | 1:27:A:VAL:H    | 1:74:A:ALA:HB1   | 9        | 0.32          |
| (3,152)  | 1:27:A:VAL:H    | 1:74:A:ALA:HB1   | 14       | 0.32          |
| (3,147)  | 1:71:A:LEU:H    | 1:66:A:LEU:HD22  | 5        | 0.32          |
| (3,143)  | 1:25:A:LYS:H    | 1:77:A:LEU:HD23  | 13       | 0.32          |
| (3,123)  | 1:50:A:ILE:HD12 | 1:79:A:THR:HA    | 13       | 0.32          |
| (3,119)  | 1:98:A:ASP:HB3  | 1:99:A:GLY:HA2   | 3        | 0.32          |
| (3,119)  | 1:98:A:ASP:HB3  | 1:99:A:GLY:HA2   | 4        | 0.32          |
| (3,119)  | 1:98:A:ASP:HB3  | 1:99:A:GLY:HA2   | 7        | 0.32          |
| (3,106)  | 1:68:A:LYS:HD2  | 1:68:A:LYS:HA    | 17       | 0.32          |
| (3,98)   | 1:64:A:MET:HE1  | 1:63:A:GLU:HG3   | 14       | 0.32          |
| (3,93)   | 1:21:A:LEU:HB3  | 1:21:A:LEU:HD12  | 7        | 0.32          |
| (3,92)   | 1:88:A:VAL:HG23 | 1:87:A:GLY:HA2   | 14       | 0.32          |
| (3,83)   | 1:114:A:ARG:HB2 | 1:113:A:ALA:HB3  | 10       | 0.32          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (3,83)   | 1:114:A:ARG:HB2  | 1:113:A:ALA:HB2  | 12       | 0.32          |
| (3,83)   | 1:114:A:ARG:HB2  | 1:113:A:ALA:HB3  | 14       | 0.32          |
| (3,72)   | 1:117:A:LEU:HG   | 1:117:A:LEU:H    | 11       | 0.32          |
| (3,72)   | 1:117:A:LEU:HG   | 1:117:A:LEU:H    | 17       | 0.32          |
| (3,69)   | 1:57:A:VAL:HA    | 1:71:A:LEU:HB2   | 14       | 0.32          |
| (3,59)   | 1:117:A:LEU:HA   | 1:85:A:LEU:HD22  | 4        | 0.32          |
| (3,52)   | 1:95:A:VAL:HG22  | 1:37:A:HIS:HB2   | 1        | 0.32          |
| (3,31)   | 1:22:A:ASN:HD21  | 1:22:A:ASN:HB2   | 11       | 0.32          |
| (1,4300) | 1:92:A:ALA:H     | 1:105:A:LEU:HD23 | 2        | 0.32          |
| (1,4300) | 1:92:A:ALA:H     | 1:105:A:LEU:HD23 | 8        | 0.32          |
| (1,4280) | 1:112:A:HIS:HA   | 1:116:A:GLN:H    | 1        | 0.32          |
| (1,4255) | 1:75:A:LEU:HD22  | 1:54:A:GLN:H     | 2        | 0.32          |
| (1,4247) | 1:54:A:GLN:HE22  | 1:57:A:VAL:HG11  | 15       | 0.32          |
| (1,4230) | 1:128:A:ARG:HA   | 1:128:A:ARG:H    | 4        | 0.32          |
| (1,4210) | 1:110:A:VAL:HG12 | 1:113:A:ALA:H    | 1        | 0.32          |
| (1,4210) | 1:110:A:VAL:HG13 | 1:113:A:ALA:H    | 2        | 0.32          |
| (1,4210) | 1:110:A:VAL:HG12 | 1:113:A:ALA:H    | 9        | 0.32          |
| (1,4210) | 1:110:A:VAL:HG13 | 1:113:A:ALA:H    | 11       | 0.32          |
| (1,4210) | 1:110:A:VAL:HG11 | 1:113:A:ALA:H    | 12       | 0.32          |
| (1,4210) | 1:110:A:VAL:HG11 | 1:113:A:ALA:H    | 13       | 0.32          |
| (1,4210) | 1:110:A:VAL:HG13 | 1:113:A:ALA:H    | 16       | 0.32          |
| (1,4171) | 1:48:A:LEU:HD21  | 1:49:A:LYS:H     | 4        | 0.32          |
| (1,4153) | 1:18:A:GLN:HB3   | 1:18:A:GLN:H     | 4        | 0.32          |
| (1,4153) | 1:18:A:GLN:HB3   | 1:18:A:GLN:H     | 12       | 0.32          |
| (1,4119) | 1:66:A:LEU:HB2   | 1:70:A:GLN:HE22  | 11       | 0.32          |
| (1,4084) | 1:20:A:LYS:HB3   | 1:22:A:ASN:HD22  | 17       | 0.32          |
| (1,4006) | 1:42:A:GLU:HB3   | 1:41:A:ALA:H     | 9        | 0.32          |
| (1,3972) | 1:53:A:PHE:H     | 1:56:A:LEU:HB3   | 17       | 0.32          |
| (1,3889) | 1:100:A:ASN:HB3  | 1:100:A:ASN:HD21 | 6        | 0.32          |
| (1,3738) | 1:103:A:GLY:HA3  | 1:104:A:GLU:H    | 4        | 0.32          |
| (1,3738) | 1:103:A:GLY:HA3  | 1:104:A:GLU:H    | 8        | 0.32          |
| (1,3738) | 1:103:A:GLY:HA3  | 1:104:A:GLU:H    | 9        | 0.32          |
| (1,3738) | 1:103:A:GLY:HA3  | 1:104:A:GLU:H    | 12       | 0.32          |
| (1,3738) | 1:103:A:GLY:HA3  | 1:104:A:GLU:H    | 13       | 0.32          |
| (1,3738) | 1:103:A:GLY:HA3  | 1:104:A:GLU:H    | 15       | 0.32          |
| (1,3733) | 1:27:A:VAL:HG11  | 1:26:A:GLU:H     | 7        | 0.32          |
| (1,3733) | 1:27:A:VAL:HG11  | 1:26:A:GLU:H     | 11       | 0.32          |
| (1,3733) | 1:27:A:VAL:HG11  | 1:26:A:GLU:H     | 13       | 0.32          |
| (1,3733) | 1:27:A:VAL:HG12  | 1:26:A:GLU:H     | 15       | 0.32          |
| (1,3728) | 1:29:A:ALA:HA    | 1:30:A:PHE:H     | 3        | 0.32          |
| (1,3728) | 1:29:A:ALA:HA    | 1:30:A:PHE:H     | 8        | 0.32          |
| (1,3678) | 1:95:A:VAL:H     | 1:96:A:ASP:H     | 2        | 0.32          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3678) | 1:95:A:VAL:H     | 1:96:A:ASP:H     | 8        | 0.32          |
| (1,3678) | 1:95:A:VAL:H     | 1:96:A:ASP:H     | 12       | 0.32          |
| (1,3678) | 1:95:A:VAL:H     | 1:96:A:ASP:H     | 14       | 0.32          |
| (1,3678) | 1:95:A:VAL:H     | 1:96:A:ASP:H     | 16       | 0.32          |
| (1,3627) | 1:100:A:ASN:H    | 1:100:A:ASN:HD21 | 15       | 0.32          |
| (1,3612) | 1:120:A:ALA:HB2  | 1:120:A:ALA:HA   | 13       | 0.32          |
| (1,3606) | 1:117:A:LEU:HA   | 1:82:A:TRP:HZ2   | 16       | 0.32          |
| (1,3599) | 1:92:A:ALA:HB3   | 1:113:A:ALA:HB3  | 2        | 0.32          |
| (1,3599) | 1:92:A:ALA:HB2   | 1:113:A:ALA:HB2  | 12       | 0.32          |
| (1,3584) | 1:110:A:VAL:HA   | 1:105:A:LEU:HD22 | 1        | 0.32          |
| (1,3584) | 1:110:A:VAL:HA   | 1:105:A:LEU:HD23 | 3        | 0.32          |
| (1,3584) | 1:110:A:VAL:HA   | 1:105:A:LEU:HD21 | 6        | 0.32          |
| (1,3584) | 1:110:A:VAL:HA   | 1:105:A:LEU:HD23 | 7        | 0.32          |
| (1,3584) | 1:110:A:VAL:HA   | 1:105:A:LEU:HD21 | 9        | 0.32          |
| (1,3584) | 1:110:A:VAL:HA   | 1:105:A:LEU:HD23 | 14       | 0.32          |
| (1,3564) | 1:105:A:LEU:HB3  | 1:104:A:GLU:HG2  | 4        | 0.32          |
| (1,3564) | 1:105:A:LEU:HB3  | 1:104:A:GLU:HG2  | 6        | 0.32          |
| (1,3564) | 1:105:A:LEU:HB3  | 1:104:A:GLU:HG2  | 14       | 0.32          |
| (1,3564) | 1:105:A:LEU:HB3  | 1:104:A:GLU:HG2  | 15       | 0.32          |
| (1,3564) | 1:105:A:LEU:HB3  | 1:104:A:GLU:HG2  | 16       | 0.32          |
| (1,3531) | 1:65:A:ASN:H     | 1:65:A:ASN:HA    | 4        | 0.32          |
| (1,3505) | 1:124:A:VAL:HG13 | 1:124:A:VAL:HG23 | 1        | 0.32          |
| (1,3505) | 1:124:A:VAL:HG11 | 1:124:A:VAL:HG22 | 3        | 0.32          |
| (1,3505) | 1:124:A:VAL:HG13 | 1:124:A:VAL:HG23 | 8        | 0.32          |
| (1,3505) | 1:124:A:VAL:HG12 | 1:124:A:VAL:HG22 | 17       | 0.32          |
| (1,3497) | 1:27:A:VAL:HA    | 1:27:A:VAL:HG11  | 9        | 0.32          |
| (1,3495) | 1:54:A:GLN:H     | 1:75:A:LEU:HD12  | 5        | 0.32          |
| (1,3495) | 1:54:A:GLN:H     | 1:75:A:LEU:HD13  | 14       | 0.32          |
| (1,3495) | 1:54:A:GLN:H     | 1:75:A:LEU:HD11  | 15       | 0.32          |
| (1,3465) | 1:88:A:VAL:HG21  | 1:85:A:LEU:HB3   | 3        | 0.32          |
| (1,3446) | 1:65:A:ASN:HD22  | 1:20:A:LYS:HG2   | 4        | 0.32          |
| (1,3416) | 1:117:A:LEU:HD13 | 1:117:A:LEU:HB3  | 1        | 0.32          |
| (1,3414) | 1:86:A:TYR:H     | 1:117:A:LEU:HD12 | 17       | 0.32          |
| (1,3402) | 1:58:A:ASP:H     | 1:55:A:ASP:HA    | 14       | 0.32          |
| (1,3402) | 1:58:A:ASP:H     | 1:55:A:ASP:HA    | 17       | 0.32          |
| (1,3401) | 1:86:A:TYR:HE2   | 1:86:A:TYR:HA    | 3        | 0.32          |
| (1,3396) | 1:71:A:LEU:HA    | 1:74:A:ALA:HB2   | 17       | 0.32          |
| (1,3330) | 1:25:A:LYS:HE3   | 1:77:A:LEU:HD12  | 1        | 0.32          |
| (1,3273) | 1:42:A:GLU:HG2   | 1:43:A:GLY:H     | 12       | 0.32          |
| (1,3264) | 1:121:A:LYS:HG2  | 1:121:A:LYS:H    | 3        | 0.32          |
| (1,3264) | 1:121:A:LYS:HG2  | 1:121:A:LYS:H    | 5        | 0.32          |
| (1,3264) | 1:121:A:LYS:HG2  | 1:121:A:LYS:H    | 7        | 0.32          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3264) | 1:121:A:LYS:HG2 | 1:121:A:LYS:H    | 17       | 0.32          |
| (1,3253) | 1:92:A:ALA:HB3  | 1:91:A:GLY:H     | 1        | 0.32          |
| (1,3223) | 1:84:A:TYR:HE1  | 1:79:A:THR:HA    | 9        | 0.32          |
| (1,3223) | 1:84:A:TYR:HE2  | 1:79:A:THR:HA    | 15       | 0.32          |
| (1,3216) | 1:48:A:LEU:HG   | 1:84:A:TYR:HD1   | 14       | 0.32          |
| (1,3198) | 1:114:A:ARG:HA  | 1:113:A:ALA:HB3  | 3        | 0.32          |
| (1,3198) | 1:114:A:ARG:HA  | 1:113:A:ALA:HB1  | 17       | 0.32          |
| (1,3197) | 1:87:A:GLY:HA3  | 1:113:A:ALA:HB1  | 1        | 0.32          |
| (1,3189) | 1:110:A:VAL:HA  | 1:105:A:LEU:HD13 | 12       | 0.32          |
| (1,3161) | 1:82:A:TRP:HH2  | 1:120:A:ALA:HB2  | 9        | 0.32          |
| (1,3135) | 1:68:A:LYS:HD3  | 1:68:A:LYS:HB2   | 14       | 0.32          |
| (1,3115) | 1:58:A:ASP:HA   | 1:57:A:VAL:HG23  | 2        | 0.32          |
| (1,3115) | 1:58:A:ASP:HA   | 1:57:A:VAL:HG22  | 4        | 0.32          |
| (1,3115) | 1:58:A:ASP:HA   | 1:57:A:VAL:HG22  | 9        | 0.32          |
| (1,3114) | 1:57:A:VAL:HG21 | 1:57:A:VAL:HG12  | 5        | 0.32          |
| (1,3114) | 1:57:A:VAL:HG23 | 1:57:A:VAL:HG12  | 10       | 0.32          |
| (1,3114) | 1:57:A:VAL:HG21 | 1:57:A:VAL:HG11  | 15       | 0.32          |
| (1,3114) | 1:57:A:VAL:HG22 | 1:57:A:VAL:HG11  | 16       | 0.32          |
| (1,3092) | 1:55:A:ASP:HA   | 1:56:A:LEU:HB3   | 1        | 0.32          |
| (1,3092) | 1:55:A:ASP:HA   | 1:56:A:LEU:HB3   | 11       | 0.32          |
| (1,3092) | 1:55:A:ASP:HA   | 1:56:A:LEU:HB3   | 16       | 0.32          |
| (1,3077) | 1:54:A:GLN:HB2  | 1:57:A:VAL:HG12  | 11       | 0.32          |
| (1,3061) | 1:31:A:LEU:HD11 | 1:28:A:ILE:HG23  | 2        | 0.32          |
| (1,3061) | 1:31:A:LEU:HD11 | 1:28:A:ILE:HG22  | 10       | 0.32          |
| (1,3027) | 1:57:A:VAL:HA   | 1:71:A:LEU:HD11  | 1        | 0.32          |
| (1,3027) | 1:57:A:VAL:HA   | 1:71:A:LEU:HD13  | 5        | 0.32          |
| (1,3027) | 1:57:A:VAL:HA   | 1:71:A:LEU:HD11  | 15       | 0.32          |
| (1,3025) | 1:21:A:LEU:HG   | 1:64:A:MET:HE2   | 7        | 0.32          |
| (1,3022) | 1:64:A:MET:HE2  | 1:30:A:PHE:HA    | 14       | 0.32          |
| (1,3022) | 1:64:A:MET:HE3  | 1:30:A:PHE:HA    | 15       | 0.32          |
| (1,2991) | 1:54:A:GLN:HE22 | 1:54:A:GLN:HG2   | 13       | 0.32          |
| (1,2942) | 1:57:A:VAL:HG21 | 1:57:A:VAL:HB    | 10       | 0.32          |
| (1,2942) | 1:57:A:VAL:HG23 | 1:57:A:VAL:HB    | 15       | 0.32          |
| (1,2942) | 1:57:A:VAL:HG21 | 1:57:A:VAL:HB    | 17       | 0.32          |
| (1,2931) | 1:88:A:VAL:HG22 | 1:85:A:LEU:H     | 2        | 0.32          |
| (1,2931) | 1:88:A:VAL:HG22 | 1:85:A:LEU:H     | 10       | 0.32          |
| (1,2891) | 1:32:A:ALA:HB3  | 1:28:A:ILE:HG22  | 14       | 0.32          |
| (1,2890) | 1:33:A:GLU:HB3  | 1:32:A:ALA:HB3   | 2        | 0.32          |
| (1,2873) | 1:126:A:ALA:HA  | 1:126:A:ALA:HB2  | 4        | 0.32          |
| (1,2863) | 1:78:A:TYR:HE2  | 1:84:A:TYR:HD1   | 6        | 0.32          |
| (1,2863) | 1:78:A:TYR:HE2  | 1:84:A:TYR:HD1   | 13       | 0.32          |
| (1,2842) | 1:28:A:ILE:H    | 1:27:A:VAL:HG13  | 1        | 0.32          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2842) | 1:28:A:ILE:H     | 1:27:A:VAL:HG11  | 4        | 0.32          |
| (1,2842) | 1:28:A:ILE:H     | 1:27:A:VAL:HG13  | 16       | 0.32          |
| (1,2841) | 1:110:A:VAL:HG11 | 1:109:A:HIS:H    | 10       | 0.32          |
| (1,2830) | 1:39:A:PHE:HZ    | 1:97:A:LEU:HD23  | 6        | 0.32          |
| (1,2830) | 1:39:A:PHE:HZ    | 1:97:A:LEU:HD23  | 12       | 0.32          |
| (1,2829) | 1:97:A:LEU:HD23  | 1:97:A:LEU:HB2   | 8        | 0.32          |
| (1,2785) | 1:50:A:ILE:HG23  | 1:51:A:GLY:HA3   | 17       | 0.32          |
| (1,2720) | 1:86:A:TYR:HB3   | 1:117:A:LEU:HD11 | 11       | 0.32          |
| (1,2662) | 1:97:A:LEU:HD11  | 1:57:A:VAL:H     | 12       | 0.32          |
| (1,2598) | 1:27:A:VAL:HG21  | 1:27:A:VAL:HG11  | 7        | 0.32          |
| (1,2597) | 1:21:A:LEU:HD23  | 1:27:A:VAL:HG11  | 1        | 0.32          |
| (1,2597) | 1:21:A:LEU:HD23  | 1:27:A:VAL:HG11  | 9        | 0.32          |
| (1,2597) | 1:21:A:LEU:HD22  | 1:27:A:VAL:HG11  | 12       | 0.32          |
| (1,2597) | 1:21:A:LEU:HD22  | 1:27:A:VAL:HG12  | 13       | 0.32          |
| (1,2597) | 1:21:A:LEU:HD21  | 1:27:A:VAL:HG13  | 17       | 0.32          |
| (1,2569) | 1:82:A:TRP:HZ2   | 1:124:A:VAL:HG21 | 15       | 0.32          |
| (1,2542) | 1:21:A:LEU:HD12  | 1:30:A:PHE:HA    | 1        | 0.32          |
| (1,2513) | 1:122:A:ALA:HA   | 1:122:A:ALA:HB2  | 10       | 0.32          |
| (1,2513) | 1:122:A:ALA:HA   | 1:122:A:ALA:HB1  | 14       | 0.32          |
| (1,2513) | 1:122:A:ALA:HA   | 1:122:A:ALA:HB1  | 15       | 0.32          |
| (1,2502) | 1:42:A:GLU:HA    | 1:43:A:GLY:H     | 7        | 0.32          |
| (1,2418) | 1:113:A:ALA:HB1  | 1:110:A:VAL:HG11 | 3        | 0.32          |
| (1,2418) | 1:113:A:ALA:HB3  | 1:110:A:VAL:HG12 | 7        | 0.32          |
| (1,2418) | 1:113:A:ALA:HB1  | 1:110:A:VAL:HG12 | 14       | 0.32          |
| (1,2415) | 1:45:A:ALA:HB3   | 1:84:A:TYR:HD2   | 7        | 0.32          |
| (1,2415) | 1:45:A:ALA:HB3   | 1:84:A:TYR:HD1   | 11       | 0.32          |
| (1,2412) | 1:45:A:ALA:HB1   | 1:78:A:TYR:HB3   | 2        | 0.32          |
| (1,2412) | 1:45:A:ALA:HB1   | 1:78:A:TYR:HB3   | 6        | 0.32          |
| (1,2412) | 1:45:A:ALA:HB2   | 1:78:A:TYR:HB3   | 13       | 0.32          |
| (1,2369) | 1:52:A:ILE:HD13  | 1:56:A:LEU:H     | 12       | 0.32          |
| (1,2367) | 1:52:A:ILE:H     | 1:52:A:ILE:HD11  | 12       | 0.32          |
| (1,2350) | 1:110:A:VAL:HG22 | 1:110:A:VAL:HA   | 2        | 0.32          |
| (1,2350) | 1:110:A:VAL:HG21 | 1:110:A:VAL:HA   | 4        | 0.32          |
| (1,2350) | 1:110:A:VAL:HG23 | 1:110:A:VAL:HA   | 6        | 0.32          |
| (1,2350) | 1:110:A:VAL:HG21 | 1:110:A:VAL:HA   | 9        | 0.32          |
| (1,2350) | 1:110:A:VAL:HG22 | 1:110:A:VAL:HA   | 10       | 0.32          |
| (1,2350) | 1:110:A:VAL:HG21 | 1:110:A:VAL:HA   | 12       | 0.32          |
| (1,2350) | 1:110:A:VAL:HG21 | 1:110:A:VAL:HA   | 16       | 0.32          |
| (1,2344) | 1:104:A:GLU:HG2  | 1:105:A:LEU:HD23 | 6        | 0.32          |
| (1,2331) | 1:54:A:GLN:HG2   | 1:55:A:ASP:HA    | 1        | 0.32          |
| (1,2331) | 1:54:A:GLN:HG2   | 1:55:A:ASP:HA    | 2        | 0.32          |
| (1,2331) | 1:54:A:GLN:HG2   | 1:55:A:ASP:HA    | 3        | 0.32          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2331) | 1:54:A:GLN:HG2   | 1:55:A:ASP:HA    | 4        | 0.32          |
| (1,2331) | 1:54:A:GLN:HG2   | 1:55:A:ASP:HA    | 9        | 0.32          |
| (1,2268) | 1:110:A:VAL:HG12 | 1:89:A:LYS:H     | 1        | 0.32          |
| (1,2190) | 1:61:A:ALA:HB2   | 1:62:A:GLY:HA2   | 12       | 0.32          |
| (1,2178) | 1:48:A:LEU:HB2   | 1:52:A:ILE:HG21  | 13       | 0.32          |
| (1,2178) | 1:48:A:LEU:HB2   | 1:52:A:ILE:HG21  | 16       | 0.32          |
| (1,2163) | 1:78:A:TYR:HA    | 1:78:A:TYR:HD2   | 1        | 0.32          |
| (1,2163) | 1:78:A:TYR:HA    | 1:78:A:TYR:HD1   | 16       | 0.32          |
| (1,2149) | 1:21:A:LEU:HD22  | 1:30:A:PHE:HD1   | 14       | 0.32          |
| (1,2099) | 1:21:A:LEU:HB2   | 1:21:A:LEU:HD22  | 10       | 0.32          |
| (1,2098) | 1:21:A:LEU:HD23  | 1:27:A:VAL:HG11  | 6        | 0.32          |
| (1,2098) | 1:21:A:LEU:HD23  | 1:27:A:VAL:HG13  | 15       | 0.32          |
| (1,2094) | 1:95:A:VAL:HG22  | 1:97:A:LEU:HD22  | 8        | 0.32          |
| (1,2088) | 1:82:A:TRP:HZ2   | 1:124:A:VAL:HG21 | 7        | 0.32          |
| (1,2088) | 1:82:A:TRP:HZ2   | 1:124:A:VAL:HG21 | 12       | 0.32          |
| (1,2088) | 1:82:A:TRP:HZ2   | 1:124:A:VAL:HG22 | 17       | 0.32          |
| (1,2036) | 1:97:A:LEU:HD22  | 1:97:A:LEU:HB2   | 3        | 0.32          |
| (1,2036) | 1:97:A:LEU:HD23  | 1:97:A:LEU:HB2   | 4        | 0.32          |
| (1,2036) | 1:97:A:LEU:HD22  | 1:97:A:LEU:HB2   | 10       | 0.32          |
| (1,2036) | 1:97:A:LEU:HD23  | 1:97:A:LEU:HB2   | 13       | 0.32          |
| (1,2036) | 1:97:A:LEU:HD22  | 1:97:A:LEU:HB2   | 15       | 0.32          |
| (1,2036) | 1:97:A:LEU:HD22  | 1:97:A:LEU:HB2   | 17       | 0.32          |
| (1,2005) | 1:95:A:VAL:HG22  | 1:48:A:LEU:HD11  | 9        | 0.32          |
| (1,1994) | 1:91:A:GLY:HA2   | 1:91:A:GLY:H     | 5        | 0.32          |
| (1,1955) | 1:92:A:ALA:HB3   | 1:113:A:ALA:HB3  | 3        | 0.32          |
| (1,1945) | 1:105:A:LEU:HB3  | 1:110:A:VAL:HG21 | 5        | 0.32          |
| (1,1945) | 1:105:A:LEU:HB3  | 1:110:A:VAL:HG22 | 14       | 0.32          |
| (1,1881) | 1:113:A:ALA:HB3  | 1:88:A:VAL:HA    | 1        | 0.32          |
| (1,1879) | 1:124:A:VAL:HG13 | 1:124:A:VAL:HG21 | 6        | 0.32          |
| (1,1879) | 1:124:A:VAL:HG12 | 1:124:A:VAL:HG21 | 10       | 0.32          |
| (1,1879) | 1:124:A:VAL:HG12 | 1:124:A:VAL:HG21 | 15       | 0.32          |
| (1,1879) | 1:124:A:VAL:HG12 | 1:124:A:VAL:HG23 | 16       | 0.32          |
| (1,1870) | 1:86:A:TYR:HE2   | 1:85:A:LEU:HD21  | 5        | 0.32          |
| (1,1870) | 1:86:A:TYR:HE1   | 1:85:A:LEU:HD21  | 6        | 0.32          |
| (1,1870) | 1:86:A:TYR:HE2   | 1:85:A:LEU:HD21  | 16       | 0.32          |
| (1,1866) | 1:83:A:ARG:HD3   | 1:45:A:ALA:HB1   | 9        | 0.32          |
| (1,1865) | 1:45:A:ALA:HB2   | 1:44:A:GLU:HB3   | 14       | 0.32          |
| (1,1813) | 1:117:A:LEU:HD11 | 1:117:A:LEU:HB3  | 10       | 0.32          |
| (1,1813) | 1:117:A:LEU:HD11 | 1:117:A:LEU:HB3  | 13       | 0.32          |
| (1,1813) | 1:117:A:LEU:HD11 | 1:117:A:LEU:HB3  | 16       | 0.32          |
| (1,1799) | 1:71:A:LEU:HA    | 1:74:A:ALA:HB3   | 7        | 0.32          |
| (1,1790) | 1:90:A:PRO:HA    | 1:92:A:ALA:HB2   | 15       | 0.32          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1698) | 1:44:A:GLU:HG2   | 1:45:A:ALA:HB1  | 7        | 0.32          |
| (1,1686) | 1:85:A:LEU:HD12  | 1:85:A:LEU:HD21 | 5        | 0.32          |
| (1,1686) | 1:85:A:LEU:HD13  | 1:85:A:LEU:HD23 | 9        | 0.32          |
| (1,1684) | 1:48:A:LEU:HD13  | 1:50:A:ILE:HA   | 5        | 0.32          |
| (1,1656) | 1:31:A:LEU:HB2   | 1:39:A:PHE:HE2  | 11       | 0.32          |
| (1,1656) | 1:31:A:LEU:HB2   | 1:39:A:PHE:HE1  | 14       | 0.32          |
| (1,1545) | 1:56:A:LEU:HD13  | 1:60:A:VAL:HB   | 12       | 0.32          |
| (1,1521) | 1:30:A:PHE:HB3   | 1:29:A:ALA:HB3  | 12       | 0.32          |
| (1,1521) | 1:30:A:PHE:HB3   | 1:29:A:ALA:HB3  | 15       | 0.32          |
| (1,1516) | 1:31:A:LEU:HD11  | 1:28:A:ILE:HG22 | 15       | 0.32          |
| (1,1490) | 1:78:A:TYR:HH    | 1:45:A:ALA:HB1  | 8        | 0.32          |
| (1,1485) | 1:71:A:LEU:HD12  | 1:72:A:ARG:HA   | 8        | 0.32          |
| (1,1485) | 1:71:A:LEU:HD12  | 1:72:A:ARG:HA   | 17       | 0.32          |
| (1,1484) | 1:57:A:VAL:HA    | 1:71:A:LEU:HD11 | 6        | 0.32          |
| (1,1484) | 1:57:A:VAL:HA    | 1:71:A:LEU:HD11 | 14       | 0.32          |
| (1,1482) | 1:64:A:MET:HE1   | 1:27:A:VAL:HA   | 4        | 0.32          |
| (1,1480) | 1:64:A:MET:HE1   | 1:63:A:GLU:H    | 3        | 0.32          |
| (1,1450) | 1:54:A:GLN:HE22  | 1:54:A:GLN:HG2  | 14       | 0.32          |
| (1,1403) | 1:95:A:VAL:HG23  | 1:95:A:VAL:HG11 | 13       | 0.32          |
| (1,1400) | 1:95:A:VAL:HG22  | 1:99:A:GLY:H    | 2        | 0.32          |
| (1,1400) | 1:95:A:VAL:HG22  | 1:99:A:GLY:H    | 10       | 0.32          |
| (1,1400) | 1:95:A:VAL:HG23  | 1:99:A:GLY:H    | 12       | 0.32          |
| (1,1400) | 1:95:A:VAL:HG21  | 1:99:A:GLY:H    | 14       | 0.32          |
| (1,1375) | 1:110:A:VAL:HG11 | 1:91:A:GLY:HA2  | 2        | 0.32          |
| (1,1375) | 1:110:A:VAL:HG12 | 1:91:A:GLY:HA2  | 4        | 0.32          |
| (1,1375) | 1:110:A:VAL:HG12 | 1:91:A:GLY:HA2  | 13       | 0.32          |
| (1,1365) | 1:32:A:ALA:HB2   | 1:28:A:ILE:HG23 | 13       | 0.32          |
| (1,1365) | 1:32:A:ALA:HB2   | 1:28:A:ILE:HG23 | 17       | 0.32          |
| (1,1331) | 1:78:A:TYR:HE2   | 1:84:A:TYR:HD1  | 9        | 0.32          |
| (1,1307) | 1:97:A:LEU:HD23  | 1:97:A:LEU:HB2  | 9        | 0.32          |
| (1,1307) | 1:97:A:LEU:HD22  | 1:97:A:LEU:HB2  | 12       | 0.32          |
| (1,1304) | 1:97:A:LEU:HD22  | 1:56:A:LEU:HA   | 10       | 0.32          |
| (1,1304) | 1:97:A:LEU:HD22  | 1:56:A:LEU:HA   | 14       | 0.32          |
| (1,1303) | 1:97:A:LEU:HD11  | 1:35:A:PHE:HE2  | 6        | 0.32          |
| (1,1124) | 1:97:A:LEU:HD12  | 1:57:A:VAL:H    | 15       | 0.32          |
| (1,1110) | 1:77:A:LEU:HD23  | 1:77:A:LEU:HB2  | 3        | 0.32          |
| (1,1110) | 1:77:A:LEU:HD22  | 1:77:A:LEU:HB2  | 5        | 0.32          |
| (1,1110) | 1:77:A:LEU:HD21  | 1:77:A:LEU:HB2  | 7        | 0.32          |
| (1,1110) | 1:77:A:LEU:HD23  | 1:77:A:LEU:HB2  | 13       | 0.32          |
| (1,1110) | 1:77:A:LEU:HD22  | 1:77:A:LEU:HB2  | 15       | 0.32          |
| (1,1110) | 1:77:A:LEU:HD22  | 1:77:A:LEU:HB2  | 16       | 0.32          |
| (1,1110) | 1:77:A:LEU:HD22  | 1:77:A:LEU:HB2  | 17       | 0.32          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1081) | 1:71:A:LEU:HD11  | 1:57:A:VAL:H     | 17       | 0.32          |
| (1,1062) | 1:27:A:VAL:HG23  | 1:27:A:VAL:HG13  | 16       | 0.32          |
| (1,1060) | 1:74:A:ALA:HB1   | 1:27:A:VAL:HG11  | 2        | 0.32          |
| (1,1060) | 1:74:A:ALA:HB3   | 1:27:A:VAL:HG11  | 4        | 0.32          |
| (1,1060) | 1:74:A:ALA:HB1   | 1:27:A:VAL:HG13  | 9        | 0.32          |
| (1,1048) | 1:124:A:VAL:HG22 | 1:120:A:ALA:HA   | 2        | 0.32          |
| (1,1048) | 1:124:A:VAL:HG22 | 1:120:A:ALA:HA   | 6        | 0.32          |
| (1,979)  | 1:122:A:ALA:HA   | 1:122:A:ALA:HB1  | 2        | 0.32          |
| (1,979)  | 1:122:A:ALA:HA   | 1:122:A:ALA:HB3  | 11       | 0.32          |
| (1,909)  | 1:53:A:PHE:HE2   | 1:72:A:ARG:HG3   | 3        | 0.32          |
| (1,909)  | 1:53:A:PHE:HE2   | 1:72:A:ARG:HG3   | 7        | 0.32          |
| (1,909)  | 1:53:A:PHE:HE2   | 1:72:A:ARG:HG3   | 13       | 0.32          |
| (1,895)  | 1:129:A:ALA:HB2  | 1:129:A:ALA:HA   | 4        | 0.32          |
| (1,852)  | 1:65:A:ASN:HB3   | 1:65:A:ASN:HD21  | 8        | 0.32          |
| (1,829)  | 1:41:A:ALA:HB2   | 1:41:A:ALA:H     | 1        | 0.32          |
| (1,790)  | 1:50:A:ILE:HG21  | 1:50:A:ILE:H     | 2        | 0.32          |
| (1,790)  | 1:50:A:ILE:HG22  | 1:50:A:ILE:H     | 17       | 0.32          |
| (1,788)  | 1:52:A:ILE:HD12  | 1:56:A:LEU:H     | 9        | 0.32          |
| (1,788)  | 1:52:A:ILE:HD13  | 1:56:A:LEU:H     | 16       | 0.32          |
| (1,575)  | 1:31:A:LEU:H     | 1:28:A:ILE:HD11  | 13       | 0.32          |
| (1,552)  | 1:65:A:ASN:H     | 1:65:A:ASN:HD21  | 9        | 0.32          |
| (1,532)  | 1:116:A:GLN:HG3  | 1:116:A:GLN:HE21 | 2        | 0.32          |
| (1,488)  | 1:21:A:LEU:HD13  | 1:23:A:SER:H     | 1        | 0.32          |
| (1,410)  | 1:53:A:PHE:H     | 1:56:A:LEU:HB3   | 8        | 0.32          |
| (1,410)  | 1:53:A:PHE:H     | 1:56:A:LEU:HB3   | 16       | 0.32          |
| (1,116)  | 1:21:A:LEU:HD12  | 1:30:A:PHE:H     | 1        | 0.32          |
| (3,148)  | 1:22:A:ASN:H     | 1:22:A:ASN:HB2   | 17       | 0.31          |
| (3,143)  | 1:25:A:LYS:H     | 1:77:A:LEU:HD21  | 7        | 0.31          |
| (3,143)  | 1:25:A:LYS:H     | 1:77:A:LEU:HD21  | 10       | 0.31          |
| (3,135)  | 1:123:A:ARG:HB3  | 1:120:A:ALA:HA   | 4        | 0.31          |
| (3,135)  | 1:123:A:ARG:HB3  | 1:120:A:ALA:HA   | 16       | 0.31          |
| (3,126)  | 1:21:A:LEU:HD21  | 1:22:A:ASN:H     | 5        | 0.31          |
| (3,126)  | 1:21:A:LEU:HD22  | 1:22:A:ASN:H     | 6        | 0.31          |
| (3,119)  | 1:98:A:ASP:HB3   | 1:99:A:GLY:HA2   | 11       | 0.31          |
| (3,112)  | 1:82:A:TRP:HA    | 1:117:A:LEU:HD12 | 11       | 0.31          |
| (3,83)   | 1:114:A:ARG:HB2  | 1:113:A:ALA:HB1  | 4        | 0.31          |
| (3,72)   | 1:117:A:LEU:HG   | 1:117:A:LEU:H    | 3        | 0.31          |
| (3,72)   | 1:117:A:LEU:HG   | 1:117:A:LEU:H    | 9        | 0.31          |
| (3,72)   | 1:117:A:LEU:HG   | 1:117:A:LEU:H    | 12       | 0.31          |
| (3,51)   | 1:95:A:VAL:HG22  | 1:49:A:LYS:HA    | 16       | 0.31          |
| (3,36)   | 1:50:A:ILE:HG21  | 1:49:A:LYS:HB2   | 15       | 0.31          |
| (3,34)   | 1:97:A:LEU:HD22  | 1:31:A:LEU:HD11  | 16       | 0.31          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,4342) | 1:38:A:CYS:H     | 1:95:A:VAL:HG13  | 15       | 0.31          |
| (1,4310) | 1:64:A:MET:HA    | 1:65:A:ASN:H     | 14       | 0.31          |
| (1,4300) | 1:92:A:ALA:H     | 1:105:A:LEU:HD23 | 17       | 0.31          |
| (1,4255) | 1:75:A:LEU:HD23  | 1:54:A:GLN:H     | 3        | 0.31          |
| (1,4255) | 1:75:A:LEU:HD23  | 1:54:A:GLN:H     | 9        | 0.31          |
| (1,4230) | 1:128:A:ARG:HA   | 1:128:A:ARG:H    | 3        | 0.31          |
| (1,4230) | 1:128:A:ARG:HA   | 1:128:A:ARG:H    | 16       | 0.31          |
| (1,4210) | 1:110:A:VAL:HG11 | 1:113:A:ALA:H    | 4        | 0.31          |
| (1,4210) | 1:110:A:VAL:HG12 | 1:113:A:ALA:H    | 7        | 0.31          |
| (1,4210) | 1:110:A:VAL:HG13 | 1:113:A:ALA:H    | 8        | 0.31          |
| (1,4210) | 1:110:A:VAL:HG12 | 1:113:A:ALA:H    | 14       | 0.31          |
| (1,4140) | 1:118:A:GLU:HA   | 1:118:A:GLU:H    | 8        | 0.31          |
| (1,4140) | 1:118:A:GLU:HA   | 1:118:A:GLU:H    | 13       | 0.31          |
| (1,4132) | 1:60:A:VAL:HG12  | 1:34:A:ARG:HE    | 17       | 0.31          |
| (1,4126) | 1:59:A:ARG:HE    | 1:97:A:LEU:HD11  | 11       | 0.31          |
| (1,4037) | 1:27:A:VAL:HG23  | 1:29:A:ALA:H     | 7        | 0.31          |
| (1,3786) | 1:27:A:VAL:HG11  | 1:21:A:LEU:H     | 9        | 0.31          |
| (1,3769) | 1:130:A:GLU:H    | 1:129:A:ALA:HB3  | 12       | 0.31          |
| (1,3744) | 1:35:A:PHE:HD1   | 1:39:A:PHE:H     | 6        | 0.31          |
| (1,3741) | 1:28:A:ILE:HG13  | 1:28:A:ILE:H     | 4        | 0.31          |
| (1,3738) | 1:103:A:GLY:HA3  | 1:104:A:GLU:H    | 3        | 0.31          |
| (1,3728) | 1:29:A:ALA:HA    | 1:30:A:PHE:H     | 2        | 0.31          |
| (1,3728) | 1:29:A:ALA:HA    | 1:30:A:PHE:H     | 7        | 0.31          |
| (1,3728) | 1:29:A:ALA:HA    | 1:30:A:PHE:H     | 10       | 0.31          |
| (1,3728) | 1:29:A:ALA:HA    | 1:30:A:PHE:H     | 11       | 0.31          |
| (1,3728) | 1:29:A:ALA:HA    | 1:30:A:PHE:H     | 14       | 0.31          |
| (1,3606) | 1:117:A:LEU:HA   | 1:82:A:TRP:HZ2   | 4        | 0.31          |
| (1,3584) | 1:110:A:VAL:HA   | 1:105:A:LEU:HD22 | 4        | 0.31          |
| (1,3584) | 1:110:A:VAL:HA   | 1:105:A:LEU:HD21 | 8        | 0.31          |
| (1,3584) | 1:110:A:VAL:HA   | 1:105:A:LEU:HD21 | 11       | 0.31          |
| (1,3584) | 1:110:A:VAL:HA   | 1:105:A:LEU:HD22 | 12       | 0.31          |
| (1,3584) | 1:110:A:VAL:HA   | 1:105:A:LEU:HD23 | 13       | 0.31          |
| (1,3584) | 1:110:A:VAL:HA   | 1:105:A:LEU:HD21 | 17       | 0.31          |
| (1,3564) | 1:105:A:LEU:HB3  | 1:104:A:GLU:HG2  | 8        | 0.31          |
| (1,3564) | 1:105:A:LEU:HB3  | 1:104:A:GLU:HG2  | 12       | 0.31          |
| (1,3531) | 1:65:A:ASN:H     | 1:65:A:ASN:HA    | 9        | 0.31          |
| (1,3513) | 1:72:A:ARG:HG3   | 1:73:A:SER:HB3   | 4        | 0.31          |
| (1,3513) | 1:72:A:ARG:HG3   | 1:73:A:SER:HB3   | 7        | 0.31          |
| (1,3513) | 1:72:A:ARG:HG3   | 1:73:A:SER:HB3   | 10       | 0.31          |
| (1,3513) | 1:72:A:ARG:HG3   | 1:73:A:SER:HB3   | 15       | 0.31          |
| (1,3513) | 1:72:A:ARG:HG3   | 1:73:A:SER:HB3   | 16       | 0.31          |
| (1,3513) | 1:72:A:ARG:HG3   | 1:73:A:SER:HB3   | 17       | 0.31          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3505) | 1:124:A:VAL:HG13 | 1:124:A:VAL:HG21 | 4        | 0.31          |
| (1,3501) | 1:27:A:VAL:HG23  | 1:28:A:ILE:HA    | 2        | 0.31          |
| (1,3497) | 1:27:A:VAL:HA    | 1:27:A:VAL:HG12  | 7        | 0.31          |
| (1,3495) | 1:54:A:GLN:H     | 1:75:A:LEU:HD13  | 1        | 0.31          |
| (1,3495) | 1:54:A:GLN:H     | 1:75:A:LEU:HD11  | 4        | 0.31          |
| (1,3495) | 1:54:A:GLN:H     | 1:75:A:LEU:HD13  | 6        | 0.31          |
| (1,3495) | 1:54:A:GLN:H     | 1:75:A:LEU:HD12  | 12       | 0.31          |
| (1,3491) | 1:86:A:TYR:HE1   | 1:85:A:LEU:HD22  | 14       | 0.31          |
| (1,3465) | 1:88:A:VAL:HG23  | 1:85:A:LEU:HB3   | 7        | 0.31          |
| (1,3430) | 1:45:A:ALA:HB3   | 1:84:A:TYR:HA    | 10       | 0.31          |
| (1,3427) | 1:117:A:LEU:HA   | 1:117:A:LEU:H    | 2        | 0.31          |
| (1,3427) | 1:117:A:LEU:HA   | 1:117:A:LEU:H    | 11       | 0.31          |
| (1,3417) | 1:117:A:LEU:HG   | 1:117:A:LEU:HD11 | 15       | 0.31          |
| (1,3416) | 1:117:A:LEU:HD12 | 1:117:A:LEU:HB3  | 5        | 0.31          |
| (1,3416) | 1:117:A:LEU:HD11 | 1:117:A:LEU:HB3  | 6        | 0.31          |
| (1,3416) | 1:117:A:LEU:HD12 | 1:117:A:LEU:HB3  | 14       | 0.31          |
| (1,3414) | 1:86:A:TYR:H     | 1:117:A:LEU:HD13 | 3        | 0.31          |
| (1,3414) | 1:86:A:TYR:H     | 1:117:A:LEU:HD13 | 9        | 0.31          |
| (1,3402) | 1:58:A:ASP:H     | 1:55:A:ASP:HA    | 4        | 0.31          |
| (1,3402) | 1:58:A:ASP:H     | 1:55:A:ASP:HA    | 6        | 0.31          |
| (1,3402) | 1:58:A:ASP:H     | 1:55:A:ASP:HA    | 9        | 0.31          |
| (1,3401) | 1:86:A:TYR:HE2   | 1:86:A:TYR:HA    | 12       | 0.31          |
| (1,3373) | 1:88:A:VAL:HA    | 1:93:A:THR:HG21  | 11       | 0.31          |
| (1,3330) | 1:25:A:LYS:HE3   | 1:77:A:LEU:HD12  | 2        | 0.31          |
| (1,3323) | 1:66:A:LEU:HD21  | 1:66:A:LEU:H     | 5        | 0.31          |
| (1,3319) | 1:66:A:LEU:HD23  | 1:27:A:VAL:HG13  | 2        | 0.31          |
| (1,3319) | 1:66:A:LEU:HD21  | 1:27:A:VAL:HG12  | 6        | 0.31          |
| (1,3319) | 1:66:A:LEU:HD22  | 1:27:A:VAL:HG12  | 9        | 0.31          |
| (1,3282) | 1:44:A:GLU:HG2   | 1:45:A:ALA:HB3   | 14       | 0.31          |
| (1,3273) | 1:42:A:GLU:HG2   | 1:43:A:GLY:H     | 6        | 0.31          |
| (1,3264) | 1:121:A:LYS:HG2  | 1:121:A:LYS:H    | 6        | 0.31          |
| (1,3264) | 1:121:A:LYS:HG2  | 1:121:A:LYS:H    | 9        | 0.31          |
| (1,3264) | 1:121:A:LYS:HG2  | 1:121:A:LYS:H    | 10       | 0.31          |
| (1,3264) | 1:121:A:LYS:HG2  | 1:121:A:LYS:H    | 16       | 0.31          |
| (1,3228) | 1:31:A:LEU:HB2   | 1:39:A:PHE:HE2   | 2        | 0.31          |
| (1,3228) | 1:31:A:LEU:HB2   | 1:39:A:PHE:HE2   | 4        | 0.31          |
| (1,3198) | 1:114:A:ARG:HA   | 1:113:A:ALA:HB1  | 6        | 0.31          |
| (1,3198) | 1:114:A:ARG:HA   | 1:113:A:ALA:HB1  | 16       | 0.31          |
| (1,3196) | 1:64:A:MET:HB2   | 1:64:A:MET:HA    | 4        | 0.31          |
| (1,3196) | 1:64:A:MET:HB2   | 1:64:A:MET:HA    | 9        | 0.31          |
| (1,3189) | 1:110:A:VAL:HA   | 1:105:A:LEU:HD13 | 5        | 0.31          |
| (1,3189) | 1:110:A:VAL:HA   | 1:105:A:LEU:HD12 | 14       | 0.31          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3189) | 1:110:A:VAL:HA   | 1:105:A:LEU:HD12 | 16       | 0.31          |
| (1,3114) | 1:57:A:VAL:HG22  | 1:57:A:VAL:HG11  | 6        | 0.31          |
| (1,3114) | 1:57:A:VAL:HG23  | 1:57:A:VAL:HG12  | 11       | 0.31          |
| (1,3113) | 1:57:A:VAL:HG13  | 1:61:A:ALA:H     | 12       | 0.31          |
| (1,3103) | 1:56:A:LEU:HD13  | 1:60:A:VAL:HB    | 17       | 0.31          |
| (1,3092) | 1:55:A:ASP:HA    | 1:56:A:LEU:HB3   | 7        | 0.31          |
| (1,3081) | 1:97:A:LEU:HD11  | 1:55:A:ASP:HA    | 16       | 0.31          |
| (1,3077) | 1:54:A:GLN:HB2   | 1:57:A:VAL:HG12  | 8        | 0.31          |
| (1,3077) | 1:54:A:GLN:HB2   | 1:57:A:VAL:HG13  | 17       | 0.31          |
| (1,3058) | 1:52:A:ILE:HG21  | 1:48:A:LEU:HG    | 17       | 0.31          |
| (1,3036) | 1:78:A:TYR:HH    | 1:45:A:ALA:HB3   | 1        | 0.31          |
| (1,3036) | 1:78:A:TYR:HH    | 1:45:A:ALA:HB1   | 14       | 0.31          |
| (1,3027) | 1:57:A:VAL:HA    | 1:71:A:LEU:HD12  | 4        | 0.31          |
| (1,3022) | 1:64:A:MET:HE3   | 1:30:A:PHE:HA    | 6        | 0.31          |
| (1,2991) | 1:54:A:GLN:HE22  | 1:54:A:GLN:HG2   | 5        | 0.31          |
| (1,2991) | 1:54:A:GLN:HE22  | 1:54:A:GLN:HG2   | 7        | 0.31          |
| (1,2942) | 1:57:A:VAL:HG23  | 1:57:A:VAL:HB    | 2        | 0.31          |
| (1,2942) | 1:57:A:VAL:HG23  | 1:57:A:VAL:HB    | 8        | 0.31          |
| (1,2940) | 1:99:A:GLY:HA3   | 1:95:A:VAL:HG12  | 4        | 0.31          |
| (1,2933) | 1:95:A:VAL:HG22  | 1:99:A:GLY:H     | 3        | 0.31          |
| (1,2931) | 1:88:A:VAL:HG22  | 1:85:A:LEU:H     | 8        | 0.31          |
| (1,2931) | 1:88:A:VAL:HG22  | 1:85:A:LEU:H     | 13       | 0.31          |
| (1,2909) | 1:110:A:VAL:HG12 | 1:91:A:GLY:HA2   | 17       | 0.31          |
| (1,2905) | 1:88:A:VAL:HG23  | 1:84:A:TYR:HD1   | 1        | 0.31          |
| (1,2891) | 1:32:A:ALA:HB1   | 1:28:A:ILE:HG21  | 2        | 0.31          |
| (1,2873) | 1:126:A:ALA:HA   | 1:126:A:ALA:HB1  | 13       | 0.31          |
| (1,2863) | 1:78:A:TYR:HE1   | 1:84:A:TYR:HD2   | 3        | 0.31          |
| (1,2863) | 1:78:A:TYR:HE1   | 1:84:A:TYR:HD1   | 12       | 0.31          |
| (1,2861) | 1:84:A:TYR:HE2   | 1:84:A:TYR:HA    | 1        | 0.31          |
| (1,2842) | 1:28:A:ILE:H     | 1:27:A:VAL:HG13  | 8        | 0.31          |
| (1,2842) | 1:28:A:ILE:H     | 1:27:A:VAL:HG13  | 9        | 0.31          |
| (1,2842) | 1:28:A:ILE:H     | 1:27:A:VAL:HG12  | 15       | 0.31          |
| (1,2831) | 1:97:A:LEU:HD22  | 1:35:A:PHE:HD1   | 12       | 0.31          |
| (1,2830) | 1:39:A:PHE:HZ    | 1:97:A:LEU:HD21  | 11       | 0.31          |
| (1,2830) | 1:39:A:PHE:HZ    | 1:97:A:LEU:HD23  | 15       | 0.31          |
| (1,2824) | 1:97:A:LEU:HD22  | 1:56:A:LEU:HA    | 5        | 0.31          |
| (1,2824) | 1:97:A:LEU:HD22  | 1:56:A:LEU:HA    | 6        | 0.31          |
| (1,2782) | 1:61:A:ALA:HB1   | 1:62:A:GLY:HA2   | 5        | 0.31          |
| (1,2679) | 1:53:A:PHE:HA    | 1:53:A:PHE:HE1   | 5        | 0.31          |
| (1,2675) | 1:85:A:LEU:HB2   | 1:86:A:TYR:HD2   | 12       | 0.31          |
| (1,2650) | 1:77:A:LEU:HD23  | 1:77:A:LEU:HB2   | 4        | 0.31          |
| (1,2650) | 1:77:A:LEU:HD23  | 1:77:A:LEU:HB2   | 6        | 0.31          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2650) | 1:77:A:LEU:HD21  | 1:77:A:LEU:HB2   | 9        | 0.31          |
| (1,2597) | 1:21:A:LEU:HD23  | 1:27:A:VAL:HG11  | 8        | 0.31          |
| (1,2597) | 1:21:A:LEU:HD23  | 1:27:A:VAL:HG12  | 10       | 0.31          |
| (1,2596) | 1:74:A:ALA:HB1   | 1:27:A:VAL:HG11  | 13       | 0.31          |
| (1,2576) | 1:124:A:VAL:HG22 | 1:120:A:ALA:HA   | 13       | 0.31          |
| (1,2547) | 1:11:A:SER:HA    | 1:12:A:GLN:HG3   | 3        | 0.31          |
| (1,2547) | 1:11:A:SER:HA    | 1:12:A:GLN:HG3   | 9        | 0.31          |
| (1,2542) | 1:21:A:LEU:HD13  | 1:30:A:PHE:HA    | 5        | 0.31          |
| (1,2542) | 1:21:A:LEU:HD13  | 1:30:A:PHE:HA    | 15       | 0.31          |
| (1,2502) | 1:42:A:GLU:HA    | 1:43:A:GLY:H     | 1        | 0.31          |
| (1,2502) | 1:42:A:GLU:HA    | 1:43:A:GLY:H     | 15       | 0.31          |
| (1,2502) | 1:42:A:GLU:HA    | 1:43:A:GLY:H     | 16       | 0.31          |
| (1,2480) | 1:71:A:LEU:HB2   | 1:27:A:VAL:HG12  | 1        | 0.31          |
| (1,2480) | 1:71:A:LEU:HB2   | 1:27:A:VAL:HG12  | 8        | 0.31          |
| (1,2480) | 1:71:A:LEU:HB2   | 1:27:A:VAL:HG13  | 13       | 0.31          |
| (1,2468) | 1:53:A:PHE:HE2   | 1:72:A:ARG:HG3   | 4        | 0.31          |
| (1,2468) | 1:53:A:PHE:HE1   | 1:72:A:ARG:HG3   | 14       | 0.31          |
| (1,2418) | 1:113:A:ALA:HB2  | 1:110:A:VAL:HG11 | 4        | 0.31          |
| (1,2418) | 1:113:A:ALA:HB3  | 1:110:A:VAL:HG11 | 12       | 0.31          |
| (1,2418) | 1:113:A:ALA:HB2  | 1:110:A:VAL:HG13 | 16       | 0.31          |
| (1,2415) | 1:45:A:ALA:HB1   | 1:84:A:TYR:HD2   | 15       | 0.31          |
| (1,2412) | 1:45:A:ALA:HB2   | 1:78:A:TYR:HB3   | 10       | 0.31          |
| (1,2412) | 1:45:A:ALA:HB3   | 1:78:A:TYR:HB3   | 14       | 0.31          |
| (1,2408) | 1:52:A:ILE:HD13  | 1:96:A:ASP:HA    | 13       | 0.31          |
| (1,2369) | 1:52:A:ILE:HD13  | 1:56:A:LEU:H     | 7        | 0.31          |
| (1,2367) | 1:52:A:ILE:H     | 1:52:A:ILE:HD12  | 17       | 0.31          |
| (1,2358) | 1:107:A:GLU:HA   | 1:111:A:GLU:H    | 7        | 0.31          |
| (1,2350) | 1:110:A:VAL:HG22 | 1:110:A:VAL:HA   | 13       | 0.31          |
| (1,2350) | 1:110:A:VAL:HG22 | 1:110:A:VAL:HA   | 14       | 0.31          |
| (1,2346) | 1:105:A:LEU:HD13 | 1:107:A:GLU:HA   | 7        | 0.31          |
| (1,2331) | 1:54:A:GLN:HG2   | 1:55:A:ASP:HA    | 11       | 0.31          |
| (1,2331) | 1:54:A:GLN:HG2   | 1:55:A:ASP:HA    | 15       | 0.31          |
| (1,2331) | 1:54:A:GLN:HG2   | 1:55:A:ASP:HA    | 17       | 0.31          |
| (1,2221) | 1:31:A:LEU:HA    | 1:60:A:VAL:HB    | 11       | 0.31          |
| (1,2190) | 1:61:A:ALA:HB1   | 1:62:A:GLY:HA2   | 16       | 0.31          |
| (1,2178) | 1:48:A:LEU:HB2   | 1:52:A:ILE:HG21  | 10       | 0.31          |
| (1,2149) | 1:21:A:LEU:HD22  | 1:30:A:PHE:HD1   | 3        | 0.31          |
| (1,2099) | 1:21:A:LEU:HB2   | 1:21:A:LEU:HD21  | 14       | 0.31          |
| (1,2098) | 1:21:A:LEU:HD23  | 1:27:A:VAL:HG11  | 1        | 0.31          |
| (1,2098) | 1:21:A:LEU:HD21  | 1:27:A:VAL:HG12  | 3        | 0.31          |
| (1,2098) | 1:21:A:LEU:HD22  | 1:27:A:VAL:HG12  | 5        | 0.31          |
| (1,2098) | 1:21:A:LEU:HD23  | 1:27:A:VAL:HG11  | 9        | 0.31          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2028) | 1:97:A:LEU:HD21  | 1:97:A:LEU:H     | 3        | 0.31          |
| (1,2028) | 1:97:A:LEU:HD22  | 1:97:A:LEU:H     | 4        | 0.31          |
| (1,2005) | 1:95:A:VAL:HG23  | 1:48:A:LEU:HD12  | 3        | 0.31          |
| (1,2005) | 1:95:A:VAL:HG22  | 1:48:A:LEU:HD12  | 17       | 0.31          |
| (1,1994) | 1:91:A:GLY:HA2   | 1:91:A:GLY:H     | 11       | 0.31          |
| (1,1994) | 1:91:A:GLY:HA2   | 1:91:A:GLY:H     | 14       | 0.31          |
| (1,1960) | 1:121:A:LYS:HG3  | 1:117:A:LEU:HD13 | 13       | 0.31          |
| (1,1955) | 1:92:A:ALA:HB3   | 1:113:A:ALA:HB3  | 14       | 0.31          |
| (1,1945) | 1:105:A:LEU:HB3  | 1:110:A:VAL:HG22 | 10       | 0.31          |
| (1,1945) | 1:105:A:LEU:HB3  | 1:110:A:VAL:HG22 | 11       | 0.31          |
| (1,1903) | 1:122:A:ALA:HB3  | 1:121:A:LYS:HE3  | 3        | 0.31          |
| (1,1903) | 1:122:A:ALA:HB2  | 1:121:A:LYS:HE3  | 4        | 0.31          |
| (1,1903) | 1:122:A:ALA:HB1  | 1:121:A:LYS:HE3  | 5        | 0.31          |
| (1,1903) | 1:122:A:ALA:HB1  | 1:121:A:LYS:HE3  | 10       | 0.31          |
| (1,1903) | 1:122:A:ALA:HB3  | 1:121:A:LYS:HE3  | 11       | 0.31          |
| (1,1881) | 1:113:A:ALA:HB3  | 1:88:A:VAL:HA    | 4        | 0.31          |
| (1,1881) | 1:113:A:ALA:HB1  | 1:88:A:VAL:HA    | 7        | 0.31          |
| (1,1879) | 1:124:A:VAL:HG11 | 1:124:A:VAL:HG22 | 5        | 0.31          |
| (1,1879) | 1:124:A:VAL:HG11 | 1:124:A:VAL:HG21 | 7        | 0.31          |
| (1,1879) | 1:124:A:VAL:HG11 | 1:124:A:VAL:HG21 | 13       | 0.31          |
| (1,1874) | 1:70:A:GLN:HE21  | 1:27:A:VAL:HG13  | 7        | 0.31          |
| (1,1874) | 1:70:A:GLN:HE21  | 1:27:A:VAL:HG11  | 15       | 0.31          |
| (1,1870) | 1:86:A:TYR:HE1   | 1:85:A:LEU:HD22  | 2        | 0.31          |
| (1,1870) | 1:86:A:TYR:HE2   | 1:85:A:LEU:HD22  | 3        | 0.31          |
| (1,1870) | 1:86:A:TYR:HE1   | 1:85:A:LEU:HD23  | 4        | 0.31          |
| (1,1870) | 1:86:A:TYR:HE1   | 1:85:A:LEU:HD22  | 7        | 0.31          |
| (1,1870) | 1:86:A:TYR:HE1   | 1:85:A:LEU:HD23  | 13       | 0.31          |
| (1,1870) | 1:86:A:TYR:HE1   | 1:85:A:LEU:HD22  | 15       | 0.31          |
| (1,1813) | 1:117:A:LEU:HD11 | 1:117:A:LEU:HB3  | 4        | 0.31          |
| (1,1793) | 1:88:A:VAL:HG23  | 1:84:A:TYR:HA    | 17       | 0.31          |
| (1,1752) | 1:41:A:ALA:HB3   | 1:28:A:ILE:HG21  | 12       | 0.31          |
| (1,1746) | 1:71:A:LEU:HD23  | 1:74:A:ALA:H     | 8        | 0.31          |
| (1,1746) | 1:71:A:LEU:HD21  | 1:74:A:ALA:H     | 10       | 0.31          |
| (1,1737) | 1:77:A:LEU:HG    | 1:77:A:LEU:HD13  | 13       | 0.31          |
| (1,1735) | 1:66:A:LEU:HD23  | 1:67:A:SER:H     | 6        | 0.31          |
| (1,1723) | 1:68:A:LYS:HD3   | 1:57:A:VAL:HG13  | 3        | 0.31          |
| (1,1686) | 1:85:A:LEU:HD13  | 1:85:A:LEU:HD23  | 11       | 0.31          |
| (1,1656) | 1:31:A:LEU:HB2   | 1:39:A:PHE:HE2   | 1        | 0.31          |
| (1,1656) | 1:31:A:LEU:HB2   | 1:39:A:PHE:HE2   | 3        | 0.31          |
| (1,1656) | 1:31:A:LEU:HB2   | 1:39:A:PHE:HE1   | 5        | 0.31          |
| (1,1656) | 1:31:A:LEU:HB2   | 1:39:A:PHE:HE1   | 13       | 0.31          |
| (1,1553) | 1:57:A:VAL:HG13  | 1:61:A:ALA:H     | 10       | 0.31          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1521) | 1:30:A:PHE:HB3   | 1:29:A:ALA:HB3  | 3        | 0.31          |
| (1,1521) | 1:30:A:PHE:HB3   | 1:29:A:ALA:HB3  | 17       | 0.31          |
| (1,1502) | 1:52:A:ILE:HG13  | 1:54:A:GLN:HE21 | 16       | 0.31          |
| (1,1485) | 1:71:A:LEU:HD11  | 1:72:A:ARG:HA   | 10       | 0.31          |
| (1,1485) | 1:71:A:LEU:HD11  | 1:72:A:ARG:HA   | 12       | 0.31          |
| (1,1485) | 1:71:A:LEU:HD11  | 1:72:A:ARG:HA   | 16       | 0.31          |
| (1,1480) | 1:64:A:MET:HE2   | 1:63:A:GLU:H    | 6        | 0.31          |
| (1,1450) | 1:54:A:GLN:HE22  | 1:54:A:GLN:HG2  | 6        | 0.31          |
| (1,1408) | 1:57:A:VAL:HG22  | 1:57:A:VAL:HB   | 4        | 0.31          |
| (1,1408) | 1:57:A:VAL:HG22  | 1:57:A:VAL:HB   | 9        | 0.31          |
| (1,1408) | 1:57:A:VAL:HG23  | 1:57:A:VAL:HB   | 16       | 0.31          |
| (1,1403) | 1:95:A:VAL:HG21  | 1:95:A:VAL:HG13 | 12       | 0.31          |
| (1,1400) | 1:95:A:VAL:HG22  | 1:99:A:GLY:H    | 13       | 0.31          |
| (1,1398) | 1:88:A:VAL:HG23  | 1:85:A:LEU:H    | 5        | 0.31          |
| (1,1398) | 1:88:A:VAL:HG22  | 1:85:A:LEU:H    | 11       | 0.31          |
| (1,1375) | 1:110:A:VAL:HG13 | 1:91:A:GLY:HA2  | 1        | 0.31          |
| (1,1375) | 1:110:A:VAL:HG12 | 1:91:A:GLY:HA2  | 3        | 0.31          |
| (1,1375) | 1:110:A:VAL:HG13 | 1:91:A:GLY:HA2  | 7        | 0.31          |
| (1,1375) | 1:110:A:VAL:HG13 | 1:91:A:GLY:HA2  | 9        | 0.31          |
| (1,1365) | 1:32:A:ALA:HB1   | 1:28:A:ILE:HG23 | 3        | 0.31          |
| (1,1365) | 1:32:A:ALA:HB2   | 1:28:A:ILE:HG22 | 9        | 0.31          |
| (1,1342) | 1:48:A:LEU:HD13  | 1:84:A:TYR:HE2  | 2        | 0.31          |
| (1,1334) | 1:81:A:SER:HB3   | 1:84:A:TYR:HD1  | 4        | 0.31          |
| (1,1309) | 1:97:A:LEU:HD21  | 1:97:A:LEU:H    | 3        | 0.31          |
| (1,1307) | 1:97:A:LEU:HD22  | 1:97:A:LEU:HB2  | 3        | 0.31          |
| (1,1307) | 1:97:A:LEU:HD23  | 1:97:A:LEU:HB2  | 4        | 0.31          |
| (1,1307) | 1:97:A:LEU:HD23  | 1:97:A:LEU:HB2  | 13       | 0.31          |
| (1,1307) | 1:97:A:LEU:HD22  | 1:97:A:LEU:HB2  | 15       | 0.31          |
| (1,1307) | 1:97:A:LEU:HD22  | 1:97:A:LEU:HB2  | 17       | 0.31          |
| (1,1304) | 1:97:A:LEU:HD23  | 1:56:A:LEU:HA   | 9        | 0.31          |
| (1,1304) | 1:97:A:LEU:HD23  | 1:56:A:LEU:HA   | 13       | 0.31          |
| (1,1231) | 1:97:A:LEU:HD13  | 1:59:A:ARG:HD3  | 13       | 0.31          |
| (1,1136) | 1:31:A:LEU:HD13  | 1:35:A:PHE:HD2  | 1        | 0.31          |
| (1,1124) | 1:97:A:LEU:HD12  | 1:57:A:VAL:H    | 5        | 0.31          |
| (1,1110) | 1:77:A:LEU:HD23  | 1:77:A:LEU:HB2  | 2        | 0.31          |
| (1,1110) | 1:77:A:LEU:HD21  | 1:77:A:LEU:HB2  | 8        | 0.31          |
| (1,1110) | 1:77:A:LEU:HD21  | 1:77:A:LEU:HB2  | 10       | 0.31          |
| (1,1110) | 1:77:A:LEU:HD21  | 1:77:A:LEU:HB2  | 11       | 0.31          |
| (1,1081) | 1:71:A:LEU:HD11  | 1:57:A:VAL:H    | 2        | 0.31          |
| (1,1081) | 1:71:A:LEU:HD13  | 1:57:A:VAL:H    | 9        | 0.31          |
| (1,1062) | 1:27:A:VAL:HG21  | 1:27:A:VAL:HG13 | 9        | 0.31          |
| (1,1062) | 1:27:A:VAL:HG23  | 1:27:A:VAL:HG11 | 11       | 0.31          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1060) | 1:74:A:ALA:HB1   | 1:27:A:VAL:HG11  | 5        | 0.31          |
| (1,1048) | 1:124:A:VAL:HG23 | 1:120:A:ALA:HA   | 5        | 0.31          |
| (1,1048) | 1:124:A:VAL:HG22 | 1:120:A:ALA:HA   | 12       | 0.31          |
| (1,909)  | 1:53:A:PHE:HE1   | 1:72:A:ARG:HG3   | 1        | 0.31          |
| (1,909)  | 1:53:A:PHE:HE2   | 1:72:A:ARG:HG3   | 12       | 0.31          |
| (1,895)  | 1:129:A:ALA:HB2  | 1:129:A:ALA:HA   | 12       | 0.31          |
| (1,790)  | 1:50:A:ILE:HG22  | 1:50:A:ILE:H     | 4        | 0.31          |
| (1,788)  | 1:52:A:ILE:HD13  | 1:56:A:LEU:H     | 3        | 0.31          |
| (1,618)  | 1:95:A:VAL:H     | 1:48:A:LEU:HD11  | 16       | 0.31          |
| (1,575)  | 1:31:A:LEU:H     | 1:28:A:ILE:HD13  | 6        | 0.31          |
| (1,564)  | 1:59:A:ARG:HE    | 1:97:A:LEU:HD13  | 2        | 0.31          |
| (1,532)  | 1:116:A:GLN:HG3  | 1:116:A:GLN:HE21 | 7        | 0.31          |
| (1,532)  | 1:116:A:GLN:HG3  | 1:116:A:GLN:HE21 | 11       | 0.31          |
| (1,532)  | 1:116:A:GLN:HG3  | 1:116:A:GLN:HE21 | 17       | 0.31          |
| (1,527)  | 1:65:A:ASN:HB3   | 1:65:A:ASN:HD21  | 2        | 0.31          |
| (1,524)  | 1:20:A:LYS:HB3   | 1:22:A:ASN:HD22  | 15       | 0.31          |
| (1,300)  | 1:100:A:ASN:HB3  | 1:100:A:ASN:HD21 | 11       | 0.31          |
| (1,154)  | 1:130:A:GLU:H    | 1:129:A:ALA:HB1  | 9        | 0.31          |
| (1,154)  | 1:130:A:GLU:H    | 1:129:A:ALA:HB1  | 10       | 0.31          |
| (1,154)  | 1:130:A:GLU:H    | 1:129:A:ALA:HB3  | 17       | 0.31          |
| (1,116)  | 1:21:A:LEU:HD12  | 1:30:A:PHE:H     | 3        | 0.31          |
| (1,116)  | 1:21:A:LEU:HD13  | 1:30:A:PHE:H     | 5        | 0.31          |
| (1,116)  | 1:21:A:LEU:HD11  | 1:30:A:PHE:H     | 6        | 0.31          |
| (1,116)  | 1:21:A:LEU:HD13  | 1:30:A:PHE:H     | 13       | 0.31          |
| (1,116)  | 1:21:A:LEU:HD13  | 1:30:A:PHE:H     | 15       | 0.31          |
| (3,152)  | 1:27:A:VAL:H     | 1:74:A:ALA:HB3   | 12       | 0.3           |
| (3,143)  | 1:25:A:LYS:H     | 1:77:A:LEU:HD23  | 6        | 0.3           |
| (3,135)  | 1:123:A:ARG:HB3  | 1:120:A:ALA:HA   | 7        | 0.3           |
| (3,122)  | 1:27:A:VAL:HG22  | 1:28:A:ILE:HD12  | 12       | 0.3           |
| (3,98)   | 1:64:A:MET:HE1   | 1:63:A:GLU:HG3   | 11       | 0.3           |
| (3,72)   | 1:117:A:LEU:HG   | 1:117:A:LEU:H    | 7        | 0.3           |
| (3,72)   | 1:117:A:LEU:HG   | 1:117:A:LEU:H    | 15       | 0.3           |
| (3,34)   | 1:97:A:LEU:HD23  | 1:31:A:LEU:HD12  | 7        | 0.3           |
| (3,15)   | 1:85:A:LEU:HB3   | 1:82:A:TRP:HA    | 1        | 0.3           |
| (1,4342) | 1:38:A:CYS:H     | 1:95:A:VAL:HG12  | 9        | 0.3           |
| (1,4300) | 1:92:A:ALA:H     | 1:105:A:LEU:HD22 | 3        | 0.3           |
| (1,4300) | 1:92:A:ALA:H     | 1:105:A:LEU:HD23 | 11       | 0.3           |
| (1,4280) | 1:112:A:HIS:HA   | 1:116:A:GLN:H    | 2        | 0.3           |
| (1,4255) | 1:75:A:LEU:HD22  | 1:54:A:GLN:H     | 4        | 0.3           |
| (1,4255) | 1:75:A:LEU:HD22  | 1:54:A:GLN:H     | 7        | 0.3           |
| (1,4255) | 1:75:A:LEU:HD21  | 1:54:A:GLN:H     | 16       | 0.3           |
| (1,4230) | 1:128:A:ARG:HA   | 1:128:A:ARG:H    | 1        | 0.3           |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,4230) | 1:128:A:ARG:HA  | 1:128:A:ARG:H    | 7        | 0.3           |
| (1,4230) | 1:128:A:ARG:HA  | 1:128:A:ARG:H    | 10       | 0.3           |
| (1,4197) | 1:66:A:LEU:HD22 | 1:67:A:SER:H     | 2        | 0.3           |
| (1,4153) | 1:18:A:GLN:HB3  | 1:18:A:GLN:H     | 16       | 0.3           |
| (1,4141) | 1:98:A:ASP:HB2  | 1:100:A:ASN:HD21 | 5        | 0.3           |
| (1,4140) | 1:118:A:GLU:HA  | 1:118:A:GLU:H    | 1        | 0.3           |
| (1,4114) | 1:65:A:ASN:H    | 1:65:A:ASN:HD21  | 4        | 0.3           |
| (1,4114) | 1:65:A:ASN:H    | 1:65:A:ASN:HD21  | 14       | 0.3           |
| (1,4087) | 1:65:A:ASN:HB2  | 1:65:A:ASN:HD21  | 12       | 0.3           |
| (1,4087) | 1:65:A:ASN:HB2  | 1:65:A:ASN:HD21  | 17       | 0.3           |
| (1,4007) | 1:41:A:ALA:HB1  | 1:41:A:ALA:H     | 17       | 0.3           |
| (1,4006) | 1:42:A:GLU:HB3  | 1:41:A:ALA:H     | 11       | 0.3           |
| (1,4006) | 1:42:A:GLU:HB3  | 1:41:A:ALA:H     | 15       | 0.3           |
| (1,4006) | 1:42:A:GLU:HB3  | 1:41:A:ALA:H     | 17       | 0.3           |
| (1,3972) | 1:53:A:PHE:H    | 1:56:A:LEU:HB3   | 12       | 0.3           |
| (1,3889) | 1:100:A:ASN:HB3 | 1:100:A:ASN:HD21 | 2        | 0.3           |
| (1,3889) | 1:100:A:ASN:HB3 | 1:100:A:ASN:HD21 | 5        | 0.3           |
| (1,3889) | 1:100:A:ASN:HB3 | 1:100:A:ASN:HD21 | 13       | 0.3           |
| (1,3889) | 1:100:A:ASN:HB3 | 1:100:A:ASN:HD21 | 17       | 0.3           |
| (1,3839) | 1:65:A:ASN:HB3  | 1:65:A:ASN:HD21  | 1        | 0.3           |
| (1,3839) | 1:65:A:ASN:HB3  | 1:65:A:ASN:HD21  | 11       | 0.3           |
| (1,3816) | 1:105:A:LEU:H   | 1:105:A:LEU:HD23 | 10       | 0.3           |
| (1,3784) | 1:21:A:LEU:HG   | 1:21:A:LEU:H     | 9        | 0.3           |
| (1,3783) | 1:117:A:LEU:HB3 | 1:117:A:LEU:H    | 15       | 0.3           |
| (1,3744) | 1:35:A:PHE:HD1  | 1:39:A:PHE:H     | 11       | 0.3           |
| (1,3741) | 1:28:A:ILE:HG13 | 1:28:A:ILE:H     | 1        | 0.3           |
| (1,3741) | 1:28:A:ILE:HG13 | 1:28:A:ILE:H     | 2        | 0.3           |
| (1,3741) | 1:28:A:ILE:HG13 | 1:28:A:ILE:H     | 5        | 0.3           |
| (1,3741) | 1:28:A:ILE:HG13 | 1:28:A:ILE:H     | 6        | 0.3           |
| (1,3741) | 1:28:A:ILE:HG13 | 1:28:A:ILE:H     | 7        | 0.3           |
| (1,3741) | 1:28:A:ILE:HG13 | 1:28:A:ILE:H     | 9        | 0.3           |
| (1,3741) | 1:28:A:ILE:HG13 | 1:28:A:ILE:H     | 11       | 0.3           |
| (1,3741) | 1:28:A:ILE:HG13 | 1:28:A:ILE:H     | 16       | 0.3           |
| (1,3741) | 1:28:A:ILE:HG13 | 1:28:A:ILE:H     | 17       | 0.3           |
| (1,3738) | 1:103:A:GLY:HA3 | 1:104:A:GLU:H    | 11       | 0.3           |
| (1,3733) | 1:27:A:VAL:HG13 | 1:26:A:GLU:H     | 1        | 0.3           |
| (1,3733) | 1:27:A:VAL:HG11 | 1:26:A:GLU:H     | 5        | 0.3           |
| (1,3733) | 1:27:A:VAL:HG13 | 1:26:A:GLU:H     | 9        | 0.3           |
| (1,3733) | 1:27:A:VAL:HG11 | 1:26:A:GLU:H     | 14       | 0.3           |
| (1,3728) | 1:29:A:ALA:HA   | 1:30:A:PHE:H     | 6        | 0.3           |
| (1,3728) | 1:29:A:ALA:HA   | 1:30:A:PHE:H     | 12       | 0.3           |
| (1,3728) | 1:29:A:ALA:HA   | 1:30:A:PHE:H     | 15       | 0.3           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3728) | 1:29:A:ALA:HA    | 1:30:A:PHE:H     | 16       | 0.3           |
| (1,3728) | 1:29:A:ALA:HA    | 1:30:A:PHE:H     | 17       | 0.3           |
| (1,3668) | 1:84:A:TYR:H     | 1:84:A:TYR:HD2   | 6        | 0.3           |
| (1,3610) | 1:121:A:LYS:HG3  | 1:117:A:LEU:HD13 | 10       | 0.3           |
| (1,3610) | 1:121:A:LYS:HG3  | 1:117:A:LEU:HD13 | 16       | 0.3           |
| (1,3599) | 1:92:A:ALA:HB3   | 1:113:A:ALA:HB3  | 3        | 0.3           |
| (1,3599) | 1:92:A:ALA:HB2   | 1:113:A:ALA:HB1  | 6        | 0.3           |
| (1,3599) | 1:92:A:ALA:HB2   | 1:113:A:ALA:HB1  | 17       | 0.3           |
| (1,3584) | 1:110:A:VAL:HA   | 1:105:A:LEU:HD23 | 5        | 0.3           |
| (1,3584) | 1:110:A:VAL:HA   | 1:105:A:LEU:HD22 | 15       | 0.3           |
| (1,3564) | 1:105:A:LEU:HB3  | 1:104:A:GLU:HG2  | 2        | 0.3           |
| (1,3564) | 1:105:A:LEU:HB3  | 1:104:A:GLU:HG2  | 13       | 0.3           |
| (1,3548) | 1:64:A:MET:HE3   | 1:65:A:ASN:HB2   | 14       | 0.3           |
| (1,3534) | 1:122:A:ALA:HB1  | 1:121:A:LYS:HE3  | 15       | 0.3           |
| (1,3513) | 1:72:A:ARG:HG3   | 1:73:A:SER:HB3   | 3        | 0.3           |
| (1,3513) | 1:72:A:ARG:HG3   | 1:73:A:SER:HB3   | 5        | 0.3           |
| (1,3513) | 1:72:A:ARG:HG3   | 1:73:A:SER:HB3   | 13       | 0.3           |
| (1,3505) | 1:124:A:VAL:HG13 | 1:124:A:VAL:HG21 | 6        | 0.3           |
| (1,3505) | 1:124:A:VAL:HG12 | 1:124:A:VAL:HG21 | 10       | 0.3           |
| (1,3505) | 1:124:A:VAL:HG12 | 1:124:A:VAL:HG21 | 11       | 0.3           |
| (1,3505) | 1:124:A:VAL:HG11 | 1:124:A:VAL:HG21 | 12       | 0.3           |
| (1,3505) | 1:124:A:VAL:HG12 | 1:124:A:VAL:HG23 | 16       | 0.3           |
| (1,3501) | 1:27:A:VAL:HG22  | 1:28:A:ILE:HA    | 13       | 0.3           |
| (1,3497) | 1:27:A:VAL:HA    | 1:27:A:VAL:HG12  | 4        | 0.3           |
| (1,3495) | 1:54:A:GLN:H     | 1:75:A:LEU:HD13  | 2        | 0.3           |
| (1,3495) | 1:54:A:GLN:H     | 1:75:A:LEU:HD13  | 9        | 0.3           |
| (1,3495) | 1:54:A:GLN:H     | 1:75:A:LEU:HD12  | 10       | 0.3           |
| (1,3495) | 1:54:A:GLN:H     | 1:75:A:LEU:HD11  | 13       | 0.3           |
| (1,3495) | 1:54:A:GLN:H     | 1:75:A:LEU:HD11  | 16       | 0.3           |
| (1,3495) | 1:54:A:GLN:H     | 1:75:A:LEU:HD11  | 17       | 0.3           |
| (1,3481) | 1:83:A:ARG:HD3   | 1:45:A:ALA:HB3   | 2        | 0.3           |
| (1,3430) | 1:45:A:ALA:HB3   | 1:84:A:TYR:HA    | 12       | 0.3           |
| (1,3430) | 1:45:A:ALA:HB2   | 1:84:A:TYR:HA    | 17       | 0.3           |
| (1,3427) | 1:117:A:LEU:HA   | 1:117:A:LEU:H    | 3        | 0.3           |
| (1,3427) | 1:117:A:LEU:HA   | 1:117:A:LEU:H    | 7        | 0.3           |
| (1,3427) | 1:117:A:LEU:HA   | 1:117:A:LEU:H    | 15       | 0.3           |
| (1,3427) | 1:117:A:LEU:HA   | 1:117:A:LEU:H    | 17       | 0.3           |
| (1,3421) | 1:53:A:PHE:HA    | 1:75:A:LEU:HD23  | 1        | 0.3           |
| (1,3421) | 1:53:A:PHE:HA    | 1:75:A:LEU:HD21  | 11       | 0.3           |
| (1,3421) | 1:53:A:PHE:HA    | 1:75:A:LEU:HD23  | 14       | 0.3           |
| (1,3416) | 1:117:A:LEU:HD11 | 1:117:A:LEU:HB3  | 13       | 0.3           |
| (1,3414) | 1:86:A:TYR:H     | 1:117:A:LEU:HD13 | 12       | 0.3           |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3402) | 1:58:A:ASP:H    | 1:55:A:ASP:HA    | 11       | 0.3           |
| (1,3402) | 1:58:A:ASP:H    | 1:55:A:ASP:HA    | 13       | 0.3           |
| (1,3401) | 1:86:A:TYR:HE2  | 1:86:A:TYR:HA    | 17       | 0.3           |
| (1,3396) | 1:71:A:LEU:HA   | 1:74:A:ALA:HB2   | 3        | 0.3           |
| (1,3386) | 1:90:A:PRO:HA   | 1:92:A:ALA:HB3   | 1        | 0.3           |
| (1,3345) | 1:29:A:ALA:HA   | 1:29:A:ALA:HB2   | 6        | 0.3           |
| (1,3336) | 1:71:A:LEU:HD22 | 1:74:A:ALA:H     | 17       | 0.3           |
| (1,3319) | 1:66:A:LEU:HD23 | 1:27:A:VAL:HG12  | 16       | 0.3           |
| (1,3266) | 1:85:A:LEU:HD13 | 1:85:A:LEU:HD22  | 1        | 0.3           |
| (1,3266) | 1:85:A:LEU:HD12 | 1:85:A:LEU:HD21  | 5        | 0.3           |
| (1,3264) | 1:121:A:LYS:HG2 | 1:121:A:LYS:H    | 4        | 0.3           |
| (1,3264) | 1:121:A:LYS:HG2 | 1:121:A:LYS:H    | 8        | 0.3           |
| (1,3264) | 1:121:A:LYS:HG2 | 1:121:A:LYS:H    | 13       | 0.3           |
| (1,3258) | 1:48:A:LEU:HD12 | 1:50:A:ILE:HA    | 14       | 0.3           |
| (1,3228) | 1:31:A:LEU:HB2  | 1:39:A:PHE:HE1   | 16       | 0.3           |
| (1,3223) | 1:84:A:TYR:HE1  | 1:79:A:THR:HA    | 5        | 0.3           |
| (1,3223) | 1:84:A:TYR:HE1  | 1:79:A:THR:HA    | 11       | 0.3           |
| (1,3216) | 1:48:A:LEU:HG   | 1:84:A:TYR:HD1   | 5        | 0.3           |
| (1,3200) | 1:116:A:GLN:HG3 | 1:113:A:ALA:HB1  | 12       | 0.3           |
| (1,3198) | 1:114:A:ARG:HA  | 1:113:A:ALA:HB1  | 11       | 0.3           |
| (1,3189) | 1:110:A:VAL:HA  | 1:105:A:LEU:HD13 | 2        | 0.3           |
| (1,3189) | 1:110:A:VAL:HA  | 1:105:A:LEU:HD11 | 3        | 0.3           |
| (1,3189) | 1:110:A:VAL:HA  | 1:105:A:LEU:HD12 | 8        | 0.3           |
| (1,3189) | 1:110:A:VAL:HA  | 1:105:A:LEU:HD12 | 9        | 0.3           |
| (1,3189) | 1:110:A:VAL:HA  | 1:105:A:LEU:HD13 | 10       | 0.3           |
| (1,3189) | 1:110:A:VAL:HA  | 1:105:A:LEU:HD11 | 17       | 0.3           |
| (1,3180) | 1:111:A:GLU:HG2 | 1:111:A:GLU:HA   | 8        | 0.3           |
| (1,3178) | 1:116:A:GLN:HA  | 1:116:A:GLN:H    | 13       | 0.3           |
| (1,3123) | 1:59:A:ARG:HB2  | 1:59:A:ARG:HA    | 14       | 0.3           |
| (1,3123) | 1:59:A:ARG:HB2  | 1:59:A:ARG:HA    | 16       | 0.3           |
| (1,3115) | 1:58:A:ASP:HA   | 1:57:A:VAL:HG23  | 14       | 0.3           |
| (1,3115) | 1:58:A:ASP:HA   | 1:57:A:VAL:HG23  | 16       | 0.3           |
| (1,3114) | 1:57:A:VAL:HG21 | 1:57:A:VAL:HG11  | 2        | 0.3           |
| (1,3114) | 1:57:A:VAL:HG23 | 1:57:A:VAL:HG13  | 7        | 0.3           |
| (1,3114) | 1:57:A:VAL:HG22 | 1:57:A:VAL:HG12  | 8        | 0.3           |
| (1,3103) | 1:56:A:LEU:HD11 | 1:60:A:VAL:HB    | 2        | 0.3           |
| (1,3081) | 1:97:A:LEU:HD11 | 1:55:A:ASP:HA    | 14       | 0.3           |
| (1,3077) | 1:54:A:GLN:HB2  | 1:57:A:VAL:HG12  | 5        | 0.3           |
| (1,3061) | 1:31:A:LEU:HD11 | 1:28:A:ILE:HG21  | 1        | 0.3           |
| (1,3052) | 1:39:A:PHE:HZ   | 1:52:A:ILE:HG22  | 11       | 0.3           |
| (1,3036) | 1:78:A:TYR:HH   | 1:45:A:ALA:HB3   | 4        | 0.3           |
| (1,3036) | 1:78:A:TYR:HH   | 1:45:A:ALA:HB3   | 13       | 0.3           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3023) | 1:64:A:MET:HE3   | 1:27:A:VAL:HA    | 9        | 0.3           |
| (1,3019) | 1:64:A:MET:HE3   | 1:66:A:LEU:H     | 7        | 0.3           |
| (1,2992) | 1:20:A:LYS:HB3   | 1:20:A:LYS:H     | 12       | 0.3           |
| (1,2942) | 1:57:A:VAL:HG23  | 1:57:A:VAL:HB    | 12       | 0.3           |
| (1,2933) | 1:95:A:VAL:HG23  | 1:99:A:GLY:H     | 8        | 0.3           |
| (1,2933) | 1:95:A:VAL:HG21  | 1:99:A:GLY:H     | 9        | 0.3           |
| (1,2931) | 1:88:A:VAL:HG23  | 1:85:A:LEU:H     | 7        | 0.3           |
| (1,2931) | 1:88:A:VAL:HG22  | 1:85:A:LEU:H     | 15       | 0.3           |
| (1,2909) | 1:110:A:VAL:HG11 | 1:91:A:GLY:HA2   | 8        | 0.3           |
| (1,2909) | 1:110:A:VAL:HG12 | 1:91:A:GLY:HA2   | 12       | 0.3           |
| (1,2909) | 1:110:A:VAL:HG11 | 1:91:A:GLY:HA2   | 15       | 0.3           |
| (1,2863) | 1:78:A:TYR:HE1   | 1:84:A:TYR:HD1   | 14       | 0.3           |
| (1,2852) | 1:81:A:SER:HB3   | 1:84:A:TYR:HD2   | 2        | 0.3           |
| (1,2829) | 1:97:A:LEU:HD22  | 1:97:A:LEU:HB2   | 6        | 0.3           |
| (1,2829) | 1:97:A:LEU:HD23  | 1:97:A:LEU:HB2   | 11       | 0.3           |
| (1,2824) | 1:97:A:LEU:HD22  | 1:56:A:LEU:HA    | 3        | 0.3           |
| (1,2782) | 1:61:A:ALA:HB1   | 1:62:A:GLY:HA2   | 3        | 0.3           |
| (1,2769) | 1:43:A:GLY:HA2   | 1:42:A:GLU:HB2   | 3        | 0.3           |
| (1,2769) | 1:43:A:GLY:HA2   | 1:42:A:GLU:HB2   | 16       | 0.3           |
| (1,2753) | 1:97:A:LEU:HD13  | 1:59:A:ARG:HD3   | 4        | 0.3           |
| (1,2753) | 1:97:A:LEU:HD12  | 1:59:A:ARG:HD3   | 12       | 0.3           |
| (1,2753) | 1:97:A:LEU:HD13  | 1:59:A:ARG:HD3   | 15       | 0.3           |
| (1,2720) | 1:86:A:TYR:HB3   | 1:117:A:LEU:HD13 | 12       | 0.3           |
| (1,2679) | 1:53:A:PHE:HA    | 1:53:A:PHE:HE2   | 3        | 0.3           |
| (1,2662) | 1:97:A:LEU:HD12  | 1:57:A:VAL:H     | 1        | 0.3           |
| (1,2662) | 1:97:A:LEU:HD13  | 1:57:A:VAL:H     | 6        | 0.3           |
| (1,2662) | 1:97:A:LEU:HD12  | 1:57:A:VAL:H     | 14       | 0.3           |
| (1,2662) | 1:97:A:LEU:HD13  | 1:57:A:VAL:H     | 17       | 0.3           |
| (1,2650) | 1:77:A:LEU:HD21  | 1:77:A:LEU:HB2   | 12       | 0.3           |
| (1,2650) | 1:77:A:LEU:HD23  | 1:77:A:LEU:HB2   | 13       | 0.3           |
| (1,2650) | 1:77:A:LEU:HD22  | 1:77:A:LEU:HB2   | 15       | 0.3           |
| (1,2650) | 1:77:A:LEU:HD22  | 1:77:A:LEU:HB2   | 16       | 0.3           |
| (1,2598) | 1:27:A:VAL:HG23  | 1:27:A:VAL:HG13  | 16       | 0.3           |
| (1,2597) | 1:21:A:LEU:HD23  | 1:27:A:VAL:HG12  | 2        | 0.3           |
| (1,2597) | 1:21:A:LEU:HD21  | 1:27:A:VAL:HG12  | 11       | 0.3           |
| (1,2597) | 1:21:A:LEU:HD22  | 1:27:A:VAL:HG12  | 14       | 0.3           |
| (1,2597) | 1:21:A:LEU:HD22  | 1:27:A:VAL:HG11  | 16       | 0.3           |
| (1,2596) | 1:74:A:ALA:HB3   | 1:27:A:VAL:HG11  | 7        | 0.3           |
| (1,2576) | 1:124:A:VAL:HG21 | 1:120:A:ALA:HA   | 8        | 0.3           |
| (1,2542) | 1:21:A:LEU:HD11  | 1:30:A:PHE:HA    | 6        | 0.3           |
| (1,2513) | 1:122:A:ALA:HA   | 1:122:A:ALA:HB3  | 11       | 0.3           |
| (1,2502) | 1:42:A:GLU:HA    | 1:43:A:GLY:H     | 4        | 0.3           |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2502) | 1:42:A:GLU:HA   | 1:43:A:GLY:H     | 9        | 0.3           |
| (1,2502) | 1:42:A:GLU:HA   | 1:43:A:GLY:H     | 10       | 0.3           |
| (1,2484) | 1:93:A:THR:HB   | 1:95:A:VAL:HG13  | 12       | 0.3           |
| (1,2480) | 1:71:A:LEU:HB2  | 1:27:A:VAL:HG13  | 3        | 0.3           |
| (1,2468) | 1:53:A:PHE:HE2  | 1:72:A:ARG:HG3   | 10       | 0.3           |
| (1,2468) | 1:53:A:PHE:HE2  | 1:72:A:ARG:HG3   | 11       | 0.3           |
| (1,2423) | 1:64:A:MET:HA   | 1:64:A:MET:HE1   | 3        | 0.3           |
| (1,2418) | 1:113:A:ALA:HB3 | 1:110:A:VAL:HG12 | 9        | 0.3           |
| (1,2418) | 1:113:A:ALA:HB1 | 1:110:A:VAL:HG11 | 13       | 0.3           |
| (1,2412) | 1:45:A:ALA:HB2  | 1:78:A:TYR:HB3   | 3        | 0.3           |
| (1,2409) | 1:49:A:LYS:H    | 1:52:A:ILE:HD13  | 2        | 0.3           |
| (1,2369) | 1:52:A:ILE:HD12 | 1:56:A:LEU:H     | 2        | 0.3           |
| (1,2369) | 1:52:A:ILE:HD11 | 1:56:A:LEU:H     | 13       | 0.3           |
| (1,2369) | 1:52:A:ILE:HD13 | 1:56:A:LEU:H     | 15       | 0.3           |
| (1,2358) | 1:107:A:GLU:HA  | 1:111:A:GLU:H    | 1        | 0.3           |
| (1,2344) | 1:104:A:GLU:HG2 | 1:105:A:LEU:HD21 | 4        | 0.3           |
| (1,2344) | 1:104:A:GLU:HG2 | 1:105:A:LEU:HD22 | 5        | 0.3           |
| (1,2344) | 1:104:A:GLU:HG2 | 1:105:A:LEU:HD21 | 12       | 0.3           |
| (1,2344) | 1:104:A:GLU:HG2 | 1:105:A:LEU:HD22 | 14       | 0.3           |
| (1,2344) | 1:104:A:GLU:HG2 | 1:105:A:LEU:HD21 | 16       | 0.3           |
| (1,2336) | 1:64:A:MET:HE3  | 1:31:A:LEU:HA    | 4        | 0.3           |
| (1,2336) | 1:64:A:MET:HE1  | 1:31:A:LEU:HA    | 14       | 0.3           |
| (1,2230) | 1:28:A:ILE:H    | 1:28:A:ILE:HG22  | 1        | 0.3           |
| (1,2201) | 1:64:A:MET:HB2  | 1:21:A:LEU:HD23  | 14       | 0.3           |
| (1,2190) | 1:61:A:ALA:HB2  | 1:62:A:GLY:HA2   | 10       | 0.3           |
| (1,2179) | 1:52:A:ILE:HG22 | 1:48:A:LEU:HB3   | 8        | 0.3           |
| (1,2163) | 1:78:A:TYR:HA   | 1:78:A:TYR:HD1   | 11       | 0.3           |
| (1,2098) | 1:21:A:LEU:HD22 | 1:27:A:VAL:HG11  | 12       | 0.3           |
| (1,2098) | 1:21:A:LEU:HD22 | 1:27:A:VAL:HG12  | 13       | 0.3           |
| (1,2098) | 1:21:A:LEU:HD21 | 1:27:A:VAL:HG13  | 17       | 0.3           |
| (1,2028) | 1:97:A:LEU:HD21 | 1:97:A:LEU:H     | 6        | 0.3           |
| (1,2028) | 1:97:A:LEU:HD22 | 1:97:A:LEU:H     | 9        | 0.3           |
| (1,2028) | 1:97:A:LEU:HD22 | 1:97:A:LEU:H     | 13       | 0.3           |
| (1,2028) | 1:97:A:LEU:HD21 | 1:97:A:LEU:H     | 15       | 0.3           |
| (1,2025) | 1:97:A:LEU:HD23 | 1:35:A:PHE:HD2   | 4        | 0.3           |
| (1,2005) | 1:95:A:VAL:HG21 | 1:48:A:LEU:HD12  | 1        | 0.3           |
| (1,1994) | 1:91:A:GLY:HA2  | 1:91:A:GLY:H     | 6        | 0.3           |
| (1,1955) | 1:92:A:ALA:HB3  | 1:113:A:ALA:HB3  | 4        | 0.3           |
| (1,1955) | 1:92:A:ALA:HB1  | 1:113:A:ALA:HB3  | 16       | 0.3           |
| (1,1947) | 1:93:A:THR:HB   | 1:88:A:VAL:HG13  | 2        | 0.3           |
| (1,1945) | 1:105:A:LEU:HB3 | 1:110:A:VAL:HG21 | 1        | 0.3           |
| (1,1903) | 1:122:A:ALA:HB1 | 1:121:A:LYS:HE3  | 2        | 0.3           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1903) | 1:122:A:ALA:HB3  | 1:121:A:LYS:HE3  | 7        | 0.3           |
| (1,1903) | 1:122:A:ALA:HB2  | 1:121:A:LYS:HE3  | 12       | 0.3           |
| (1,1903) | 1:122:A:ALA:HB1  | 1:121:A:LYS:HE3  | 17       | 0.3           |
| (1,1879) | 1:124:A:VAL:HG12 | 1:124:A:VAL:HG22 | 14       | 0.3           |
| (1,1870) | 1:86:A:TYR:HE1   | 1:85:A:LEU:HD23  | 9        | 0.3           |
| (1,1870) | 1:86:A:TYR:HE1   | 1:85:A:LEU:HD23  | 10       | 0.3           |
| (1,1870) | 1:86:A:TYR:HE1   | 1:85:A:LEU:HD23  | 11       | 0.3           |
| (1,1870) | 1:86:A:TYR:HE2   | 1:85:A:LEU:HD21  | 12       | 0.3           |
| (1,1870) | 1:86:A:TYR:HE2   | 1:85:A:LEU:HD22  | 17       | 0.3           |
| (1,1866) | 1:83:A:ARG:HD3   | 1:45:A:ALA:HB1   | 13       | 0.3           |
| (1,1865) | 1:45:A:ALA:HB1   | 1:44:A:GLU:HB3   | 10       | 0.3           |
| (1,1865) | 1:45:A:ALA:HB2   | 1:44:A:GLU:HB3   | 15       | 0.3           |
| (1,1865) | 1:45:A:ALA:HB2   | 1:44:A:GLU:HB3   | 17       | 0.3           |
| (1,1813) | 1:117:A:LEU:HD11 | 1:117:A:LEU:HB3  | 8        | 0.3           |
| (1,1799) | 1:71:A:LEU:HA    | 1:74:A:ALA:HB3   | 8        | 0.3           |
| (1,1746) | 1:71:A:LEU:HD21  | 1:74:A:ALA:H     | 7        | 0.3           |
| (1,1746) | 1:71:A:LEU:HD23  | 1:74:A:ALA:H     | 16       | 0.3           |
| (1,1737) | 1:77:A:LEU:HG    | 1:77:A:LEU:HD12  | 1        | 0.3           |
| (1,1737) | 1:77:A:LEU:HG    | 1:77:A:LEU:HD12  | 5        | 0.3           |
| (1,1737) | 1:77:A:LEU:HG    | 1:77:A:LEU:HD13  | 6        | 0.3           |
| (1,1737) | 1:77:A:LEU:HG    | 1:77:A:LEU:HD13  | 16       | 0.3           |
| (1,1723) | 1:68:A:LYS:HD3   | 1:57:A:VAL:HG11  | 5        | 0.3           |
| (1,1686) | 1:85:A:LEU:HD13  | 1:85:A:LEU:HD21  | 12       | 0.3           |
| (1,1679) | 1:92:A:ALA:HB3   | 1:91:A:GLY:H     | 14       | 0.3           |
| (1,1656) | 1:31:A:LEU:HB2   | 1:39:A:PHE:HE1   | 15       | 0.3           |
| (1,1613) | 1:124:A:VAL:HG23 | 1:121:A:LYS:HA   | 3        | 0.3           |
| (1,1613) | 1:124:A:VAL:HG21 | 1:121:A:LYS:HA   | 9        | 0.3           |
| (1,1553) | 1:57:A:VAL:HG11  | 1:61:A:ALA:H     | 14       | 0.3           |
| (1,1545) | 1:56:A:LEU:HD12  | 1:60:A:VAL:HB    | 7        | 0.3           |
| (1,1516) | 1:31:A:LEU:HD11  | 1:28:A:ILE:HG22  | 5        | 0.3           |
| (1,1516) | 1:31:A:LEU:HD11  | 1:28:A:ILE:HG21  | 9        | 0.3           |
| (1,1490) | 1:78:A:TYR:HH    | 1:45:A:ALA:HB2   | 6        | 0.3           |
| (1,1485) | 1:71:A:LEU:HD13  | 1:72:A:ARG:HA    | 6        | 0.3           |
| (1,1414) | 1:74:A:ALA:HB3   | 1:75:A:LEU:HD13  | 5        | 0.3           |
| (1,1363) | 1:29:A:ALA:HA    | 1:32:A:ALA:HB1   | 9        | 0.3           |
| (1,1357) | 1:74:A:ALA:HB2   | 1:31:A:LEU:HD12  | 15       | 0.3           |
| (1,1331) | 1:78:A:TYR:HE1   | 1:84:A:TYR:HD2   | 16       | 0.3           |
| (1,1309) | 1:97:A:LEU:HD22  | 1:97:A:LEU:H     | 4        | 0.3           |
| (1,1309) | 1:97:A:LEU:HD21  | 1:97:A:LEU:H     | 6        | 0.3           |
| (1,1309) | 1:97:A:LEU:HD22  | 1:97:A:LEU:H     | 9        | 0.3           |
| (1,1309) | 1:97:A:LEU:HD22  | 1:97:A:LEU:H     | 13       | 0.3           |
| (1,1308) | 1:97:A:LEU:HD22  | 1:35:A:PHE:HD1   | 2        | 0.3           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1308) | 1:97:A:LEU:HD22  | 1:35:A:PHE:HD2   | 14       | 0.3           |
| (1,1307) | 1:97:A:LEU:HD22  | 1:97:A:LEU:HB2   | 10       | 0.3           |
| (1,1304) | 1:97:A:LEU:HD23  | 1:56:A:LEU:HA    | 4        | 0.3           |
| (1,1304) | 1:97:A:LEU:HD23  | 1:56:A:LEU:HA    | 8        | 0.3           |
| (1,1304) | 1:97:A:LEU:HD22  | 1:56:A:LEU:HA    | 12       | 0.3           |
| (1,1304) | 1:97:A:LEU:HD22  | 1:56:A:LEU:HA    | 17       | 0.3           |
| (1,1124) | 1:97:A:LEU:HD12  | 1:57:A:VAL:H     | 4        | 0.3           |
| (1,1110) | 1:77:A:LEU:HD22  | 1:77:A:LEU:HB2   | 1        | 0.3           |
| (1,1110) | 1:77:A:LEU:HD22  | 1:77:A:LEU:HB2   | 14       | 0.3           |
| (1,1062) | 1:27:A:VAL:HG23  | 1:27:A:VAL:HG11  | 4        | 0.3           |
| (1,1062) | 1:27:A:VAL:HG21  | 1:27:A:VAL:HG11  | 10       | 0.3           |
| (1,1060) | 1:74:A:ALA:HB2   | 1:27:A:VAL:HG11  | 3        | 0.3           |
| (1,1060) | 1:74:A:ALA:HB3   | 1:27:A:VAL:HG13  | 6        | 0.3           |
| (1,1060) | 1:74:A:ALA:HB2   | 1:27:A:VAL:HG11  | 11       | 0.3           |
| (1,1060) | 1:74:A:ALA:HB3   | 1:27:A:VAL:HG13  | 16       | 0.3           |
| (1,1048) | 1:124:A:VAL:HG22 | 1:120:A:ALA:HA   | 11       | 0.3           |
| (1,895)  | 1:129:A:ALA:HB2  | 1:129:A:ALA:HA   | 2        | 0.3           |
| (1,895)  | 1:129:A:ALA:HB3  | 1:129:A:ALA:HA   | 9        | 0.3           |
| (1,895)  | 1:129:A:ALA:HB2  | 1:129:A:ALA:HA   | 17       | 0.3           |
| (1,829)  | 1:41:A:ALA:HB3   | 1:41:A:ALA:H     | 4        | 0.3           |
| (1,819)  | 1:28:A:ILE:HD11  | 1:74:A:ALA:HA    | 11       | 0.3           |
| (1,819)  | 1:28:A:ILE:HD13  | 1:74:A:ALA:HA    | 17       | 0.3           |
| (1,788)  | 1:52:A:ILE:HD13  | 1:56:A:LEU:H     | 11       | 0.3           |
| (1,643)  | 1:110:A:VAL:HG11 | 1:113:A:ALA:H    | 6        | 0.3           |
| (1,552)  | 1:65:A:ASN:H     | 1:65:A:ASN:HD21  | 2        | 0.3           |
| (1,552)  | 1:65:A:ASN:H     | 1:65:A:ASN:HD21  | 8        | 0.3           |
| (1,532)  | 1:116:A:GLN:HG3  | 1:116:A:GLN:HE21 | 3        | 0.3           |
| (1,532)  | 1:116:A:GLN:HG3  | 1:116:A:GLN:HE21 | 12       | 0.3           |
| (1,532)  | 1:116:A:GLN:HG3  | 1:116:A:GLN:HE21 | 15       | 0.3           |
| (1,527)  | 1:65:A:ASN:HB3   | 1:65:A:ASN:HD21  | 8        | 0.3           |
| (1,451)  | 1:32:A:ALA:HB2   | 1:35:A:PHE:H     | 9        | 0.3           |
| (1,410)  | 1:53:A:PHE:H     | 1:56:A:LEU:HB3   | 1        | 0.3           |
| (1,410)  | 1:53:A:PHE:H     | 1:56:A:LEU:HB3   | 13       | 0.3           |
| (1,410)  | 1:53:A:PHE:H     | 1:56:A:LEU:HB3   | 15       | 0.3           |
| (1,241)  | 1:95:A:VAL:HG11  | 1:96:A:ASP:H     | 14       | 0.3           |
| (1,116)  | 1:21:A:LEU:HD13  | 1:30:A:PHE:H     | 2        | 0.3           |
| (1,116)  | 1:21:A:LEU:HD11  | 1:30:A:PHE:H     | 11       | 0.3           |
| (1,116)  | 1:21:A:LEU:HD11  | 1:30:A:PHE:H     | 14       | 0.3           |
| (1,116)  | 1:21:A:LEU:HD12  | 1:30:A:PHE:H     | 16       | 0.3           |
| (1,12)   | 1:100:A:ASN:H    | 1:100:A:ASN:HD21 | 3        | 0.3           |
| (3,148)  | 1:22:A:ASN:H     | 1:22:A:ASN:HB2   | 10       | 0.29          |
| (3,135)  | 1:123:A:ARG:HB3  | 1:120:A:ALA:HA   | 15       | 0.29          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (3,109)  | 1:92:A:ALA:H     | 1:110:A:VAL:HB   | 8        | 0.29          |
| (3,109)  | 1:92:A:ALA:H     | 1:110:A:VAL:HB   | 15       | 0.29          |
| (3,109)  | 1:92:A:ALA:H     | 1:110:A:VAL:HB   | 17       | 0.29          |
| (3,87)   | 1:117:A:LEU:HD12 | 1:121:A:LYS:H    | 4        | 0.29          |
| (3,87)   | 1:117:A:LEU:HD12 | 1:121:A:LYS:H    | 13       | 0.29          |
| (3,83)   | 1:114:A:ARG:HB2  | 1:113:A:ALA:HB1  | 11       | 0.29          |
| (3,16)   | 1:90:A:PRO:HA    | 1:110:A:VAL:HG13 | 2        | 0.29          |
| (3,16)   | 1:90:A:PRO:HA    | 1:110:A:VAL:HG11 | 12       | 0.29          |
| (1,4310) | 1:64:A:MET:HA    | 1:65:A:ASN:H     | 3        | 0.29          |
| (1,4310) | 1:64:A:MET:HA    | 1:65:A:ASN:H     | 5        | 0.29          |
| (1,4310) | 1:64:A:MET:HA    | 1:65:A:ASN:H     | 6        | 0.29          |
| (1,4310) | 1:64:A:MET:HA    | 1:65:A:ASN:H     | 15       | 0.29          |
| (1,4300) | 1:92:A:ALA:H     | 1:105:A:LEU:HD21 | 4        | 0.29          |
| (1,4280) | 1:112:A:HIS:HA   | 1:116:A:GLN:H    | 4        | 0.29          |
| (1,4280) | 1:112:A:HIS:HA   | 1:116:A:GLN:H    | 5        | 0.29          |
| (1,4280) | 1:112:A:HIS:HA   | 1:116:A:GLN:H    | 16       | 0.29          |
| (1,4255) | 1:75:A:LEU:HD21  | 1:54:A:GLN:H     | 8        | 0.29          |
| (1,4255) | 1:75:A:LEU:HD23  | 1:54:A:GLN:H     | 10       | 0.29          |
| (1,4255) | 1:75:A:LEU:HD21  | 1:54:A:GLN:H     | 12       | 0.29          |
| (1,4255) | 1:75:A:LEU:HD21  | 1:54:A:GLN:H     | 15       | 0.29          |
| (1,4255) | 1:75:A:LEU:HD22  | 1:54:A:GLN:H     | 17       | 0.29          |
| (1,4230) | 1:128:A:ARG:HA   | 1:128:A:ARG:H    | 2        | 0.29          |
| (1,4230) | 1:128:A:ARG:HA   | 1:128:A:ARG:H    | 9        | 0.29          |
| (1,4230) | 1:128:A:ARG:HA   | 1:128:A:ARG:H    | 12       | 0.29          |
| (1,4230) | 1:128:A:ARG:HA   | 1:128:A:ARG:H    | 17       | 0.29          |
| (1,4202) | 1:127:A:GLN:H    | 1:127:A:GLN:HB3  | 16       | 0.29          |
| (1,4202) | 1:127:A:GLN:H    | 1:127:A:GLN:HB3  | 17       | 0.29          |
| (1,4180) | 1:95:A:VAL:H     | 1:48:A:LEU:HD12  | 10       | 0.29          |
| (1,4180) | 1:95:A:VAL:H     | 1:48:A:LEU:HD11  | 13       | 0.29          |
| (1,4171) | 1:48:A:LEU:HD23  | 1:49:A:LYS:H     | 17       | 0.29          |
| (1,4141) | 1:98:A:ASP:HB2   | 1:100:A:ASN:HD21 | 3        | 0.29          |
| (1,4141) | 1:98:A:ASP:HB2   | 1:100:A:ASN:HD21 | 4        | 0.29          |
| (1,4141) | 1:98:A:ASP:HB2   | 1:100:A:ASN:HD21 | 9        | 0.29          |
| (1,4141) | 1:98:A:ASP:HB2   | 1:100:A:ASN:HD21 | 15       | 0.29          |
| (1,4140) | 1:118:A:GLU:HA   | 1:118:A:GLU:H    | 12       | 0.29          |
| (1,4126) | 1:59:A:ARG:HE    | 1:97:A:LEU:HD11  | 1        | 0.29          |
| (1,4126) | 1:59:A:ARG:HE    | 1:97:A:LEU:HD11  | 6        | 0.29          |
| (1,4114) | 1:65:A:ASN:H     | 1:65:A:ASN:HD21  | 3        | 0.29          |
| (1,4114) | 1:65:A:ASN:H     | 1:65:A:ASN:HD21  | 5        | 0.29          |
| (1,4114) | 1:65:A:ASN:H     | 1:65:A:ASN:HD21  | 6        | 0.29          |
| (1,4087) | 1:65:A:ASN:HB2   | 1:65:A:ASN:HD21  | 10       | 0.29          |
| (1,4084) | 1:20:A:LYS:HB3   | 1:22:A:ASN:HD22  | 13       | 0.29          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,4017) | 1:32:A:ALA:HB2  | 1:35:A:PHE:H     | 6        | 0.29          |
| (1,4017) | 1:32:A:ALA:HB2  | 1:35:A:PHE:H     | 15       | 0.29          |
| (1,4006) | 1:42:A:GLU:HB3  | 1:41:A:ALA:H     | 1        | 0.29          |
| (1,4006) | 1:42:A:GLU:HB3  | 1:41:A:ALA:H     | 13       | 0.29          |
| (1,3889) | 1:100:A:ASN:HB3 | 1:100:A:ASN:HD21 | 1        | 0.29          |
| (1,3889) | 1:100:A:ASN:HB3 | 1:100:A:ASN:HD21 | 3        | 0.29          |
| (1,3889) | 1:100:A:ASN:HB3 | 1:100:A:ASN:HD21 | 4        | 0.29          |
| (1,3889) | 1:100:A:ASN:HB3 | 1:100:A:ASN:HD21 | 8        | 0.29          |
| (1,3889) | 1:100:A:ASN:HB3 | 1:100:A:ASN:HD21 | 9        | 0.29          |
| (1,3889) | 1:100:A:ASN:HB3 | 1:100:A:ASN:HD21 | 10       | 0.29          |
| (1,3889) | 1:100:A:ASN:HB3 | 1:100:A:ASN:HD21 | 12       | 0.29          |
| (1,3889) | 1:100:A:ASN:HB3 | 1:100:A:ASN:HD21 | 14       | 0.29          |
| (1,3889) | 1:100:A:ASN:HB3 | 1:100:A:ASN:HD21 | 15       | 0.29          |
| (1,3845) | 1:95:A:VAL:HG13 | 1:96:A:ASP:H     | 17       | 0.29          |
| (1,3839) | 1:65:A:ASN:HB3  | 1:65:A:ASN:HD21  | 5        | 0.29          |
| (1,3839) | 1:65:A:ASN:HB3  | 1:65:A:ASN:HD21  | 15       | 0.29          |
| (1,3786) | 1:27:A:VAL:HG12 | 1:21:A:LEU:H     | 13       | 0.29          |
| (1,3783) | 1:117:A:LEU:HB3 | 1:117:A:LEU:H    | 7        | 0.29          |
| (1,3783) | 1:117:A:LEU:HB3 | 1:117:A:LEU:H    | 12       | 0.29          |
| (1,3769) | 1:130:A:GLU:H   | 1:129:A:ALA:HB3  | 2        | 0.29          |
| (1,3769) | 1:130:A:GLU:H   | 1:129:A:ALA:HB1  | 8        | 0.29          |
| (1,3741) | 1:28:A:ILE:HG13 | 1:28:A:ILE:H     | 3        | 0.29          |
| (1,3741) | 1:28:A:ILE:HG13 | 1:28:A:ILE:H     | 8        | 0.29          |
| (1,3741) | 1:28:A:ILE:HG13 | 1:28:A:ILE:H     | 12       | 0.29          |
| (1,3741) | 1:28:A:ILE:HG13 | 1:28:A:ILE:H     | 13       | 0.29          |
| (1,3741) | 1:28:A:ILE:HG13 | 1:28:A:ILE:H     | 14       | 0.29          |
| (1,3741) | 1:28:A:ILE:HG13 | 1:28:A:ILE:H     | 15       | 0.29          |
| (1,3733) | 1:27:A:VAL:HG13 | 1:26:A:GLU:H     | 6        | 0.29          |
| (1,3732) | 1:21:A:LEU:HD13 | 1:30:A:PHE:H     | 10       | 0.29          |
| (1,3732) | 1:21:A:LEU:HD12 | 1:30:A:PHE:H     | 17       | 0.29          |
| (1,3728) | 1:29:A:ALA:HA   | 1:30:A:PHE:H     | 5        | 0.29          |
| (1,3728) | 1:29:A:ALA:HA   | 1:30:A:PHE:H     | 13       | 0.29          |
| (1,3627) | 1:100:A:ASN:H   | 1:100:A:ASN:HD21 | 8        | 0.29          |
| (1,3627) | 1:100:A:ASN:H   | 1:100:A:ASN:HD21 | 13       | 0.29          |
| (1,3610) | 1:121:A:LYS:HG3 | 1:117:A:LEU:HD12 | 1        | 0.29          |
| (1,3606) | 1:117:A:LEU:HA  | 1:82:A:TRP:HZ2   | 1        | 0.29          |
| (1,3606) | 1:117:A:LEU:HA  | 1:82:A:TRP:HZ2   | 5        | 0.29          |
| (1,3606) | 1:117:A:LEU:HA  | 1:82:A:TRP:HZ2   | 6        | 0.29          |
| (1,3606) | 1:117:A:LEU:HA  | 1:82:A:TRP:HZ2   | 10       | 0.29          |
| (1,3606) | 1:117:A:LEU:HA  | 1:82:A:TRP:HZ2   | 13       | 0.29          |
| (1,3599) | 1:92:A:ALA:HB3  | 1:113:A:ALA:HB3  | 14       | 0.29          |
| (1,3588) | 1:105:A:LEU:HB3 | 1:110:A:VAL:HG21 | 5        | 0.29          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3588) | 1:105:A:LEU:HB3  | 1:110:A:VAL:HG22 | 14       | 0.29          |
| (1,3564) | 1:105:A:LEU:HB3  | 1:104:A:GLU:HG2  | 10       | 0.29          |
| (1,3564) | 1:105:A:LEU:HB3  | 1:104:A:GLU:HG2  | 17       | 0.29          |
| (1,3531) | 1:65:A:ASN:H     | 1:65:A:ASN:HA    | 2        | 0.29          |
| (1,3531) | 1:65:A:ASN:H     | 1:65:A:ASN:HA    | 7        | 0.29          |
| (1,3531) | 1:65:A:ASN:H     | 1:65:A:ASN:HA    | 8        | 0.29          |
| (1,3531) | 1:65:A:ASN:H     | 1:65:A:ASN:HA    | 10       | 0.29          |
| (1,3531) | 1:65:A:ASN:H     | 1:65:A:ASN:HA    | 12       | 0.29          |
| (1,3531) | 1:65:A:ASN:H     | 1:65:A:ASN:HA    | 13       | 0.29          |
| (1,3531) | 1:65:A:ASN:H     | 1:65:A:ASN:HA    | 16       | 0.29          |
| (1,3531) | 1:65:A:ASN:H     | 1:65:A:ASN:HA    | 17       | 0.29          |
| (1,3505) | 1:124:A:VAL:HG11 | 1:124:A:VAL:HG22 | 5        | 0.29          |
| (1,3505) | 1:124:A:VAL:HG11 | 1:124:A:VAL:HG21 | 7        | 0.29          |
| (1,3505) | 1:124:A:VAL:HG11 | 1:124:A:VAL:HG21 | 13       | 0.29          |
| (1,3505) | 1:124:A:VAL:HG12 | 1:124:A:VAL:HG21 | 15       | 0.29          |
| (1,3495) | 1:54:A:GLN:H     | 1:75:A:LEU:HD12  | 11       | 0.29          |
| (1,3491) | 1:86:A:TYR:HE2   | 1:85:A:LEU:HD22  | 1        | 0.29          |
| (1,3481) | 1:83:A:ARG:HD3   | 1:45:A:ALA:HB3   | 6        | 0.29          |
| (1,3465) | 1:88:A:VAL:HG22  | 1:85:A:LEU:HB3   | 15       | 0.29          |
| (1,3465) | 1:88:A:VAL:HG21  | 1:85:A:LEU:HB3   | 16       | 0.29          |
| (1,3452) | 1:95:A:VAL:HA    | 1:93:A:THR:HG21  | 5        | 0.29          |
| (1,3430) | 1:45:A:ALA:HB2   | 1:84:A:TYR:HA    | 6        | 0.29          |
| (1,3427) | 1:117:A:LEU:HA   | 1:117:A:LEU:H    | 9        | 0.29          |
| (1,3427) | 1:117:A:LEU:HA   | 1:117:A:LEU:H    | 12       | 0.29          |
| (1,3421) | 1:53:A:PHE:HA    | 1:75:A:LEU:HD23  | 5        | 0.29          |
| (1,3421) | 1:53:A:PHE:HA    | 1:75:A:LEU:HD23  | 6        | 0.29          |
| (1,3421) | 1:53:A:PHE:HA    | 1:75:A:LEU:HD22  | 13       | 0.29          |
| (1,3421) | 1:53:A:PHE:HA    | 1:75:A:LEU:HD21  | 16       | 0.29          |
| (1,3416) | 1:117:A:LEU:HD11 | 1:117:A:LEU:HB3  | 4        | 0.29          |
| (1,3416) | 1:117:A:LEU:HD11 | 1:117:A:LEU:HB3  | 10       | 0.29          |
| (1,3416) | 1:117:A:LEU:HD11 | 1:117:A:LEU:HB3  | 16       | 0.29          |
| (1,3396) | 1:71:A:LEU:HA    | 1:74:A:ALA:HB3   | 7        | 0.29          |
| (1,3319) | 1:66:A:LEU:HD21  | 1:27:A:VAL:HG13  | 13       | 0.29          |
| (1,3302) | 1:83:A:ARG:HB2   | 1:86:A:TYR:HD2   | 10       | 0.29          |
| (1,3266) | 1:85:A:LEU:HD13  | 1:85:A:LEU:HD23  | 9        | 0.29          |
| (1,3266) | 1:85:A:LEU:HD13  | 1:85:A:LEU:HD23  | 11       | 0.29          |
| (1,3264) | 1:121:A:LYS:HG2  | 1:121:A:LYS:H    | 1        | 0.29          |
| (1,3223) | 1:84:A:TYR:HE2   | 1:79:A:THR:HA    | 3        | 0.29          |
| (1,3223) | 1:84:A:TYR:HE1   | 1:79:A:THR:HA    | 8        | 0.29          |
| (1,3223) | 1:84:A:TYR:HE1   | 1:79:A:THR:HA    | 10       | 0.29          |
| (1,3216) | 1:48:A:LEU:HG    | 1:84:A:TYR:HD1   | 12       | 0.29          |
| (1,3198) | 1:114:A:ARG:HA   | 1:113:A:ALA:HB2  | 9        | 0.29          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3198) | 1:114:A:ARG:HA   | 1:113:A:ALA:HB3  | 14       | 0.29          |
| (1,3189) | 1:110:A:VAL:HA   | 1:105:A:LEU:HD13 | 1        | 0.29          |
| (1,3189) | 1:110:A:VAL:HA   | 1:105:A:LEU:HD11 | 4        | 0.29          |
| (1,3189) | 1:110:A:VAL:HA   | 1:105:A:LEU:HD13 | 7        | 0.29          |
| (1,3189) | 1:110:A:VAL:HA   | 1:105:A:LEU:HD12 | 13       | 0.29          |
| (1,3189) | 1:110:A:VAL:HA   | 1:105:A:LEU:HD12 | 15       | 0.29          |
| (1,3178) | 1:116:A:GLN:HA   | 1:116:A:GLN:H    | 1        | 0.29          |
| (1,3178) | 1:116:A:GLN:HA   | 1:116:A:GLN:H    | 2        | 0.29          |
| (1,3178) | 1:116:A:GLN:HA   | 1:116:A:GLN:H    | 4        | 0.29          |
| (1,3178) | 1:116:A:GLN:HA   | 1:116:A:GLN:H    | 5        | 0.29          |
| (1,3178) | 1:116:A:GLN:HA   | 1:116:A:GLN:H    | 7        | 0.29          |
| (1,3178) | 1:116:A:GLN:HA   | 1:116:A:GLN:H    | 8        | 0.29          |
| (1,3178) | 1:116:A:GLN:HA   | 1:116:A:GLN:H    | 11       | 0.29          |
| (1,3178) | 1:116:A:GLN:HA   | 1:116:A:GLN:H    | 15       | 0.29          |
| (1,3178) | 1:116:A:GLN:HA   | 1:116:A:GLN:H    | 17       | 0.29          |
| (1,3132) | 1:68:A:LYS:HB2   | 1:53:A:PHE:HE1   | 4        | 0.29          |
| (1,3132) | 1:68:A:LYS:HB2   | 1:53:A:PHE:HE1   | 9        | 0.29          |
| (1,3123) | 1:59:A:ARG:HB2   | 1:59:A:ARG:HA    | 2        | 0.29          |
| (1,3123) | 1:59:A:ARG:HB2   | 1:59:A:ARG:HA    | 6        | 0.29          |
| (1,3123) | 1:59:A:ARG:HB2   | 1:59:A:ARG:HA    | 8        | 0.29          |
| (1,3123) | 1:59:A:ARG:HB2   | 1:59:A:ARG:HA    | 10       | 0.29          |
| (1,3123) | 1:59:A:ARG:HB2   | 1:59:A:ARG:HA    | 12       | 0.29          |
| (1,3114) | 1:57:A:VAL:HG23  | 1:57:A:VAL:HG13  | 17       | 0.29          |
| (1,3103) | 1:56:A:LEU:HD12  | 1:60:A:VAL:HB    | 13       | 0.29          |
| (1,3077) | 1:54:A:GLN:HB2   | 1:57:A:VAL:HG12  | 10       | 0.29          |
| (1,3061) | 1:31:A:LEU:HD13  | 1:28:A:ILE:HG22  | 13       | 0.29          |
| (1,3058) | 1:52:A:ILE:HG23  | 1:48:A:LEU:HG    | 2        | 0.29          |
| (1,3036) | 1:78:A:TYR:HH    | 1:45:A:ALA:HB1   | 15       | 0.29          |
| (1,3027) | 1:57:A:VAL:HA    | 1:71:A:LEU:HD13  | 2        | 0.29          |
| (1,3027) | 1:57:A:VAL:HA    | 1:71:A:LEU:HD11  | 6        | 0.29          |
| (1,3027) | 1:57:A:VAL:HA    | 1:71:A:LEU:HD11  | 14       | 0.29          |
| (1,3021) | 1:64:A:MET:HE2   | 1:63:A:GLU:H     | 2        | 0.29          |
| (1,2991) | 1:54:A:GLN:HE22  | 1:54:A:GLN:HG2   | 14       | 0.29          |
| (1,2945) | 1:110:A:VAL:HB   | 1:110:A:VAL:HG12 | 1        | 0.29          |
| (1,2937) | 1:95:A:VAL:HG21  | 1:95:A:VAL:HG13  | 12       | 0.29          |
| (1,2937) | 1:95:A:VAL:HG23  | 1:95:A:VAL:HG11  | 13       | 0.29          |
| (1,2933) | 1:95:A:VAL:HG21  | 1:99:A:GLY:H     | 7        | 0.29          |
| (1,2909) | 1:110:A:VAL:HG11 | 1:91:A:GLY:HA2   | 2        | 0.29          |
| (1,2909) | 1:110:A:VAL:HG13 | 1:91:A:GLY:HA2   | 10       | 0.29          |
| (1,2909) | 1:110:A:VAL:HG12 | 1:91:A:GLY:HA2   | 13       | 0.29          |
| (1,2909) | 1:110:A:VAL:HG11 | 1:91:A:GLY:HA2   | 16       | 0.29          |
| (1,2891) | 1:32:A:ALA:HB2   | 1:28:A:ILE:HG23  | 13       | 0.29          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2891) | 1:32:A:ALA:HB2  | 1:28:A:ILE:HG23  | 17       | 0.29          |
| (1,2842) | 1:28:A:ILE:H    | 1:27:A:VAL:HG11  | 7        | 0.29          |
| (1,2829) | 1:97:A:LEU:HD22 | 1:97:A:LEU:HB2   | 3        | 0.29          |
| (1,2829) | 1:97:A:LEU:HD23 | 1:97:A:LEU:HB2   | 4        | 0.29          |
| (1,2829) | 1:97:A:LEU:HD23 | 1:97:A:LEU:HB2   | 9        | 0.29          |
| (1,2829) | 1:97:A:LEU:HD22 | 1:97:A:LEU:HB2   | 12       | 0.29          |
| (1,2829) | 1:97:A:LEU:HD22 | 1:97:A:LEU:HB2   | 15       | 0.29          |
| (1,2824) | 1:97:A:LEU:HD23 | 1:56:A:LEU:HA    | 11       | 0.29          |
| (1,2824) | 1:97:A:LEU:HD22 | 1:56:A:LEU:HA    | 15       | 0.29          |
| (1,2824) | 1:97:A:LEU:HD21 | 1:56:A:LEU:HA    | 16       | 0.29          |
| (1,2769) | 1:43:A:GLY:HA2  | 1:42:A:GLU:HB2   | 8        | 0.29          |
| (1,2769) | 1:43:A:GLY:HA2  | 1:42:A:GLU:HB2   | 10       | 0.29          |
| (1,2754) | 1:60:A:VAL:HG12 | 1:59:A:ARG:HD3   | 7        | 0.29          |
| (1,2753) | 1:97:A:LEU:HD13 | 1:59:A:ARG:HD3   | 3        | 0.29          |
| (1,2753) | 1:97:A:LEU:HD12 | 1:59:A:ARG:HD3   | 9        | 0.29          |
| (1,2720) | 1:86:A:TYR:HB3  | 1:117:A:LEU:HD13 | 9        | 0.29          |
| (1,2720) | 1:86:A:TYR:HB3  | 1:117:A:LEU:HD11 | 15       | 0.29          |
| (1,2679) | 1:53:A:PHE:HA   | 1:53:A:PHE:HE1   | 1        | 0.29          |
| (1,2679) | 1:53:A:PHE:HA   | 1:53:A:PHE:HE1   | 2        | 0.29          |
| (1,2662) | 1:97:A:LEU:HD13 | 1:57:A:VAL:H     | 10       | 0.29          |
| (1,2662) | 1:97:A:LEU:HD12 | 1:57:A:VAL:H     | 13       | 0.29          |
| (1,2650) | 1:77:A:LEU:HD23 | 1:77:A:LEU:HB2   | 3        | 0.29          |
| (1,2650) | 1:77:A:LEU:HD22 | 1:77:A:LEU:HB2   | 5        | 0.29          |
| (1,2650) | 1:77:A:LEU:HD21 | 1:77:A:LEU:HB2   | 7        | 0.29          |
| (1,2650) | 1:77:A:LEU:HD21 | 1:77:A:LEU:HB2   | 10       | 0.29          |
| (1,2650) | 1:77:A:LEU:HD21 | 1:77:A:LEU:HB2   | 11       | 0.29          |
| (1,2650) | 1:77:A:LEU:HD22 | 1:77:A:LEU:HB2   | 17       | 0.29          |
| (1,2622) | 1:71:A:LEU:HD11 | 1:57:A:VAL:H     | 8        | 0.29          |
| (1,2622) | 1:71:A:LEU:HD12 | 1:57:A:VAL:H     | 14       | 0.29          |
| (1,2618) | 1:34:A:ARG:HG3  | 1:34:A:ARG:H     | 16       | 0.29          |
| (1,2596) | 1:74:A:ALA:HB1  | 1:27:A:VAL:HG11  | 2        | 0.29          |
| (1,2596) | 1:74:A:ALA:HB3  | 1:27:A:VAL:HG11  | 4        | 0.29          |
| (1,2583) | 1:60:A:VAL:HG12 | 1:34:A:ARG:HG2   | 8        | 0.29          |
| (1,2513) | 1:122:A:ALA:HA  | 1:122:A:ALA:HB1  | 2        | 0.29          |
| (1,2502) | 1:42:A:GLU:HA   | 1:43:A:GLY:H     | 8        | 0.29          |
| (1,2502) | 1:42:A:GLU:HA   | 1:43:A:GLY:H     | 12       | 0.29          |
| (1,2502) | 1:42:A:GLU:HA   | 1:43:A:GLY:H     | 13       | 0.29          |
| (1,2484) | 1:93:A:THR:HB   | 1:95:A:VAL:HG13  | 16       | 0.29          |
| (1,2480) | 1:71:A:LEU:HB2  | 1:27:A:VAL:HG13  | 11       | 0.29          |
| (1,2480) | 1:71:A:LEU:HB2  | 1:27:A:VAL:HG11  | 15       | 0.29          |
| (1,2468) | 1:53:A:PHE:HE1  | 1:72:A:ARG:HG3   | 8        | 0.29          |
| (1,2468) | 1:53:A:PHE:HE2  | 1:72:A:ARG:HG3   | 17       | 0.29          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2412) | 1:45:A:ALA:HB2   | 1:78:A:TYR:HB3   | 5        | 0.29          |
| (1,2403) | 1:28:A:ILE:HD11  | 1:78:A:TYR:HB3   | 2        | 0.29          |
| (1,2367) | 1:52:A:ILE:H     | 1:52:A:ILE:HD12  | 13       | 0.29          |
| (1,2358) | 1:107:A:GLU:HA   | 1:111:A:GLU:H    | 8        | 0.29          |
| (1,2346) | 1:105:A:LEU:HD12 | 1:107:A:GLU:HA   | 8        | 0.29          |
| (1,2344) | 1:104:A:GLU:HG2  | 1:105:A:LEU:HD23 | 2        | 0.29          |
| (1,2331) | 1:54:A:GLN:HG2   | 1:55:A:ASP:HA    | 7        | 0.29          |
| (1,2307) | 1:117:A:LEU:HD11 | 1:86:A:TYR:HB2   | 8        | 0.29          |
| (1,2212) | 1:110:A:VAL:HG22 | 1:114:A:ARG:H    | 7        | 0.29          |
| (1,2201) | 1:64:A:MET:HB2   | 1:21:A:LEU:HD23  | 13       | 0.29          |
| (1,2179) | 1:52:A:ILE:HG21  | 1:48:A:LEU:HB3   | 12       | 0.29          |
| (1,2178) | 1:48:A:LEU:HB2   | 1:52:A:ILE:HG21  | 12       | 0.29          |
| (1,2178) | 1:48:A:LEU:HB2   | 1:52:A:ILE:HG22  | 15       | 0.29          |
| (1,2149) | 1:21:A:LEU:HD22  | 1:30:A:PHE:HD1   | 17       | 0.29          |
| (1,2099) | 1:21:A:LEU:HB2   | 1:21:A:LEU:HD21  | 5        | 0.29          |
| (1,2099) | 1:21:A:LEU:HB2   | 1:21:A:LEU:HD22  | 6        | 0.29          |
| (1,2098) | 1:21:A:LEU:HD23  | 1:27:A:VAL:HG12  | 2        | 0.29          |
| (1,2098) | 1:21:A:LEU:HD23  | 1:27:A:VAL:HG11  | 8        | 0.29          |
| (1,2098) | 1:21:A:LEU:HD23  | 1:27:A:VAL:HG12  | 10       | 0.29          |
| (1,2098) | 1:21:A:LEU:HD21  | 1:27:A:VAL:HG12  | 11       | 0.29          |
| (1,2088) | 1:82:A:TRP:HZ2   | 1:124:A:VAL:HG21 | 6        | 0.29          |
| (1,2088) | 1:82:A:TRP:HZ2   | 1:124:A:VAL:HG23 | 9        | 0.29          |
| (1,2075) | 1:61:A:ALA:HB3   | 1:62:A:GLY:H     | 11       | 0.29          |
| (1,2028) | 1:97:A:LEU:HD21  | 1:97:A:LEU:H     | 10       | 0.29          |
| (1,2028) | 1:97:A:LEU:HD22  | 1:97:A:LEU:H     | 11       | 0.29          |
| (1,2028) | 1:97:A:LEU:HD21  | 1:97:A:LEU:H     | 17       | 0.29          |
| (1,2006) | 1:78:A:TYR:HE2   | 1:48:A:LEU:HD11  | 4        | 0.29          |
| (1,1960) | 1:121:A:LYS:HG3  | 1:117:A:LEU:HD11 | 5        | 0.29          |
| (1,1947) | 1:93:A:THR:HB    | 1:88:A:VAL:HG12  | 17       | 0.29          |
| (1,1945) | 1:105:A:LEU:HB3  | 1:110:A:VAL:HG21 | 4        | 0.29          |
| (1,1945) | 1:105:A:LEU:HB3  | 1:110:A:VAL:HG23 | 7        | 0.29          |
| (1,1945) | 1:105:A:LEU:HB3  | 1:110:A:VAL:HG21 | 9        | 0.29          |
| (1,1945) | 1:105:A:LEU:HB3  | 1:110:A:VAL:HG22 | 13       | 0.29          |
| (1,1945) | 1:105:A:LEU:HB3  | 1:110:A:VAL:HG22 | 15       | 0.29          |
| (1,1945) | 1:105:A:LEU:HB3  | 1:110:A:VAL:HG21 | 16       | 0.29          |
| (1,1945) | 1:105:A:LEU:HB3  | 1:110:A:VAL:HG21 | 17       | 0.29          |
| (1,1940) | 1:111:A:GLU:HB2  | 1:109:A:HIS:HA   | 14       | 0.29          |
| (1,1903) | 1:122:A:ALA:HB1  | 1:121:A:LYS:HE3  | 6        | 0.29          |
| (1,1903) | 1:122:A:ALA:HB2  | 1:121:A:LYS:HE3  | 9        | 0.29          |
| (1,1903) | 1:122:A:ALA:HB1  | 1:121:A:LYS:HE3  | 14       | 0.29          |
| (1,1881) | 1:113:A:ALA:HB3  | 1:88:A:VAL:HA    | 15       | 0.29          |
| (1,1881) | 1:113:A:ALA:HB3  | 1:88:A:VAL:HA    | 17       | 0.29          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1874) | 1:70:A:GLN:HE21  | 1:27:A:VAL:HG13 | 13       | 0.29          |
| (1,1865) | 1:45:A:ALA:HB3   | 1:44:A:GLU:HB3  | 12       | 0.29          |
| (1,1799) | 1:71:A:LEU:HA    | 1:74:A:ALA:HB3  | 1        | 0.29          |
| (1,1752) | 1:41:A:ALA:HB1   | 1:28:A:ILE:HG23 | 4        | 0.29          |
| (1,1746) | 1:71:A:LEU:HD22  | 1:74:A:ALA:H    | 2        | 0.29          |
| (1,1746) | 1:71:A:LEU:HD23  | 1:74:A:ALA:H    | 6        | 0.29          |
| (1,1746) | 1:71:A:LEU:HD22  | 1:74:A:ALA:H    | 12       | 0.29          |
| (1,1746) | 1:71:A:LEU:HD21  | 1:74:A:ALA:H    | 14       | 0.29          |
| (1,1737) | 1:77:A:LEU:HG    | 1:77:A:LEU:HD12 | 2        | 0.29          |
| (1,1737) | 1:77:A:LEU:HG    | 1:77:A:LEU:HD12 | 4        | 0.29          |
| (1,1737) | 1:77:A:LEU:HG    | 1:77:A:LEU:HD11 | 12       | 0.29          |
| (1,1735) | 1:66:A:LEU:HD22  | 1:67:A:SER:H    | 2        | 0.29          |
| (1,1698) | 1:44:A:GLU:HG2   | 1:45:A:ALA:HB1  | 11       | 0.29          |
| (1,1686) | 1:85:A:LEU:HD13  | 1:85:A:LEU:HD22 | 2        | 0.29          |
| (1,1613) | 1:124:A:VAL:HG21 | 1:121:A:LYS:HA  | 1        | 0.29          |
| (1,1613) | 1:124:A:VAL:HG23 | 1:121:A:LYS:HA  | 14       | 0.29          |
| (1,1545) | 1:56:A:LEU:HD13  | 1:60:A:VAL:HB   | 16       | 0.29          |
| (1,1521) | 1:30:A:PHE:HB3   | 1:29:A:ALA:HB2  | 2        | 0.29          |
| (1,1521) | 1:30:A:PHE:HB3   | 1:29:A:ALA:HB3  | 8        | 0.29          |
| (1,1521) | 1:30:A:PHE:HB3   | 1:29:A:ALA:HB2  | 13       | 0.29          |
| (1,1485) | 1:71:A:LEU:HD12  | 1:72:A:ARG:HA   | 2        | 0.29          |
| (1,1485) | 1:71:A:LEU:HD12  | 1:72:A:ARG:HA   | 7        | 0.29          |
| (1,1485) | 1:71:A:LEU:HD11  | 1:72:A:ARG:HA   | 9        | 0.29          |
| (1,1485) | 1:71:A:LEU:HD11  | 1:72:A:ARG:HA   | 13       | 0.29          |
| (1,1485) | 1:71:A:LEU:HD13  | 1:72:A:ARG:HA   | 14       | 0.29          |
| (1,1483) | 1:21:A:LEU:HG    | 1:64:A:MET:HE1  | 4        | 0.29          |
| (1,1481) | 1:64:A:MET:HE2   | 1:30:A:PHE:HA   | 7        | 0.29          |
| (1,1414) | 1:74:A:ALA:HB2   | 1:75:A:LEU:HD11 | 6        | 0.29          |
| (1,1414) | 1:74:A:ALA:HB3   | 1:75:A:LEU:HD11 | 14       | 0.29          |
| (1,1408) | 1:57:A:VAL:HG23  | 1:57:A:VAL:HB   | 6        | 0.29          |
| (1,1408) | 1:57:A:VAL:HG23  | 1:57:A:VAL:HB   | 14       | 0.29          |
| (1,1400) | 1:95:A:VAL:HG21  | 1:99:A:GLY:H    | 16       | 0.29          |
| (1,1397) | 1:31:A:LEU:HD22  | 1:60:A:VAL:HG11 | 2        | 0.29          |
| (1,1397) | 1:31:A:LEU:HD21  | 1:60:A:VAL:HG11 | 14       | 0.29          |
| (1,1375) | 1:110:A:VAL:HG13 | 1:91:A:GLY:HA2  | 5        | 0.29          |
| (1,1375) | 1:110:A:VAL:HG12 | 1:91:A:GLY:HA2  | 6        | 0.29          |
| (1,1365) | 1:32:A:ALA:HB2   | 1:28:A:ILE:HG23 | 4        | 0.29          |
| (1,1365) | 1:32:A:ALA:HB1   | 1:28:A:ILE:HG23 | 6        | 0.29          |
| (1,1365) | 1:32:A:ALA:HB2   | 1:28:A:ILE:HG22 | 11       | 0.29          |
| (1,1309) | 1:97:A:LEU:HD22  | 1:97:A:LEU:H    | 11       | 0.29          |
| (1,1309) | 1:97:A:LEU:HD21  | 1:97:A:LEU:H    | 15       | 0.29          |
| (1,1309) | 1:97:A:LEU:HD21  | 1:97:A:LEU:H    | 17       | 0.29          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1303) | 1:97:A:LEU:HD12  | 1:35:A:PHE:HE1   | 8        | 0.29          |
| (1,1136) | 1:31:A:LEU:HD13  | 1:35:A:PHE:HD2   | 9        | 0.29          |
| (1,1082) | 1:71:A:LEU:HD12  | 1:72:A:ARG:H     | 3        | 0.29          |
| (1,1082) | 1:71:A:LEU:HD13  | 1:72:A:ARG:H     | 11       | 0.29          |
| (1,1082) | 1:71:A:LEU:HD13  | 1:72:A:ARG:H     | 14       | 0.29          |
| (1,1081) | 1:71:A:LEU:HD13  | 1:57:A:VAL:H     | 16       | 0.29          |
| (1,1062) | 1:27:A:VAL:HG21  | 1:27:A:VAL:HG11  | 3        | 0.29          |
| (1,1048) | 1:124:A:VAL:HG22 | 1:120:A:ALA:HA   | 4        | 0.29          |
| (1,1048) | 1:124:A:VAL:HG22 | 1:120:A:ALA:HA   | 7        | 0.29          |
| (1,1048) | 1:124:A:VAL:HG22 | 1:120:A:ALA:HA   | 10       | 0.29          |
| (1,1048) | 1:124:A:VAL:HG21 | 1:120:A:ALA:HA   | 16       | 0.29          |
| (1,993)  | 1:79:A:THR:HG22  | 1:75:A:LEU:HA    | 8        | 0.29          |
| (1,895)  | 1:129:A:ALA:HB3  | 1:129:A:ALA:HA   | 8        | 0.29          |
| (1,850)  | 1:86:A:TYR:HB2   | 1:117:A:LEU:HB3  | 4        | 0.29          |
| (1,850)  | 1:86:A:TYR:HB2   | 1:117:A:LEU:HB3  | 13       | 0.29          |
| (1,829)  | 1:41:A:ALA:HB2   | 1:41:A:ALA:H     | 3        | 0.29          |
| (1,829)  | 1:41:A:ALA:HB2   | 1:41:A:ALA:H     | 5        | 0.29          |
| (1,829)  | 1:41:A:ALA:HB2   | 1:41:A:ALA:H     | 6        | 0.29          |
| (1,822)  | 1:49:A:LYS:H     | 1:52:A:ILE:HD13  | 8        | 0.29          |
| (1,822)  | 1:49:A:LYS:H     | 1:52:A:ILE:HD11  | 15       | 0.29          |
| (1,819)  | 1:28:A:ILE:HD11  | 1:74:A:ALA:HA    | 2        | 0.29          |
| (1,819)  | 1:28:A:ILE:HD12  | 1:74:A:ALA:HA    | 4        | 0.29          |
| (1,819)  | 1:28:A:ILE:HD11  | 1:74:A:ALA:HA    | 9        | 0.29          |
| (1,819)  | 1:28:A:ILE:HD11  | 1:74:A:ALA:HA    | 12       | 0.29          |
| (1,790)  | 1:50:A:ILE:HG22  | 1:50:A:ILE:H     | 8        | 0.29          |
| (1,691)  | 1:75:A:LEU:HD23  | 1:54:A:GLN:H     | 1        | 0.29          |
| (1,691)  | 1:75:A:LEU:HD21  | 1:54:A:GLN:H     | 11       | 0.29          |
| (1,643)  | 1:110:A:VAL:HG11 | 1:113:A:ALA:H    | 3        | 0.29          |
| (1,643)  | 1:110:A:VAL:HG12 | 1:113:A:ALA:H    | 5        | 0.29          |
| (1,643)  | 1:110:A:VAL:HG12 | 1:113:A:ALA:H    | 10       | 0.29          |
| (1,643)  | 1:110:A:VAL:HG13 | 1:113:A:ALA:H    | 15       | 0.29          |
| (1,643)  | 1:110:A:VAL:HG11 | 1:113:A:ALA:H    | 17       | 0.29          |
| (1,618)  | 1:95:A:VAL:H     | 1:48:A:LEU:HD11  | 7        | 0.29          |
| (1,618)  | 1:95:A:VAL:H     | 1:48:A:LEU:HD12  | 15       | 0.29          |
| (1,570)  | 1:60:A:VAL:HG11  | 1:34:A:ARG:HE    | 16       | 0.29          |
| (1,532)  | 1:116:A:GLN:HG3  | 1:116:A:GLN:HE21 | 1        | 0.29          |
| (1,532)  | 1:116:A:GLN:HG3  | 1:116:A:GLN:HE21 | 13       | 0.29          |
| (1,488)  | 1:21:A:LEU:HD12  | 1:23:A:SER:H     | 8        | 0.29          |
| (1,410)  | 1:53:A:PHE:H     | 1:56:A:LEU:HB3   | 10       | 0.29          |
| (1,241)  | 1:95:A:VAL:HG13  | 1:96:A:ASP:H     | 6        | 0.29          |
| (1,172)  | 1:27:A:VAL:HG11  | 1:21:A:LEU:H     | 6        | 0.29          |
| (1,128)  | 1:35:A:PHE:HD1   | 1:39:A:PHE:H     | 8        | 0.29          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (3,135)  | 1:123:A:ARG:HB3 | 1:120:A:ALA:HA   | 6        | 0.28          |
| (3,135)  | 1:123:A:ARG:HB3 | 1:120:A:ALA:HA   | 11       | 0.28          |
| (3,119)  | 1:98:A:ASP:HB3  | 1:99:A:GLY:HA2   | 15       | 0.28          |
| (3,109)  | 1:92:A:ALA:H    | 1:110:A:VAL:HB   | 2        | 0.28          |
| (3,109)  | 1:92:A:ALA:H    | 1:110:A:VAL:HB   | 14       | 0.28          |
| (3,84)   | 1:84:A:TYR:HE2  | 1:84:A:TYR:HA    | 2        | 0.28          |
| (3,59)   | 1:117:A:LEU:HA  | 1:85:A:LEU:HD23  | 5        | 0.28          |
| (3,16)   | 1:90:A:PRO:HA   | 1:110:A:VAL:HG11 | 3        | 0.28          |
| (3,16)   | 1:90:A:PRO:HA   | 1:110:A:VAL:HG12 | 9        | 0.28          |
| (3,16)   | 1:90:A:PRO:HA   | 1:110:A:VAL:HG11 | 17       | 0.28          |
| (3,15)   | 1:85:A:LEU:HB3  | 1:82:A:TRP:HA    | 15       | 0.28          |
| (3,15)   | 1:85:A:LEU:HB3  | 1:82:A:TRP:HA    | 17       | 0.28          |
| (1,4310) | 1:64:A:MET:HA   | 1:65:A:ASN:H     | 1        | 0.28          |
| (1,4280) | 1:112:A:HIS:HA  | 1:116:A:GLN:H    | 3        | 0.28          |
| (1,4280) | 1:112:A:HIS:HA  | 1:116:A:GLN:H    | 7        | 0.28          |
| (1,4280) | 1:112:A:HIS:HA  | 1:116:A:GLN:H    | 10       | 0.28          |
| (1,4280) | 1:112:A:HIS:HA  | 1:116:A:GLN:H    | 12       | 0.28          |
| (1,4280) | 1:112:A:HIS:HA  | 1:116:A:GLN:H    | 13       | 0.28          |
| (1,4280) | 1:112:A:HIS:HA  | 1:116:A:GLN:H    | 14       | 0.28          |
| (1,4280) | 1:112:A:HIS:HA  | 1:116:A:GLN:H    | 15       | 0.28          |
| (1,4255) | 1:75:A:LEU:HD22 | 1:54:A:GLN:H     | 13       | 0.28          |
| (1,4230) | 1:128:A:ARG:HA  | 1:128:A:ARG:H    | 8        | 0.28          |
| (1,4195) | 1:61:A:ALA:HB2  | 1:67:A:SER:H     | 10       | 0.28          |
| (1,4171) | 1:48:A:LEU:HD23 | 1:49:A:LYS:H     | 2        | 0.28          |
| (1,4141) | 1:98:A:ASP:HB2  | 1:100:A:ASN:HD21 | 1        | 0.28          |
| (1,4141) | 1:98:A:ASP:HB2  | 1:100:A:ASN:HD21 | 6        | 0.28          |
| (1,4141) | 1:98:A:ASP:HB2  | 1:100:A:ASN:HD21 | 7        | 0.28          |
| (1,4141) | 1:98:A:ASP:HB2  | 1:100:A:ASN:HD21 | 11       | 0.28          |
| (1,4140) | 1:118:A:GLU:HA  | 1:118:A:GLU:H    | 4        | 0.28          |
| (1,4140) | 1:118:A:GLU:HA  | 1:118:A:GLU:H    | 6        | 0.28          |
| (1,4140) | 1:118:A:GLU:HA  | 1:118:A:GLU:H    | 14       | 0.28          |
| (1,4119) | 1:66:A:LEU:HB2  | 1:70:A:GLN:HE22  | 7        | 0.28          |
| (1,4114) | 1:65:A:ASN:H    | 1:65:A:ASN:HD21  | 1        | 0.28          |
| (1,4114) | 1:65:A:ASN:H    | 1:65:A:ASN:HD21  | 12       | 0.28          |
| (1,4113) | 1:22:A:ASN:H    | 1:22:A:ASN:HD22  | 2        | 0.28          |
| (1,4082) | 1:22:A:ASN:HD21 | 1:22:A:ASN:HB3   | 11       | 0.28          |
| (1,4016) | 1:15:A:MET:HA   | 1:15:A:MET:H     | 6        | 0.28          |
| (1,4016) | 1:15:A:MET:HA   | 1:15:A:MET:H     | 16       | 0.28          |
| (1,4006) | 1:42:A:GLU:HB3  | 1:41:A:ALA:H     | 4        | 0.28          |
| (1,4006) | 1:42:A:GLU:HB3  | 1:41:A:ALA:H     | 6        | 0.28          |
| (1,4006) | 1:42:A:GLU:HB3  | 1:41:A:ALA:H     | 10       | 0.28          |
| (1,4006) | 1:42:A:GLU:HB3  | 1:41:A:ALA:H     | 12       | 0.28          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,4006) | 1:42:A:GLU:HB3  | 1:41:A:ALA:H     | 16       | 0.28          |
| (1,3889) | 1:100:A:ASN:HB3 | 1:100:A:ASN:HD21 | 7        | 0.28          |
| (1,3889) | 1:100:A:ASN:HB3 | 1:100:A:ASN:HD21 | 16       | 0.28          |
| (1,3786) | 1:27:A:VAL:HG12 | 1:21:A:LEU:H     | 4        | 0.28          |
| (1,3783) | 1:117:A:LEU:HB3 | 1:117:A:LEU:H    | 3        | 0.28          |
| (1,3783) | 1:117:A:LEU:HB3 | 1:117:A:LEU:H    | 9        | 0.28          |
| (1,3776) | 1:121:A:LYS:HA  | 1:122:A:ALA:H    | 13       | 0.28          |
| (1,3769) | 1:130:A:GLU:H   | 1:129:A:ALA:HB3  | 3        | 0.28          |
| (1,3769) | 1:130:A:GLU:H   | 1:129:A:ALA:HB1  | 5        | 0.28          |
| (1,3769) | 1:130:A:GLU:H   | 1:129:A:ALA:HB2  | 7        | 0.28          |
| (1,3769) | 1:130:A:GLU:H   | 1:129:A:ALA:HB1  | 11       | 0.28          |
| (1,3741) | 1:28:A:ILE:HG13 | 1:28:A:ILE:H     | 10       | 0.28          |
| (1,3733) | 1:27:A:VAL:HG11 | 1:26:A:GLU:H     | 4        | 0.28          |
| (1,3728) | 1:29:A:ALA:HA   | 1:30:A:PHE:H     | 1        | 0.28          |
| (1,3716) | 1:35:A:PHE:HE1  | 1:35:A:PHE:H     | 2        | 0.28          |
| (1,3716) | 1:35:A:PHE:HE1  | 1:35:A:PHE:H     | 12       | 0.28          |
| (1,3716) | 1:35:A:PHE:HE2  | 1:35:A:PHE:H     | 14       | 0.28          |
| (1,3716) | 1:35:A:PHE:HE2  | 1:35:A:PHE:H     | 17       | 0.28          |
| (1,3678) | 1:95:A:VAL:H    | 1:96:A:ASP:H     | 11       | 0.28          |
| (1,3668) | 1:84:A:TYR:H    | 1:84:A:TYR:HD1   | 2        | 0.28          |
| (1,3668) | 1:84:A:TYR:H    | 1:84:A:TYR:HD1   | 16       | 0.28          |
| (1,3662) | 1:83:A:ARG:H    | 1:82:A:TRP:HD1   | 9        | 0.28          |
| (1,3662) | 1:83:A:ARG:H    | 1:82:A:TRP:HD1   | 11       | 0.28          |
| (1,3627) | 1:100:A:ASN:H   | 1:100:A:ASN:HD21 | 1        | 0.28          |
| (1,3627) | 1:100:A:ASN:H   | 1:100:A:ASN:HD21 | 17       | 0.28          |
| (1,3604) | 1:97:A:LEU:HB2  | 1:97:A:LEU:HA    | 8        | 0.28          |
| (1,3599) | 1:92:A:ALA:HB3  | 1:113:A:ALA:HB3  | 4        | 0.28          |
| (1,3591) | 1:93:A:THR:HB   | 1:88:A:VAL:HG11  | 4        | 0.28          |
| (1,3565) | 1:105:A:LEU:HB3 | 1:105:A:LEU:HA   | 3        | 0.28          |
| (1,3565) | 1:105:A:LEU:HB3 | 1:105:A:LEU:HA   | 7        | 0.28          |
| (1,3565) | 1:105:A:LEU:HB3 | 1:105:A:LEU:HA   | 11       | 0.28          |
| (1,3534) | 1:122:A:ALA:HB3 | 1:121:A:LYS:HE3  | 16       | 0.28          |
| (1,3508) | 1:113:A:ALA:HB3 | 1:88:A:VAL:HA    | 1        | 0.28          |
| (1,3495) | 1:54:A:GLN:H    | 1:75:A:LEU:HD12  | 7        | 0.28          |
| (1,3491) | 1:86:A:TYR:HE1  | 1:85:A:LEU:HD22  | 8        | 0.28          |
| (1,3491) | 1:86:A:TYR:HE2  | 1:85:A:LEU:HD21  | 16       | 0.28          |
| (1,3479) | 1:45:A:ALA:HB2  | 1:44:A:GLU:HB3   | 14       | 0.28          |
| (1,3465) | 1:88:A:VAL:HG22 | 1:85:A:LEU:HB3   | 6        | 0.28          |
| (1,3421) | 1:53:A:PHE:HA   | 1:75:A:LEU:HD22  | 2        | 0.28          |
| (1,3421) | 1:53:A:PHE:HA   | 1:75:A:LEU:HD22  | 4        | 0.28          |
| (1,3421) | 1:53:A:PHE:HA   | 1:75:A:LEU:HD22  | 7        | 0.28          |
| (1,3421) | 1:53:A:PHE:HA   | 1:75:A:LEU:HD23  | 9        | 0.28          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3417) | 1:117:A:LEU:HG   | 1:117:A:LEU:HD12 | 17       | 0.28          |
| (1,3416) | 1:117:A:LEU:HD11 | 1:117:A:LEU:HB3  | 8        | 0.28          |
| (1,3414) | 1:86:A:TYR:H     | 1:117:A:LEU:HD13 | 2        | 0.28          |
| (1,3402) | 1:58:A:ASP:H     | 1:55:A:ASP:HA    | 3        | 0.28          |
| (1,3402) | 1:58:A:ASP:H     | 1:55:A:ASP:HA    | 5        | 0.28          |
| (1,3396) | 1:71:A:LEU:HA    | 1:74:A:ALA:HB3   | 8        | 0.28          |
| (1,3345) | 1:29:A:ALA:HA    | 1:29:A:ALA:HB2   | 4        | 0.28          |
| (1,3341) | 1:41:A:ALA:HB3   | 1:28:A:ILE:HG21  | 12       | 0.28          |
| (1,3326) | 1:77:A:LEU:HG    | 1:77:A:LEU:HD13  | 6        | 0.28          |
| (1,3326) | 1:77:A:LEU:HG    | 1:77:A:LEU:HD13  | 13       | 0.28          |
| (1,3326) | 1:77:A:LEU:HG    | 1:77:A:LEU:HD13  | 16       | 0.28          |
| (1,3282) | 1:44:A:GLU:HG2   | 1:45:A:ALA:HB1   | 7        | 0.28          |
| (1,3257) | 1:48:A:LEU:HD12  | 1:38:A:CYS:HA    | 4        | 0.28          |
| (1,3253) | 1:92:A:ALA:HB2   | 1:91:A:GLY:H     | 6        | 0.28          |
| (1,3253) | 1:92:A:ALA:HB1   | 1:91:A:GLY:H     | 11       | 0.28          |
| (1,3228) | 1:31:A:LEU:HB2   | 1:39:A:PHE:HE2   | 6        | 0.28          |
| (1,3228) | 1:31:A:LEU:HB2   | 1:39:A:PHE:HE2   | 7        | 0.28          |
| (1,3228) | 1:31:A:LEU:HB2   | 1:39:A:PHE:HE1   | 10       | 0.28          |
| (1,3223) | 1:84:A:TYR:HE1   | 1:79:A:THR:HA    | 12       | 0.28          |
| (1,3216) | 1:48:A:LEU:HG    | 1:84:A:TYR:HD2   | 3        | 0.28          |
| (1,3198) | 1:114:A:ARG:HA   | 1:113:A:ALA:HB2  | 12       | 0.28          |
| (1,3180) | 1:111:A:GLU:HG2  | 1:111:A:GLU:HA   | 4        | 0.28          |
| (1,3180) | 1:111:A:GLU:HG2  | 1:111:A:GLU:HA   | 7        | 0.28          |
| (1,3180) | 1:111:A:GLU:HG2  | 1:111:A:GLU:HA   | 12       | 0.28          |
| (1,3180) | 1:111:A:GLU:HG2  | 1:111:A:GLU:HA   | 17       | 0.28          |
| (1,3178) | 1:116:A:GLN:HA   | 1:116:A:GLN:H    | 3        | 0.28          |
| (1,3178) | 1:116:A:GLN:HA   | 1:116:A:GLN:H    | 6        | 0.28          |
| (1,3178) | 1:116:A:GLN:HA   | 1:116:A:GLN:H    | 10       | 0.28          |
| (1,3178) | 1:116:A:GLN:HA   | 1:116:A:GLN:H    | 12       | 0.28          |
| (1,3178) | 1:116:A:GLN:HA   | 1:116:A:GLN:H    | 14       | 0.28          |
| (1,3178) | 1:116:A:GLN:HA   | 1:116:A:GLN:H    | 16       | 0.28          |
| (1,3123) | 1:59:A:ARG:HB2   | 1:59:A:ARG:HA    | 13       | 0.28          |
| (1,3123) | 1:59:A:ARG:HB2   | 1:59:A:ARG:HA    | 17       | 0.28          |
| (1,3114) | 1:57:A:VAL:HG22  | 1:57:A:VAL:HG12  | 12       | 0.28          |
| (1,3066) | 1:30:A:PHE:HB3   | 1:29:A:ALA:HB3   | 11       | 0.28          |
| (1,3058) | 1:52:A:ILE:HG22  | 1:48:A:LEU:HG    | 4        | 0.28          |
| (1,3036) | 1:78:A:TYR:HH    | 1:45:A:ALA:HB3   | 7        | 0.28          |
| (1,3036) | 1:78:A:TYR:HH    | 1:45:A:ALA:HB3   | 10       | 0.28          |
| (1,3036) | 1:78:A:TYR:HH    | 1:45:A:ALA:HB3   | 16       | 0.28          |
| (1,3025) | 1:21:A:LEU:HG    | 1:64:A:MET:HE3   | 9        | 0.28          |
| (1,2991) | 1:54:A:GLN:HE22  | 1:54:A:GLN:HG2   | 6        | 0.28          |
| (1,2989) | 1:42:A:GLU:HA    | 1:42:A:GLU:HB2   | 2        | 0.28          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2989) | 1:42:A:GLU:HA    | 1:42:A:GLU:HB2   | 12       | 0.28          |
| (1,2942) | 1:57:A:VAL:HG22  | 1:57:A:VAL:HB    | 4        | 0.28          |
| (1,2942) | 1:57:A:VAL:HG22  | 1:57:A:VAL:HB    | 9        | 0.28          |
| (1,2942) | 1:57:A:VAL:HG23  | 1:57:A:VAL:HB    | 16       | 0.28          |
| (1,2933) | 1:95:A:VAL:HG23  | 1:99:A:GLY:H     | 4        | 0.28          |
| (1,2909) | 1:110:A:VAL:HG12 | 1:91:A:GLY:HA2   | 4        | 0.28          |
| (1,2909) | 1:110:A:VAL:HG13 | 1:91:A:GLY:HA2   | 9        | 0.28          |
| (1,2891) | 1:32:A:ALA:HB1   | 1:28:A:ILE:HG23  | 3        | 0.28          |
| (1,2873) | 1:126:A:ALA:HA   | 1:126:A:ALA:HB3  | 5        | 0.28          |
| (1,2863) | 1:78:A:TYR:HE2   | 1:84:A:TYR:HD1   | 8        | 0.28          |
| (1,2863) | 1:78:A:TYR:HE1   | 1:84:A:TYR:HD1   | 11       | 0.28          |
| (1,2830) | 1:39:A:PHE:HZ    | 1:97:A:LEU:HD21  | 9        | 0.28          |
| (1,2829) | 1:97:A:LEU:HD22  | 1:97:A:LEU:HB2   | 10       | 0.28          |
| (1,2829) | 1:97:A:LEU:HD23  | 1:97:A:LEU:HB2   | 13       | 0.28          |
| (1,2829) | 1:97:A:LEU:HD22  | 1:97:A:LEU:HB2   | 17       | 0.28          |
| (1,2824) | 1:97:A:LEU:HD22  | 1:56:A:LEU:HA    | 10       | 0.28          |
| (1,2824) | 1:97:A:LEU:HD22  | 1:56:A:LEU:HA    | 14       | 0.28          |
| (1,2819) | 1:97:A:LEU:HD11  | 1:35:A:PHE:HE2   | 6        | 0.28          |
| (1,2769) | 1:43:A:GLY:HA2   | 1:42:A:GLU:HB2   | 7        | 0.28          |
| (1,2753) | 1:97:A:LEU:HD13  | 1:59:A:ARG:HD3   | 13       | 0.28          |
| (1,2720) | 1:86:A:TYR:HB3   | 1:117:A:LEU:HD12 | 17       | 0.28          |
| (1,2679) | 1:53:A:PHE:HA    | 1:53:A:PHE:HE2   | 4        | 0.28          |
| (1,2679) | 1:53:A:PHE:HA    | 1:53:A:PHE:HE2   | 11       | 0.28          |
| (1,2679) | 1:53:A:PHE:HA    | 1:53:A:PHE:HE2   | 13       | 0.28          |
| (1,2679) | 1:53:A:PHE:HA    | 1:53:A:PHE:HE1   | 14       | 0.28          |
| (1,2675) | 1:85:A:LEU:HB2   | 1:86:A:TYR:HD2   | 1        | 0.28          |
| (1,2675) | 1:85:A:LEU:HB2   | 1:86:A:TYR:HD1   | 2        | 0.28          |
| (1,2675) | 1:85:A:LEU:HB2   | 1:86:A:TYR:HD1   | 9        | 0.28          |
| (1,2675) | 1:85:A:LEU:HB2   | 1:86:A:TYR:HD1   | 11       | 0.28          |
| (1,2675) | 1:85:A:LEU:HB2   | 1:86:A:TYR:HD2   | 17       | 0.28          |
| (1,2662) | 1:97:A:LEU:HD11  | 1:57:A:VAL:H     | 8        | 0.28          |
| (1,2650) | 1:77:A:LEU:HD22  | 1:77:A:LEU:HB2   | 1        | 0.28          |
| (1,2650) | 1:77:A:LEU:HD23  | 1:77:A:LEU:HB2   | 2        | 0.28          |
| (1,2650) | 1:77:A:LEU:HD21  | 1:77:A:LEU:HB2   | 8        | 0.28          |
| (1,2650) | 1:77:A:LEU:HD22  | 1:77:A:LEU:HB2   | 14       | 0.28          |
| (1,2598) | 1:27:A:VAL:HG21  | 1:27:A:VAL:HG13  | 9        | 0.28          |
| (1,2598) | 1:27:A:VAL:HG21  | 1:27:A:VAL:HG11  | 10       | 0.28          |
| (1,2598) | 1:27:A:VAL:HG23  | 1:27:A:VAL:HG11  | 11       | 0.28          |
| (1,2596) | 1:74:A:ALA:HB1   | 1:27:A:VAL:HG11  | 5        | 0.28          |
| (1,2596) | 1:74:A:ALA:HB1   | 1:27:A:VAL:HG13  | 9        | 0.28          |
| (1,2583) | 1:60:A:VAL:HG11  | 1:34:A:ARG:HG2   | 15       | 0.28          |
| (1,2576) | 1:124:A:VAL:HG22 | 1:120:A:ALA:HA   | 2        | 0.28          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2576) | 1:124:A:VAL:HG22 | 1:120:A:ALA:HA   | 6        | 0.28          |
| (1,2559) | 1:86:A:TYR:HE1   | 1:86:A:TYR:HB2   | 8        | 0.28          |
| (1,2546) | 1:73:A:SER:HA    | 1:73:A:SER:HB3   | 11       | 0.28          |
| (1,2502) | 1:42:A:GLU:HA    | 1:43:A:GLY:H     | 2        | 0.28          |
| (1,2502) | 1:42:A:GLU:HA    | 1:43:A:GLY:H     | 5        | 0.28          |
| (1,2468) | 1:53:A:PHE:HE1   | 1:72:A:ARG:HG3   | 5        | 0.28          |
| (1,2468) | 1:53:A:PHE:HE1   | 1:72:A:ARG:HG3   | 15       | 0.28          |
| (1,2468) | 1:53:A:PHE:HE1   | 1:72:A:ARG:HG3   | 16       | 0.28          |
| (1,2418) | 1:113:A:ALA:HB2  | 1:110:A:VAL:HG13 | 11       | 0.28          |
| (1,2369) | 1:52:A:ILE:HD12  | 1:56:A:LEU:H     | 1        | 0.28          |
| (1,2369) | 1:52:A:ILE:HD12  | 1:56:A:LEU:H     | 4        | 0.28          |
| (1,2358) | 1:107:A:GLU:HA   | 1:111:A:GLU:H    | 10       | 0.28          |
| (1,2346) | 1:105:A:LEU:HD12 | 1:107:A:GLU:HA   | 16       | 0.28          |
| (1,2344) | 1:104:A:GLU:HG2  | 1:105:A:LEU:HD23 | 8        | 0.28          |
| (1,2336) | 1:64:A:MET:HE1   | 1:31:A:LEU:HA    | 1        | 0.28          |
| (1,2331) | 1:54:A:GLN:HG2   | 1:55:A:ASP:HA    | 5        | 0.28          |
| (1,2331) | 1:54:A:GLN:HG2   | 1:55:A:ASP:HA    | 6        | 0.28          |
| (1,2331) | 1:54:A:GLN:HG2   | 1:55:A:ASP:HA    | 13       | 0.28          |
| (1,2201) | 1:64:A:MET:HB2   | 1:21:A:LEU:HD22  | 3        | 0.28          |
| (1,2116) | 1:45:A:ALA:HB3   | 1:84:A:TYR:HA    | 10       | 0.28          |
| (1,2098) | 1:21:A:LEU:HD22  | 1:27:A:VAL:HG12  | 14       | 0.28          |
| (1,2098) | 1:21:A:LEU:HD22  | 1:27:A:VAL:HG11  | 16       | 0.28          |
| (1,2094) | 1:95:A:VAL:HG22  | 1:97:A:LEU:HD21  | 12       | 0.28          |
| (1,2088) | 1:82:A:TRP:HZ2   | 1:124:A:VAL:HG22 | 3        | 0.28          |
| (1,2088) | 1:82:A:TRP:HZ2   | 1:124:A:VAL:HG22 | 5        | 0.28          |
| (1,2088) | 1:82:A:TRP:HZ2   | 1:124:A:VAL:HG21 | 15       | 0.28          |
| (1,2036) | 1:97:A:LEU:HD22  | 1:97:A:LEU:HB2   | 5        | 0.28          |
| (1,2036) | 1:97:A:LEU:HD22  | 1:97:A:LEU:HB2   | 7        | 0.28          |
| (1,2036) | 1:97:A:LEU:HD21  | 1:97:A:LEU:HB2   | 16       | 0.28          |
| (1,2028) | 1:97:A:LEU:HD21  | 1:97:A:LEU:H     | 12       | 0.28          |
| (1,2025) | 1:97:A:LEU:HD23  | 1:35:A:PHE:HD1   | 8        | 0.28          |
| (1,2005) | 1:95:A:VAL:HG23  | 1:48:A:LEU:HD11  | 6        | 0.28          |
| (1,1994) | 1:91:A:GLY:HA2   | 1:91:A:GLY:H     | 2        | 0.28          |
| (1,1994) | 1:91:A:GLY:HA2   | 1:91:A:GLY:H     | 8        | 0.28          |
| (1,1994) | 1:91:A:GLY:HA2   | 1:91:A:GLY:H     | 9        | 0.28          |
| (1,1994) | 1:91:A:GLY:HA2   | 1:91:A:GLY:H     | 12       | 0.28          |
| (1,1994) | 1:91:A:GLY:HA2   | 1:91:A:GLY:H     | 13       | 0.28          |
| (1,1994) | 1:91:A:GLY:HA2   | 1:91:A:GLY:H     | 16       | 0.28          |
| (1,1960) | 1:121:A:LYS:HG3  | 1:117:A:LEU:HD13 | 6        | 0.28          |
| (1,1947) | 1:93:A:THR:HB    | 1:88:A:VAL:HG13  | 11       | 0.28          |
| (1,1945) | 1:105:A:LEU:HB3  | 1:110:A:VAL:HG22 | 2        | 0.28          |
| (1,1945) | 1:105:A:LEU:HB3  | 1:110:A:VAL:HG21 | 3        | 0.28          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1945) | 1:105:A:LEU:HB3  | 1:110:A:VAL:HG23 | 8        | 0.28          |
| (1,1940) | 1:111:A:GLU:HB2  | 1:109:A:HIS:HA   | 1        | 0.28          |
| (1,1940) | 1:111:A:GLU:HB2  | 1:109:A:HIS:HA   | 7        | 0.28          |
| (1,1940) | 1:111:A:GLU:HB2  | 1:109:A:HIS:HA   | 11       | 0.28          |
| (1,1940) | 1:111:A:GLU:HB2  | 1:109:A:HIS:HA   | 12       | 0.28          |
| (1,1903) | 1:122:A:ALA:HB2  | 1:121:A:LYS:HE3  | 8        | 0.28          |
| (1,1903) | 1:122:A:ALA:HB3  | 1:121:A:LYS:HE3  | 13       | 0.28          |
| (1,1865) | 1:45:A:ALA:HB1   | 1:44:A:GLU:HB3   | 13       | 0.28          |
| (1,1799) | 1:71:A:LEU:HA    | 1:74:A:ALA:HB2   | 10       | 0.28          |
| (1,1799) | 1:71:A:LEU:HA    | 1:74:A:ALA:HB2   | 16       | 0.28          |
| (1,1752) | 1:41:A:ALA:HB2   | 1:28:A:ILE:HG23  | 6        | 0.28          |
| (1,1752) | 1:41:A:ALA:HB1   | 1:28:A:ILE:HG21  | 7        | 0.28          |
| (1,1752) | 1:41:A:ALA:HB2   | 1:28:A:ILE:HG22  | 14       | 0.28          |
| (1,1737) | 1:77:A:LEU:HG    | 1:77:A:LEU:HD11  | 7        | 0.28          |
| (1,1737) | 1:77:A:LEU:HG    | 1:77:A:LEU:HD11  | 9        | 0.28          |
| (1,1737) | 1:77:A:LEU:HG    | 1:77:A:LEU:HD12  | 15       | 0.28          |
| (1,1723) | 1:68:A:LYS:HD3   | 1:57:A:VAL:HG13  | 9        | 0.28          |
| (1,1723) | 1:68:A:LYS:HD3   | 1:57:A:VAL:HG11  | 11       | 0.28          |
| (1,1698) | 1:44:A:GLU:HG2   | 1:45:A:ALA:HB2   | 17       | 0.28          |
| (1,1686) | 1:85:A:LEU:HD11  | 1:85:A:LEU:HD22  | 3        | 0.28          |
| (1,1684) | 1:48:A:LEU:HD12  | 1:50:A:ILE:HA    | 6        | 0.28          |
| (1,1656) | 1:31:A:LEU:HB2   | 1:39:A:PHE:HE1   | 8        | 0.28          |
| (1,1629) | 1:116:A:GLN:HG3  | 1:113:A:ALA:HB1  | 7        | 0.28          |
| (1,1521) | 1:30:A:PHE:HB3   | 1:29:A:ALA:HB2   | 7        | 0.28          |
| (1,1521) | 1:30:A:PHE:HB3   | 1:29:A:ALA:HB3   | 9        | 0.28          |
| (1,1521) | 1:30:A:PHE:HB3   | 1:29:A:ALA:HB2   | 10       | 0.28          |
| (1,1490) | 1:78:A:TYR:HH    | 1:45:A:ALA:HB1   | 17       | 0.28          |
| (1,1485) | 1:71:A:LEU:HD11  | 1:72:A:ARG:HA    | 4        | 0.28          |
| (1,1485) | 1:71:A:LEU:HD13  | 1:72:A:ARG:HA    | 15       | 0.28          |
| (1,1419) | 1:77:A:LEU:HD13  | 1:25:A:LYS:HA    | 1        | 0.28          |
| (1,1419) | 1:77:A:LEU:HD13  | 1:25:A:LYS:HA    | 2        | 0.28          |
| (1,1397) | 1:31:A:LEU:HD21  | 1:60:A:VAL:HG11  | 16       | 0.28          |
| (1,1375) | 1:110:A:VAL:HG11 | 1:91:A:GLY:HA2   | 11       | 0.28          |
| (1,1375) | 1:110:A:VAL:HG13 | 1:91:A:GLY:HA2   | 14       | 0.28          |
| (1,1365) | 1:32:A:ALA:HB3   | 1:28:A:ILE:HG22  | 1        | 0.28          |
| (1,1357) | 1:74:A:ALA:HB3   | 1:31:A:LEU:HD12  | 9        | 0.28          |
| (1,1309) | 1:97:A:LEU:HD21  | 1:97:A:LEU:H     | 10       | 0.28          |
| (1,1309) | 1:97:A:LEU:HD21  | 1:97:A:LEU:H     | 12       | 0.28          |
| (1,1304) | 1:97:A:LEU:HD22  | 1:56:A:LEU:HA    | 2        | 0.28          |
| (1,1231) | 1:97:A:LEU:HD13  | 1:59:A:ARG:HD3   | 1        | 0.28          |
| (1,1231) | 1:97:A:LEU:HD11  | 1:59:A:ARG:HD3   | 10       | 0.28          |
| (1,1136) | 1:31:A:LEU:HD11  | 1:35:A:PHE:HD1   | 8        | 0.28          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1124) | 1:97:A:LEU:HD12  | 1:57:A:VAL:H    | 3        | 0.28          |
| (1,1082) | 1:71:A:LEU:HD12  | 1:72:A:ARG:H    | 2        | 0.28          |
| (1,1082) | 1:71:A:LEU:HD11  | 1:72:A:ARG:H    | 4        | 0.28          |
| (1,1082) | 1:71:A:LEU:HD12  | 1:72:A:ARG:H    | 5        | 0.28          |
| (1,1082) | 1:71:A:LEU:HD12  | 1:72:A:ARG:H    | 7        | 0.28          |
| (1,1082) | 1:71:A:LEU:HD12  | 1:72:A:ARG:H    | 8        | 0.28          |
| (1,1082) | 1:71:A:LEU:HD11  | 1:72:A:ARG:H    | 9        | 0.28          |
| (1,1082) | 1:71:A:LEU:HD11  | 1:72:A:ARG:H    | 10       | 0.28          |
| (1,1082) | 1:71:A:LEU:HD11  | 1:72:A:ARG:H    | 13       | 0.28          |
| (1,1082) | 1:71:A:LEU:HD13  | 1:72:A:ARG:H    | 15       | 0.28          |
| (1,1082) | 1:71:A:LEU:HD11  | 1:72:A:ARG:H    | 16       | 0.28          |
| (1,1081) | 1:71:A:LEU:HD12  | 1:57:A:VAL:H    | 15       | 0.28          |
| (1,1062) | 1:27:A:VAL:HG23  | 1:27:A:VAL:HG13 | 1        | 0.28          |
| (1,1062) | 1:27:A:VAL:HG21  | 1:27:A:VAL:HG11 | 2        | 0.28          |
| (1,1062) | 1:27:A:VAL:HG23  | 1:27:A:VAL:HG11 | 13       | 0.28          |
| (1,1062) | 1:27:A:VAL:HG23  | 1:27:A:VAL:HG11 | 14       | 0.28          |
| (1,1062) | 1:27:A:VAL:HG21  | 1:27:A:VAL:HG12 | 17       | 0.28          |
| (1,1060) | 1:74:A:ALA:HB1   | 1:27:A:VAL:HG13 | 1        | 0.28          |
| (1,1060) | 1:74:A:ALA:HB2   | 1:27:A:VAL:HG11 | 10       | 0.28          |
| (1,1060) | 1:74:A:ALA:HB3   | 1:27:A:VAL:HG12 | 15       | 0.28          |
| (1,1048) | 1:124:A:VAL:HG21 | 1:120:A:ALA:HA  | 1        | 0.28          |
| (1,1048) | 1:124:A:VAL:HG22 | 1:120:A:ALA:HA  | 15       | 0.28          |
| (1,1048) | 1:124:A:VAL:HG23 | 1:120:A:ALA:HA  | 17       | 0.28          |
| (1,1030) | 1:86:A:TYR:HE1   | 1:86:A:TYR:HB2  | 4        | 0.28          |
| (1,1030) | 1:86:A:TYR:HE2   | 1:86:A:TYR:HB2  | 5        | 0.28          |
| (1,1030) | 1:86:A:TYR:HE2   | 1:86:A:TYR:HB2  | 16       | 0.28          |
| (1,1010) | 1:76:A:ARG:HB2   | 1:73:A:SER:HA   | 11       | 0.28          |
| (1,895)  | 1:129:A:ALA:HB2  | 1:129:A:ALA:HA  | 3        | 0.28          |
| (1,895)  | 1:129:A:ALA:HB1  | 1:129:A:ALA:HA  | 14       | 0.28          |
| (1,850)  | 1:86:A:TYR:HB2   | 1:117:A:LEU:HB3 | 5        | 0.28          |
| (1,850)  | 1:86:A:TYR:HB2   | 1:117:A:LEU:HB3 | 7        | 0.28          |
| (1,850)  | 1:86:A:TYR:HB2   | 1:117:A:LEU:HB3 | 8        | 0.28          |
| (1,850)  | 1:86:A:TYR:HB2   | 1:117:A:LEU:HB3 | 10       | 0.28          |
| (1,850)  | 1:86:A:TYR:HB2   | 1:117:A:LEU:HB3 | 16       | 0.28          |
| (1,850)  | 1:86:A:TYR:HB2   | 1:117:A:LEU:HB3 | 17       | 0.28          |
| (1,829)  | 1:41:A:ALA:HB2   | 1:41:A:ALA:H    | 12       | 0.28          |
| (1,819)  | 1:28:A:ILE:HD11  | 1:74:A:ALA:HA   | 7        | 0.28          |
| (1,819)  | 1:28:A:ILE:HD11  | 1:74:A:ALA:HA   | 15       | 0.28          |
| (1,815)  | 1:50:A:ILE:HD11  | 1:50:A:ILE:HA   | 4        | 0.28          |
| (1,691)  | 1:75:A:LEU:HD23  | 1:54:A:GLN:H    | 5        | 0.28          |
| (1,691)  | 1:75:A:LEU:HD23  | 1:54:A:GLN:H    | 6        | 0.28          |
| (1,691)  | 1:75:A:LEU:HD23  | 1:54:A:GLN:H    | 14       | 0.28          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,643)  | 1:110:A:VAL:HG12 | 1:113:A:ALA:H    | 1        | 0.28          |
| (1,643)  | 1:110:A:VAL:HG13 | 1:113:A:ALA:H    | 2        | 0.28          |
| (1,643)  | 1:110:A:VAL:HG12 | 1:113:A:ALA:H    | 9        | 0.28          |
| (1,643)  | 1:110:A:VAL:HG13 | 1:113:A:ALA:H    | 11       | 0.28          |
| (1,643)  | 1:110:A:VAL:HG11 | 1:113:A:ALA:H    | 12       | 0.28          |
| (1,643)  | 1:110:A:VAL:HG11 | 1:113:A:ALA:H    | 13       | 0.28          |
| (1,643)  | 1:110:A:VAL:HG13 | 1:113:A:ALA:H    | 16       | 0.28          |
| (1,610)  | 1:48:A:LEU:HD21  | 1:49:A:LYS:H     | 4        | 0.28          |
| (1,549)  | 1:97:A:LEU:HD11  | 1:98:A:ASP:H     | 16       | 0.28          |
| (1,532)  | 1:116:A:GLN:HG3  | 1:116:A:GLN:HE21 | 4        | 0.28          |
| (1,532)  | 1:116:A:GLN:HG3  | 1:116:A:GLN:HE21 | 5        | 0.28          |
| (1,532)  | 1:116:A:GLN:HG3  | 1:116:A:GLN:HE21 | 8        | 0.28          |
| (1,532)  | 1:116:A:GLN:HG3  | 1:116:A:GLN:HE21 | 9        | 0.28          |
| (1,532)  | 1:116:A:GLN:HG3  | 1:116:A:GLN:HE21 | 10       | 0.28          |
| (1,532)  | 1:116:A:GLN:HG3  | 1:116:A:GLN:HE21 | 16       | 0.28          |
| (1,300)  | 1:100:A:ASN:HB3  | 1:100:A:ASN:HD21 | 6        | 0.28          |
| (1,154)  | 1:130:A:GLU:H    | 1:129:A:ALA:HB3  | 12       | 0.28          |
| (1,117)  | 1:27:A:VAL:HG11  | 1:26:A:GLU:H     | 11       | 0.28          |
| (1,117)  | 1:27:A:VAL:HG11  | 1:26:A:GLU:H     | 13       | 0.28          |
| (1,117)  | 1:27:A:VAL:HG12  | 1:26:A:GLU:H     | 15       | 0.28          |
| (1,12)   | 1:100:A:ASN:H    | 1:100:A:ASN:HD21 | 15       | 0.28          |
| (3,148)  | 1:22:A:ASN:H     | 1:22:A:ASN:HB2   | 3        | 0.27          |
| (3,148)  | 1:22:A:ASN:H     | 1:65:A:ASN:HB3   | 5        | 0.27          |
| (3,135)  | 1:123:A:ARG:HB3  | 1:120:A:ALA:HA   | 5        | 0.27          |
| (3,130)  | 1:52:A:ILE:HG22  | 1:50:A:ILE:HA    | 14       | 0.27          |
| (3,129)  | 1:71:A:LEU:HD13  | 1:60:A:VAL:HB    | 16       | 0.27          |
| (3,123)  | 1:50:A:ILE:HD13  | 1:79:A:THR:HA    | 4        | 0.27          |
| (3,109)  | 1:92:A:ALA:H     | 1:110:A:VAL:HB   | 6        | 0.27          |
| (3,109)  | 1:92:A:ALA:H     | 1:110:A:VAL:HB   | 12       | 0.27          |
| (3,109)  | 1:92:A:ALA:H     | 1:110:A:VAL:HB   | 16       | 0.27          |
| (3,92)   | 1:88:A:VAL:HG22  | 1:87:A:GLY:HA2   | 16       | 0.27          |
| (3,86)   | 1:84:A:TYR:HE2   | 1:47:A:PRO:HB3   | 4        | 0.27          |
| (3,64)   | 1:102:A:CYS:HB2  | 1:52:A:ILE:HG22  | 6        | 0.27          |
| (3,41)   | 1:52:A:ILE:HD11  | 1:56:A:LEU:HA    | 5        | 0.27          |
| (3,34)   | 1:97:A:LEU:HD23  | 1:31:A:LEU:HD12  | 14       | 0.27          |
| (3,22)   | 1:48:A:LEU:HD11  | 1:97:A:LEU:H     | 13       | 0.27          |
| (3,15)   | 1:85:A:LEU:HB3   | 1:82:A:TRP:HA    | 7        | 0.27          |
| (3,15)   | 1:85:A:LEU:HB3   | 1:82:A:TRP:HA    | 8        | 0.27          |
| (1,4342) | 1:38:A:CYS:H     | 1:95:A:VAL:HG12  | 16       | 0.27          |
| (1,4310) | 1:64:A:MET:HA    | 1:65:A:ASN:H     | 8        | 0.27          |
| (1,4280) | 1:112:A:HIS:HA   | 1:116:A:GLN:H    | 6        | 0.27          |
| (1,4280) | 1:112:A:HIS:HA   | 1:116:A:GLN:H    | 11       | 0.27          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,4230) | 1:128:A:ARG:HA  | 1:128:A:ARG:H    | 5        | 0.27          |
| (1,4230) | 1:128:A:ARG:HA  | 1:128:A:ARG:H    | 15       | 0.27          |
| (1,4195) | 1:61:A:ALA:HB1  | 1:67:A:SER:H     | 3        | 0.27          |
| (1,4195) | 1:61:A:ALA:HB2  | 1:67:A:SER:H     | 12       | 0.27          |
| (1,4180) | 1:95:A:VAL:H    | 1:48:A:LEU:HD12  | 5        | 0.27          |
| (1,4172) | 1:105:A:LEU:H   | 1:92:A:ALA:H     | 1        | 0.27          |
| (1,4150) | 1:17:A:ASN:HB3  | 1:18:A:GLN:H     | 4        | 0.27          |
| (1,4150) | 1:17:A:ASN:HB3  | 1:18:A:GLN:H     | 7        | 0.27          |
| (1,4141) | 1:98:A:ASP:HB2  | 1:100:A:ASN:HD21 | 17       | 0.27          |
| (1,4140) | 1:118:A:GLU:HA  | 1:118:A:GLU:H    | 5        | 0.27          |
| (1,4140) | 1:118:A:GLU:HA  | 1:118:A:GLU:H    | 9        | 0.27          |
| (1,4140) | 1:118:A:GLU:HA  | 1:118:A:GLU:H    | 10       | 0.27          |
| (1,4140) | 1:118:A:GLU:HA  | 1:118:A:GLU:H    | 11       | 0.27          |
| (1,4140) | 1:118:A:GLU:HA  | 1:118:A:GLU:H    | 16       | 0.27          |
| (1,4114) | 1:65:A:ASN:H    | 1:65:A:ASN:HD21  | 11       | 0.27          |
| (1,4114) | 1:65:A:ASN:H    | 1:65:A:ASN:HD21  | 15       | 0.27          |
| (1,4113) | 1:22:A:ASN:H    | 1:22:A:ASN:HD22  | 6        | 0.27          |
| (1,4037) | 1:27:A:VAL:HG23 | 1:29:A:ALA:H     | 8        | 0.27          |
| (1,4019) | 1:33:A:GLU:HB3  | 1:34:A:ARG:H     | 10       | 0.27          |
| (1,4017) | 1:32:A:ALA:HB2  | 1:35:A:PHE:H     | 4        | 0.27          |
| (1,4017) | 1:32:A:ALA:HB3  | 1:35:A:PHE:H     | 12       | 0.27          |
| (1,4017) | 1:32:A:ALA:HB2  | 1:35:A:PHE:H     | 17       | 0.27          |
| (1,4006) | 1:42:A:GLU:HB3  | 1:41:A:ALA:H     | 3        | 0.27          |
| (1,4006) | 1:42:A:GLU:HB3  | 1:41:A:ALA:H     | 5        | 0.27          |
| (1,4006) | 1:42:A:GLU:HB3  | 1:41:A:ALA:H     | 14       | 0.27          |
| (1,3845) | 1:95:A:VAL:HG13 | 1:96:A:ASP:H     | 2        | 0.27          |
| (1,3816) | 1:105:A:LEU:H   | 1:105:A:LEU:HD23 | 8        | 0.27          |
| (1,3816) | 1:105:A:LEU:H   | 1:105:A:LEU:HD23 | 11       | 0.27          |
| (1,3816) | 1:105:A:LEU:H   | 1:105:A:LEU:HD23 | 17       | 0.27          |
| (1,3786) | 1:27:A:VAL:HG12 | 1:21:A:LEU:H     | 2        | 0.27          |
| (1,3783) | 1:117:A:LEU:HB3 | 1:117:A:LEU:H    | 17       | 0.27          |
| (1,3776) | 1:121:A:LYS:HA  | 1:122:A:ALA:H    | 1        | 0.27          |
| (1,3775) | 1:124:A:VAL:HA  | 1:125:A:GLN:H    | 2        | 0.27          |
| (1,3775) | 1:124:A:VAL:HA  | 1:125:A:GLN:H    | 13       | 0.27          |
| (1,3773) | 1:123:A:ARG:HA  | 1:124:A:VAL:H    | 2        | 0.27          |
| (1,3773) | 1:123:A:ARG:HA  | 1:124:A:VAL:H    | 13       | 0.27          |
| (1,3771) | 1:126:A:ALA:HB3 | 1:126:A:ALA:H    | 13       | 0.27          |
| (1,3769) | 1:130:A:GLU:H   | 1:129:A:ALA:HB1  | 16       | 0.27          |
| (1,3733) | 1:27:A:VAL:HG13 | 1:26:A:GLU:H     | 16       | 0.27          |
| (1,3732) | 1:21:A:LEU:HD13 | 1:30:A:PHE:H     | 12       | 0.27          |
| (1,3728) | 1:29:A:ALA:HA   | 1:30:A:PHE:H     | 4        | 0.27          |
| (1,3716) | 1:35:A:PHE:HE2  | 1:35:A:PHE:H     | 7        | 0.27          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3716) | 1:35:A:PHE:HE2   | 1:35:A:PHE:H     | 10       | 0.27          |
| (1,3678) | 1:95:A:VAL:H     | 1:96:A:ASP:H     | 9        | 0.27          |
| (1,3668) | 1:84:A:TYR:H     | 1:84:A:TYR:HD1   | 1        | 0.27          |
| (1,3668) | 1:84:A:TYR:H     | 1:84:A:TYR:HD1   | 3        | 0.27          |
| (1,3668) | 1:84:A:TYR:H     | 1:84:A:TYR:HD2   | 12       | 0.27          |
| (1,3627) | 1:100:A:ASN:H    | 1:100:A:ASN:HD21 | 5        | 0.27          |
| (1,3610) | 1:121:A:LYS:HG3  | 1:117:A:LEU:HD13 | 13       | 0.27          |
| (1,3606) | 1:117:A:LEU:HA   | 1:82:A:TRP:HZ2   | 8        | 0.27          |
| (1,3606) | 1:117:A:LEU:HA   | 1:82:A:TRP:HZ2   | 14       | 0.27          |
| (1,3604) | 1:97:A:LEU:HB2   | 1:97:A:LEU:HA    | 3        | 0.27          |
| (1,3604) | 1:97:A:LEU:HB2   | 1:97:A:LEU:HA    | 6        | 0.27          |
| (1,3604) | 1:97:A:LEU:HB2   | 1:97:A:LEU:HA    | 7        | 0.27          |
| (1,3604) | 1:97:A:LEU:HB2   | 1:97:A:LEU:HA    | 10       | 0.27          |
| (1,3604) | 1:97:A:LEU:HB2   | 1:97:A:LEU:HA    | 11       | 0.27          |
| (1,3604) | 1:97:A:LEU:HB2   | 1:97:A:LEU:HA    | 12       | 0.27          |
| (1,3604) | 1:97:A:LEU:HB2   | 1:97:A:LEU:HA    | 13       | 0.27          |
| (1,3604) | 1:97:A:LEU:HB2   | 1:97:A:LEU:HA    | 15       | 0.27          |
| (1,3604) | 1:97:A:LEU:HB2   | 1:97:A:LEU:HA    | 16       | 0.27          |
| (1,3599) | 1:92:A:ALA:HB1   | 1:113:A:ALA:HB3  | 16       | 0.27          |
| (1,3588) | 1:105:A:LEU:HB3  | 1:110:A:VAL:HG21 | 1        | 0.27          |
| (1,3588) | 1:105:A:LEU:HB3  | 1:110:A:VAL:HG22 | 10       | 0.27          |
| (1,3588) | 1:105:A:LEU:HB3  | 1:110:A:VAL:HG22 | 11       | 0.27          |
| (1,3565) | 1:105:A:LEU:HB3  | 1:105:A:LEU:HA   | 1        | 0.27          |
| (1,3565) | 1:105:A:LEU:HB3  | 1:105:A:LEU:HA   | 2        | 0.27          |
| (1,3565) | 1:105:A:LEU:HB3  | 1:105:A:LEU:HA   | 6        | 0.27          |
| (1,3565) | 1:105:A:LEU:HB3  | 1:105:A:LEU:HA   | 9        | 0.27          |
| (1,3565) | 1:105:A:LEU:HB3  | 1:105:A:LEU:HA   | 12       | 0.27          |
| (1,3565) | 1:105:A:LEU:HB3  | 1:105:A:LEU:HA   | 14       | 0.27          |
| (1,3565) | 1:105:A:LEU:HB3  | 1:105:A:LEU:HA   | 15       | 0.27          |
| (1,3548) | 1:64:A:MET:HE1   | 1:65:A:ASN:HB2   | 3        | 0.27          |
| (1,3536) | 1:66:A:LEU:HB3   | 1:62:A:GLY:HA3   | 17       | 0.27          |
| (1,3531) | 1:65:A:ASN:H     | 1:65:A:ASN:HA    | 1        | 0.27          |
| (1,3516) | 1:21:A:LEU:HG    | 1:65:A:ASN:HB3   | 12       | 0.27          |
| (1,3505) | 1:124:A:VAL:HG12 | 1:124:A:VAL:HG22 | 14       | 0.27          |
| (1,3503) | 1:27:A:VAL:HG21  | 1:31:A:LEU:H     | 12       | 0.27          |
| (1,3503) | 1:27:A:VAL:HG22  | 1:31:A:LEU:H     | 14       | 0.27          |
| (1,3503) | 1:27:A:VAL:HG23  | 1:31:A:LEU:H     | 15       | 0.27          |
| (1,3501) | 1:27:A:VAL:HG22  | 1:28:A:ILE:HA    | 1        | 0.27          |
| (1,3501) | 1:27:A:VAL:HG23  | 1:28:A:ILE:HA    | 3        | 0.27          |
| (1,3498) | 1:70:A:GLN:HE21  | 1:27:A:VAL:HG13  | 7        | 0.27          |
| (1,3495) | 1:54:A:GLN:H     | 1:75:A:LEU:HD13  | 3        | 0.27          |
| (1,3495) | 1:54:A:GLN:H     | 1:75:A:LEU:HD11  | 8        | 0.27          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3491) | 1:86:A:TYR:HE2   | 1:85:A:LEU:HD22  | 3        | 0.27          |
| (1,3491) | 1:86:A:TYR:HE1   | 1:85:A:LEU:HD23  | 4        | 0.27          |
| (1,3491) | 1:86:A:TYR:HE2   | 1:85:A:LEU:HD21  | 5        | 0.27          |
| (1,3491) | 1:86:A:TYR:HE1   | 1:85:A:LEU:HD21  | 6        | 0.27          |
| (1,3491) | 1:86:A:TYR:HE1   | 1:85:A:LEU:HD22  | 7        | 0.27          |
| (1,3491) | 1:86:A:TYR:HE1   | 1:85:A:LEU:HD22  | 15       | 0.27          |
| (1,3430) | 1:45:A:ALA:HB1   | 1:84:A:TYR:HA    | 14       | 0.27          |
| (1,3421) | 1:53:A:PHE:HA    | 1:75:A:LEU:HD23  | 3        | 0.27          |
| (1,3421) | 1:53:A:PHE:HA    | 1:75:A:LEU:HD21  | 15       | 0.27          |
| (1,3421) | 1:53:A:PHE:HA    | 1:75:A:LEU:HD22  | 17       | 0.27          |
| (1,3417) | 1:117:A:LEU:HG   | 1:117:A:LEU:HD13 | 3        | 0.27          |
| (1,3345) | 1:29:A:ALA:HA    | 1:29:A:ALA:HB3   | 2        | 0.27          |
| (1,3345) | 1:29:A:ALA:HA    | 1:29:A:ALA:HB1   | 3        | 0.27          |
| (1,3345) | 1:29:A:ALA:HA    | 1:29:A:ALA:HB3   | 10       | 0.27          |
| (1,3345) | 1:29:A:ALA:HA    | 1:29:A:ALA:HB3   | 16       | 0.27          |
| (1,3345) | 1:29:A:ALA:HA    | 1:29:A:ALA:HB1   | 17       | 0.27          |
| (1,3326) | 1:77:A:LEU:HG    | 1:77:A:LEU:HD12  | 1        | 0.27          |
| (1,3326) | 1:77:A:LEU:HG    | 1:77:A:LEU:HD12  | 2        | 0.27          |
| (1,3326) | 1:77:A:LEU:HG    | 1:77:A:LEU:HD12  | 5        | 0.27          |
| (1,3311) | 1:68:A:LYS:HD3   | 1:57:A:VAL:HG13  | 3        | 0.27          |
| (1,3311) | 1:68:A:LYS:HD3   | 1:57:A:VAL:HG11  | 5        | 0.27          |
| (1,3266) | 1:85:A:LEU:HD13  | 1:85:A:LEU:HD22  | 2        | 0.27          |
| (1,3266) | 1:85:A:LEU:HD13  | 1:85:A:LEU:HD21  | 12       | 0.27          |
| (1,3258) | 1:48:A:LEU:HD13  | 1:50:A:ILE:HA    | 5        | 0.27          |
| (1,3230) | 1:68:A:LYS:HB2   | 1:68:A:LYS:HA    | 17       | 0.27          |
| (1,3223) | 1:84:A:TYR:HE2   | 1:79:A:THR:HA    | 16       | 0.27          |
| (1,3221) | 1:37:A:HIS:HB2   | 1:99:A:GLY:HA2   | 6        | 0.27          |
| (1,3189) | 1:110:A:VAL:HA   | 1:105:A:LEU:HD11 | 11       | 0.27          |
| (1,3183) | 1:124:A:VAL:HG23 | 1:121:A:LYS:HA   | 3        | 0.27          |
| (1,3183) | 1:124:A:VAL:HG21 | 1:121:A:LYS:HA   | 9        | 0.27          |
| (1,3180) | 1:111:A:GLU:HG2  | 1:111:A:GLU:HA   | 10       | 0.27          |
| (1,3180) | 1:111:A:GLU:HG2  | 1:111:A:GLU:HA   | 14       | 0.27          |
| (1,3180) | 1:111:A:GLU:HG2  | 1:111:A:GLU:HA   | 16       | 0.27          |
| (1,3178) | 1:116:A:GLN:HA   | 1:116:A:GLN:H    | 9        | 0.27          |
| (1,3135) | 1:68:A:LYS:HD3   | 1:68:A:LYS:HB2   | 3        | 0.27          |
| (1,3123) | 1:59:A:ARG:HB2   | 1:59:A:ARG:HA    | 1        | 0.27          |
| (1,3123) | 1:59:A:ARG:HB2   | 1:59:A:ARG:HA    | 4        | 0.27          |
| (1,3123) | 1:59:A:ARG:HB2   | 1:59:A:ARG:HA    | 9        | 0.27          |
| (1,3123) | 1:59:A:ARG:HB2   | 1:59:A:ARG:HA    | 15       | 0.27          |
| (1,3115) | 1:58:A:ASP:HA    | 1:57:A:VAL:HG23  | 6        | 0.27          |
| (1,3103) | 1:56:A:LEU:HD13  | 1:60:A:VAL:HB    | 12       | 0.27          |
| (1,3081) | 1:97:A:LEU:HD11  | 1:55:A:ASP:HA    | 5        | 0.27          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3066) | 1:30:A:PHE:HB3   | 1:29:A:ALA:HB3   | 15       | 0.27          |
| (1,3061) | 1:31:A:LEU:HD11  | 1:28:A:ILE:HG22  | 15       | 0.27          |
| (1,3036) | 1:78:A:TYR:HH    | 1:45:A:ALA:HB1   | 8        | 0.27          |
| (1,3028) | 1:71:A:LEU:HD12  | 1:72:A:ARG:HA    | 8        | 0.27          |
| (1,3028) | 1:71:A:LEU:HD12  | 1:72:A:ARG:HA    | 17       | 0.27          |
| (1,3023) | 1:64:A:MET:HE1   | 1:27:A:VAL:HA    | 4        | 0.27          |
| (1,3021) | 1:64:A:MET:HE3   | 1:63:A:GLU:H     | 8        | 0.27          |
| (1,2989) | 1:42:A:GLU:HA    | 1:42:A:GLU:HB2   | 14       | 0.27          |
| (1,2989) | 1:42:A:GLU:HA    | 1:42:A:GLU:HB2   | 15       | 0.27          |
| (1,2945) | 1:110:A:VAL:HB   | 1:110:A:VAL:HG11 | 3        | 0.27          |
| (1,2945) | 1:110:A:VAL:HB   | 1:110:A:VAL:HG11 | 13       | 0.27          |
| (1,2945) | 1:110:A:VAL:HB   | 1:110:A:VAL:HG12 | 14       | 0.27          |
| (1,2942) | 1:57:A:VAL:HG23  | 1:57:A:VAL:HB    | 14       | 0.27          |
| (1,2933) | 1:95:A:VAL:HG22  | 1:99:A:GLY:H     | 2        | 0.27          |
| (1,2933) | 1:95:A:VAL:HG22  | 1:99:A:GLY:H     | 10       | 0.27          |
| (1,2933) | 1:95:A:VAL:HG23  | 1:99:A:GLY:H     | 12       | 0.27          |
| (1,2933) | 1:95:A:VAL:HG21  | 1:99:A:GLY:H     | 14       | 0.27          |
| (1,2931) | 1:88:A:VAL:HG22  | 1:85:A:LEU:H     | 11       | 0.27          |
| (1,2909) | 1:110:A:VAL:HG13 | 1:91:A:GLY:HA2   | 1        | 0.27          |
| (1,2909) | 1:110:A:VAL:HG12 | 1:91:A:GLY:HA2   | 3        | 0.27          |
| (1,2909) | 1:110:A:VAL:HG13 | 1:91:A:GLY:HA2   | 7        | 0.27          |
| (1,2891) | 1:32:A:ALA:HB2   | 1:28:A:ILE:HG22  | 9        | 0.27          |
| (1,2888) | 1:29:A:ALA:HA    | 1:32:A:ALA:HB1   | 9        | 0.27          |
| (1,2881) | 1:74:A:ALA:HB2   | 1:31:A:LEU:HD12  | 15       | 0.27          |
| (1,2832) | 1:97:A:LEU:HD21  | 1:97:A:LEU:H     | 3        | 0.27          |
| (1,2832) | 1:97:A:LEU:HD22  | 1:97:A:LEU:H     | 4        | 0.27          |
| (1,2831) | 1:97:A:LEU:HD22  | 1:35:A:PHE:HD1   | 2        | 0.27          |
| (1,2824) | 1:97:A:LEU:HD23  | 1:56:A:LEU:HA    | 9        | 0.27          |
| (1,2824) | 1:97:A:LEU:HD23  | 1:56:A:LEU:HA    | 13       | 0.27          |
| (1,2824) | 1:97:A:LEU:HD22  | 1:56:A:LEU:HA    | 17       | 0.27          |
| (1,2769) | 1:43:A:GLY:HA2   | 1:42:A:GLU:HB2   | 5        | 0.27          |
| (1,2679) | 1:53:A:PHE:HA    | 1:53:A:PHE:HE2   | 6        | 0.27          |
| (1,2679) | 1:53:A:PHE:HA    | 1:53:A:PHE:HE2   | 7        | 0.27          |
| (1,2679) | 1:53:A:PHE:HA    | 1:53:A:PHE:HE2   | 10       | 0.27          |
| (1,2679) | 1:53:A:PHE:HA    | 1:53:A:PHE:HE1   | 16       | 0.27          |
| (1,2675) | 1:85:A:LEU:HB2   | 1:86:A:TYR:HD1   | 14       | 0.27          |
| (1,2662) | 1:97:A:LEU:HD12  | 1:57:A:VAL:H     | 15       | 0.27          |
| (1,2622) | 1:71:A:LEU:HD11  | 1:57:A:VAL:H     | 2        | 0.27          |
| (1,2622) | 1:71:A:LEU:HD13  | 1:57:A:VAL:H     | 9        | 0.27          |
| (1,2622) | 1:71:A:LEU:HD11  | 1:57:A:VAL:H     | 17       | 0.27          |
| (1,2618) | 1:34:A:ARG:HG3   | 1:34:A:ARG:H     | 3        | 0.27          |
| (1,2605) | 1:31:A:LEU:HD23  | 1:30:A:PHE:HD1   | 1        | 0.27          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2605) | 1:31:A:LEU:HD22  | 1:30:A:PHE:HD2   | 11       | 0.27          |
| (1,2605) | 1:31:A:LEU:HD23  | 1:30:A:PHE:HD1   | 12       | 0.27          |
| (1,2598) | 1:27:A:VAL:HG21  | 1:27:A:VAL:HG11  | 3        | 0.27          |
| (1,2598) | 1:27:A:VAL:HG23  | 1:27:A:VAL:HG11  | 4        | 0.27          |
| (1,2596) | 1:74:A:ALA:HB3   | 1:27:A:VAL:HG13  | 6        | 0.27          |
| (1,2583) | 1:60:A:VAL:HG12  | 1:34:A:ARG:HG2   | 4        | 0.27          |
| (1,2583) | 1:60:A:VAL:HG11  | 1:34:A:ARG:HG2   | 5        | 0.27          |
| (1,2583) | 1:60:A:VAL:HG12  | 1:34:A:ARG:HG2   | 9        | 0.27          |
| (1,2583) | 1:60:A:VAL:HG12  | 1:34:A:ARG:HG2   | 13       | 0.27          |
| (1,2576) | 1:124:A:VAL:HG23 | 1:120:A:ALA:HA   | 5        | 0.27          |
| (1,2576) | 1:124:A:VAL:HG22 | 1:120:A:ALA:HA   | 12       | 0.27          |
| (1,2560) | 1:86:A:TYR:HE1   | 1:86:A:TYR:HD1   | 14       | 0.27          |
| (1,2547) | 1:11:A:SER:HA    | 1:12:A:GLN:HG3   | 1        | 0.27          |
| (1,2547) | 1:11:A:SER:HA    | 1:12:A:GLN:HG3   | 6        | 0.27          |
| (1,2546) | 1:73:A:SER:HA    | 1:73:A:SER:HB3   | 10       | 0.27          |
| (1,2546) | 1:73:A:SER:HA    | 1:73:A:SER:HB3   | 12       | 0.27          |
| (1,2546) | 1:73:A:SER:HA    | 1:73:A:SER:HB3   | 16       | 0.27          |
| (1,2546) | 1:73:A:SER:HA    | 1:73:A:SER:HB3   | 17       | 0.27          |
| (1,2502) | 1:42:A:GLU:HA    | 1:43:A:GLY:H     | 11       | 0.27          |
| (1,2480) | 1:71:A:LEU:HB2   | 1:27:A:VAL:HG12  | 6        | 0.27          |
| (1,2480) | 1:71:A:LEU:HB2   | 1:27:A:VAL:HG13  | 14       | 0.27          |
| (1,2468) | 1:53:A:PHE:HE2   | 1:72:A:ARG:HG3   | 3        | 0.27          |
| (1,2468) | 1:53:A:PHE:HE2   | 1:72:A:ARG:HG3   | 7        | 0.27          |
| (1,2468) | 1:53:A:PHE:HE2   | 1:72:A:ARG:HG3   | 13       | 0.27          |
| (1,2415) | 1:45:A:ALA:HB3   | 1:84:A:TYR:HD2   | 16       | 0.27          |
| (1,2369) | 1:52:A:ILE:HD12  | 1:56:A:LEU:H     | 9        | 0.27          |
| (1,2369) | 1:52:A:ILE:HD13  | 1:56:A:LEU:H     | 16       | 0.27          |
| (1,2363) | 1:48:A:LEU:HD11  | 1:84:A:TYR:HE1   | 4        | 0.27          |
| (1,2346) | 1:105:A:LEU:HD13 | 1:107:A:GLU:HA   | 5        | 0.27          |
| (1,2346) | 1:105:A:LEU:HD12 | 1:107:A:GLU:HA   | 9        | 0.27          |
| (1,2346) | 1:105:A:LEU:HD13 | 1:107:A:GLU:HA   | 10       | 0.27          |
| (1,2344) | 1:104:A:GLU:HG2  | 1:105:A:LEU:HD23 | 10       | 0.27          |
| (1,2344) | 1:104:A:GLU:HG2  | 1:105:A:LEU:HD22 | 13       | 0.27          |
| (1,2341) | 1:66:A:LEU:HD22  | 1:70:A:GLN:H     | 5        | 0.27          |
| (1,2331) | 1:54:A:GLN:HG2   | 1:55:A:ASP:HA    | 14       | 0.27          |
| (1,2331) | 1:54:A:GLN:HG2   | 1:55:A:ASP:HA    | 16       | 0.27          |
| (1,2190) | 1:61:A:ALA:HB2   | 1:62:A:GLY:HA2   | 6        | 0.27          |
| (1,2116) | 1:45:A:ALA:HB3   | 1:84:A:TYR:HA    | 12       | 0.27          |
| (1,2116) | 1:45:A:ALA:HB2   | 1:84:A:TYR:HA    | 17       | 0.27          |
| (1,2108) | 1:40:A:SER:H     | 1:41:A:ALA:H     | 2        | 0.27          |
| (1,2036) | 1:97:A:LEU:HD22  | 1:97:A:LEU:HB2   | 2        | 0.27          |
| (1,2036) | 1:97:A:LEU:HD22  | 1:97:A:LEU:HB2   | 14       | 0.27          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1994) | 1:91:A:GLY:HA2   | 1:91:A:GLY:H     | 1        | 0.27          |
| (1,1994) | 1:91:A:GLY:HA2   | 1:91:A:GLY:H     | 3        | 0.27          |
| (1,1994) | 1:91:A:GLY:HA2   | 1:91:A:GLY:H     | 10       | 0.27          |
| (1,1994) | 1:91:A:GLY:HA2   | 1:91:A:GLY:H     | 15       | 0.27          |
| (1,1994) | 1:91:A:GLY:HA2   | 1:91:A:GLY:H     | 17       | 0.27          |
| (1,1955) | 1:92:A:ALA:HB1   | 1:113:A:ALA:HB1  | 9        | 0.27          |
| (1,1947) | 1:93:A:THR:HB    | 1:88:A:VAL:HG12  | 6        | 0.27          |
| (1,1940) | 1:111:A:GLU:HB2  | 1:109:A:HIS:HA   | 3        | 0.27          |
| (1,1940) | 1:111:A:GLU:HB2  | 1:109:A:HIS:HA   | 4        | 0.27          |
| (1,1940) | 1:111:A:GLU:HB2  | 1:109:A:HIS:HA   | 6        | 0.27          |
| (1,1940) | 1:111:A:GLU:HB2  | 1:109:A:HIS:HA   | 8        | 0.27          |
| (1,1940) | 1:111:A:GLU:HB2  | 1:109:A:HIS:HA   | 9        | 0.27          |
| (1,1940) | 1:111:A:GLU:HB2  | 1:109:A:HIS:HA   | 10       | 0.27          |
| (1,1940) | 1:111:A:GLU:HB2  | 1:109:A:HIS:HA   | 13       | 0.27          |
| (1,1940) | 1:111:A:GLU:HB2  | 1:109:A:HIS:HA   | 16       | 0.27          |
| (1,1940) | 1:111:A:GLU:HB2  | 1:109:A:HIS:HA   | 17       | 0.27          |
| (1,1904) | 1:74:A:ALA:HB1   | 1:28:A:ILE:HA    | 4        | 0.27          |
| (1,1904) | 1:74:A:ALA:HB2   | 1:28:A:ILE:HA    | 5        | 0.27          |
| (1,1904) | 1:74:A:ALA:HB3   | 1:28:A:ILE:HA    | 10       | 0.27          |
| (1,1904) | 1:74:A:ALA:HB1   | 1:28:A:ILE:HA    | 15       | 0.27          |
| (1,1904) | 1:74:A:ALA:HB1   | 1:28:A:ILE:HA    | 16       | 0.27          |
| (1,1889) | 1:65:A:ASN:H     | 1:65:A:ASN:HB3   | 1        | 0.27          |
| (1,1889) | 1:65:A:ASN:H     | 1:65:A:ASN:HB3   | 6        | 0.27          |
| (1,1886) | 1:102:A:CYS:HB3  | 1:49:A:LYS:HA    | 5        | 0.27          |
| (1,1886) | 1:102:A:CYS:HB3  | 1:49:A:LYS:HA    | 9        | 0.27          |
| (1,1886) | 1:102:A:CYS:HB3  | 1:49:A:LYS:HA    | 14       | 0.27          |
| (1,1879) | 1:124:A:VAL:HG12 | 1:124:A:VAL:HG21 | 2        | 0.27          |
| (1,1874) | 1:70:A:GLN:HE21  | 1:27:A:VAL:HG13  | 3        | 0.27          |
| (1,1865) | 1:45:A:ALA:HB1   | 1:44:A:GLU:HB3   | 3        | 0.27          |
| (1,1799) | 1:71:A:LEU:HA    | 1:74:A:ALA:HB2   | 4        | 0.27          |
| (1,1752) | 1:41:A:ALA:HB3   | 1:28:A:ILE:HG23  | 3        | 0.27          |
| (1,1752) | 1:41:A:ALA:HB3   | 1:28:A:ILE:HG23  | 5        | 0.27          |
| (1,1752) | 1:41:A:ALA:HB2   | 1:28:A:ILE:HG22  | 9        | 0.27          |
| (1,1752) | 1:41:A:ALA:HB2   | 1:28:A:ILE:HG23  | 15       | 0.27          |
| (1,1737) | 1:77:A:LEU:HG    | 1:77:A:LEU:HD12  | 11       | 0.27          |
| (1,1737) | 1:77:A:LEU:HG    | 1:77:A:LEU:HD11  | 14       | 0.27          |
| (1,1737) | 1:77:A:LEU:HG    | 1:77:A:LEU:HD11  | 17       | 0.27          |
| (1,1723) | 1:68:A:LYS:HD3   | 1:57:A:VAL:HG13  | 2        | 0.27          |
| (1,1723) | 1:68:A:LYS:HD3   | 1:57:A:VAL:HG13  | 4        | 0.27          |
| (1,1723) | 1:68:A:LYS:HD3   | 1:57:A:VAL:HG13  | 6        | 0.27          |
| (1,1723) | 1:68:A:LYS:HD3   | 1:57:A:VAL:HG13  | 13       | 0.27          |
| (1,1723) | 1:68:A:LYS:HD3   | 1:57:A:VAL:HG12  | 17       | 0.27          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1684) | 1:48:A:LEU:HD12  | 1:50:A:ILE:HA    | 7        | 0.27          |
| (1,1656) | 1:31:A:LEU:HB2   | 1:39:A:PHE:HE2   | 9        | 0.27          |
| (1,1629) | 1:116:A:GLN:HG3  | 1:113:A:ALA:HB3  | 6        | 0.27          |
| (1,1618) | 1:109:A:HIS:HB2  | 1:110:A:VAL:HG11 | 1        | 0.27          |
| (1,1613) | 1:124:A:VAL:HG22 | 1:121:A:LYS:HA   | 4        | 0.27          |
| (1,1613) | 1:124:A:VAL:HG23 | 1:121:A:LYS:HA   | 5        | 0.27          |
| (1,1613) | 1:124:A:VAL:HG22 | 1:121:A:LYS:HA   | 11       | 0.27          |
| (1,1553) | 1:57:A:VAL:HG11  | 1:61:A:ALA:H     | 17       | 0.27          |
| (1,1521) | 1:30:A:PHE:HB3   | 1:29:A:ALA:HB1   | 14       | 0.27          |
| (1,1521) | 1:30:A:PHE:HB3   | 1:29:A:ALA:HB1   | 16       | 0.27          |
| (1,1510) | 1:52:A:ILE:HG23  | 1:50:A:ILE:H     | 10       | 0.27          |
| (1,1490) | 1:78:A:TYR:HH    | 1:45:A:ALA:HB2   | 12       | 0.27          |
| (1,1485) | 1:71:A:LEU:HD12  | 1:72:A:ARG:HA    | 3        | 0.27          |
| (1,1485) | 1:71:A:LEU:HD12  | 1:72:A:ARG:HA    | 5        | 0.27          |
| (1,1450) | 1:54:A:GLN:HE22  | 1:54:A:GLN:HG2   | 16       | 0.27          |
| (1,1399) | 1:95:A:VAL:HG23  | 1:95:A:VAL:H     | 3        | 0.27          |
| (1,1398) | 1:88:A:VAL:HG23  | 1:85:A:LEU:H     | 1        | 0.27          |
| (1,1363) | 1:29:A:ALA:HA    | 1:32:A:ALA:HB2   | 1        | 0.27          |
| (1,1363) | 1:29:A:ALA:HA    | 1:32:A:ALA:HB1   | 4        | 0.27          |
| (1,1363) | 1:29:A:ALA:HA    | 1:32:A:ALA:HB2   | 15       | 0.27          |
| (1,1331) | 1:78:A:TYR:HE1   | 1:84:A:TYR:HD2   | 15       | 0.27          |
| (1,1307) | 1:97:A:LEU:HD22  | 1:97:A:LEU:HB2   | 7        | 0.27          |
| (1,1232) | 1:60:A:VAL:HG12  | 1:59:A:ARG:HD3   | 1        | 0.27          |
| (1,1231) | 1:97:A:LEU:HD11  | 1:59:A:ARG:HD3   | 11       | 0.27          |
| (1,1136) | 1:31:A:LEU:HD12  | 1:35:A:PHE:HD2   | 3        | 0.27          |
| (1,1124) | 1:97:A:LEU:HD11  | 1:57:A:VAL:H     | 7        | 0.27          |
| (1,1124) | 1:97:A:LEU:HD11  | 1:57:A:VAL:H     | 9        | 0.27          |
| (1,1082) | 1:71:A:LEU:HD13  | 1:72:A:ARG:H     | 6        | 0.27          |
| (1,1082) | 1:71:A:LEU:HD11  | 1:72:A:ARG:H     | 12       | 0.27          |
| (1,1082) | 1:71:A:LEU:HD12  | 1:72:A:ARG:H     | 17       | 0.27          |
| (1,1081) | 1:71:A:LEU:HD11  | 1:57:A:VAL:H     | 5        | 0.27          |
| (1,1081) | 1:71:A:LEU:HD13  | 1:57:A:VAL:H     | 10       | 0.27          |
| (1,1062) | 1:27:A:VAL:HG21  | 1:27:A:VAL:HG13  | 6        | 0.27          |
| (1,1062) | 1:27:A:VAL:HG23  | 1:27:A:VAL:HG13  | 8        | 0.27          |
| (1,1060) | 1:74:A:ALA:HB3   | 1:27:A:VAL:HG12  | 17       | 0.27          |
| (1,1048) | 1:124:A:VAL:HG21 | 1:120:A:ALA:HA   | 9        | 0.27          |
| (1,1048) | 1:124:A:VAL:HG23 | 1:120:A:ALA:HA   | 14       | 0.27          |
| (1,993)  | 1:79:A:THR:HG23  | 1:75:A:LEU:HA    | 10       | 0.27          |
| (1,895)  | 1:129:A:ALA:HB2  | 1:129:A:ALA:HA   | 1        | 0.27          |
| (1,894)  | 1:133:A:ALA:HA   | 1:133:A:ALA:HB1  | 1        | 0.27          |
| (1,894)  | 1:133:A:ALA:HA   | 1:133:A:ALA:HB1  | 10       | 0.27          |
| (1,852)  | 1:65:A:ASN:HB3   | 1:65:A:ASN:HD21  | 4        | 0.27          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,850) | 1:86:A:TYR:HB2   | 1:117:A:LEU:HB3  | 6        | 0.27          |
| (1,850) | 1:86:A:TYR:HB2   | 1:117:A:LEU:HB3  | 14       | 0.27          |
| (1,850) | 1:86:A:TYR:HB2   | 1:117:A:LEU:HB3  | 15       | 0.27          |
| (1,829) | 1:41:A:ALA:HB1   | 1:41:A:ALA:H     | 9        | 0.27          |
| (1,829) | 1:41:A:ALA:HB2   | 1:41:A:ALA:H     | 10       | 0.27          |
| (1,822) | 1:49:A:LYS:H     | 1:52:A:ILE:HD11  | 3        | 0.27          |
| (1,822) | 1:49:A:LYS:H     | 1:52:A:ILE:HD11  | 7        | 0.27          |
| (1,819) | 1:28:A:ILE:HD11  | 1:74:A:ALA:HA    | 1        | 0.27          |
| (1,819) | 1:28:A:ILE:HD13  | 1:74:A:ALA:HA    | 5        | 0.27          |
| (1,819) | 1:28:A:ILE:HD12  | 1:74:A:ALA:HA    | 6        | 0.27          |
| (1,819) | 1:28:A:ILE:HD13  | 1:74:A:ALA:HA    | 14       | 0.27          |
| (1,691) | 1:75:A:LEU:HD22  | 1:54:A:GLN:H     | 2        | 0.27          |
| (1,643) | 1:110:A:VAL:HG11 | 1:113:A:ALA:H    | 4        | 0.27          |
| (1,643) | 1:110:A:VAL:HG12 | 1:113:A:ALA:H    | 7        | 0.27          |
| (1,643) | 1:110:A:VAL:HG13 | 1:113:A:ALA:H    | 8        | 0.27          |
| (1,643) | 1:110:A:VAL:HG12 | 1:113:A:ALA:H    | 14       | 0.27          |
| (1,635) | 1:127:A:GLN:H    | 1:127:A:GLN:HB3  | 16       | 0.27          |
| (1,532) | 1:116:A:GLN:HG3  | 1:116:A:GLN:HE21 | 6        | 0.27          |
| (1,532) | 1:116:A:GLN:HG3  | 1:116:A:GLN:HE21 | 14       | 0.27          |
| (1,523) | 1:21:A:LEU:HA    | 1:22:A:ASN:HD22  | 15       | 0.27          |
| (1,442) | 1:41:A:ALA:HB1   | 1:41:A:ALA:H     | 17       | 0.27          |
| (1,441) | 1:42:A:GLU:HB3   | 1:41:A:ALA:H     | 9        | 0.27          |
| (1,410) | 1:53:A:PHE:H     | 1:56:A:LEU:HB3   | 17       | 0.27          |
| (1,300) | 1:100:A:ASN:HB3  | 1:100:A:ASN:HD21 | 5        | 0.27          |
| (1,300) | 1:100:A:ASN:HB3  | 1:100:A:ASN:HD21 | 13       | 0.27          |
| (1,300) | 1:100:A:ASN:HB3  | 1:100:A:ASN:HD21 | 17       | 0.27          |
| (1,234) | 1:95:A:VAL:HG23  | 1:99:A:GLY:H     | 1        | 0.27          |
| (1,125) | 1:28:A:ILE:HG13  | 1:28:A:ILE:H     | 4        | 0.27          |
| (1,125) | 1:28:A:ILE:HG13  | 1:28:A:ILE:H     | 6        | 0.27          |
| (1,125) | 1:28:A:ILE:HG13  | 1:28:A:ILE:H     | 7        | 0.27          |
| (1,125) | 1:28:A:ILE:HG13  | 1:28:A:ILE:H     | 11       | 0.27          |
| (1,117) | 1:27:A:VAL:HG11  | 1:26:A:GLU:H     | 7        | 0.27          |
| (3,129) | 1:71:A:LEU:HD11  | 1:60:A:VAL:HB    | 3        | 0.26          |
| (3,123) | 1:50:A:ILE:HD12  | 1:79:A:THR:HA    | 1        | 0.26          |
| (3,109) | 1:92:A:ALA:H     | 1:110:A:VAL:HB   | 9        | 0.26          |
| (3,109) | 1:92:A:ALA:H     | 1:110:A:VAL:HB   | 13       | 0.26          |
| (3,62)  | 1:52:A:ILE:HG22  | 1:56:A:LEU:H     | 12       | 0.26          |
| (3,59)  | 1:117:A:LEU:HA   | 1:85:A:LEU:HD23  | 16       | 0.26          |
| (3,41)  | 1:52:A:ILE:HD11  | 1:56:A:LEU:HA    | 14       | 0.26          |
| (3,34)  | 1:97:A:LEU:HD23  | 1:31:A:LEU:HD13  | 5        | 0.26          |
| (3,34)  | 1:97:A:LEU:HD23  | 1:31:A:LEU:HD12  | 12       | 0.26          |
| (3,29)  | 1:48:A:LEU:HD22  | 1:39:A:PHE:HD2   | 10       | 0.26          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (3,15)   | 1:85:A:LEU:HB3   | 1:82:A:TRP:HA    | 5        | 0.26          |
| (3,15)   | 1:85:A:LEU:HB3   | 1:82:A:TRP:HA    | 6        | 0.26          |
| (3,15)   | 1:85:A:LEU:HB3   | 1:82:A:TRP:HA    | 10       | 0.26          |
| (3,15)   | 1:85:A:LEU:HB3   | 1:82:A:TRP:HA    | 14       | 0.26          |
| (3,15)   | 1:85:A:LEU:HB3   | 1:82:A:TRP:HA    | 16       | 0.26          |
| (3,14)   | 1:82:A:TRP:HA    | 1:85:A:LEU:HB2   | 10       | 0.26          |
| (3,14)   | 1:82:A:TRP:HA    | 1:85:A:LEU:HB2   | 14       | 0.26          |
| (1,4310) | 1:64:A:MET:HA    | 1:65:A:ASN:H     | 2        | 0.26          |
| (1,4300) | 1:92:A:ALA:H     | 1:105:A:LEU:HD22 | 13       | 0.26          |
| (1,4299) | 1:65:A:ASN:HD22  | 1:65:A:ASN:HD21  | 5        | 0.26          |
| (1,4299) | 1:65:A:ASN:HD22  | 1:65:A:ASN:HD21  | 15       | 0.26          |
| (1,4280) | 1:112:A:HIS:HA   | 1:116:A:GLN:H    | 8        | 0.26          |
| (1,4280) | 1:112:A:HIS:HA   | 1:116:A:GLN:H    | 17       | 0.26          |
| (1,4262) | 1:95:A:VAL:HG22  | 1:38:A:CYS:H     | 4        | 0.26          |
| (1,4230) | 1:128:A:ARG:HA   | 1:128:A:ARG:H    | 14       | 0.26          |
| (1,4195) | 1:61:A:ALA:HB1   | 1:67:A:SER:H     | 5        | 0.26          |
| (1,4140) | 1:118:A:GLU:HA   | 1:118:A:GLU:H    | 2        | 0.26          |
| (1,4140) | 1:118:A:GLU:HA   | 1:118:A:GLU:H    | 3        | 0.26          |
| (1,4140) | 1:118:A:GLU:HA   | 1:118:A:GLU:H    | 7        | 0.26          |
| (1,4140) | 1:118:A:GLU:HA   | 1:118:A:GLU:H    | 15       | 0.26          |
| (1,4140) | 1:118:A:GLU:HA   | 1:118:A:GLU:H    | 17       | 0.26          |
| (1,4109) | 1:97:A:LEU:HD11  | 1:98:A:ASP:H     | 3        | 0.26          |
| (1,4017) | 1:32:A:ALA:HB2   | 1:35:A:PHE:H     | 8        | 0.26          |
| (1,4016) | 1:15:A:MET:HA    | 1:15:A:MET:H     | 4        | 0.26          |
| (1,4016) | 1:15:A:MET:HA    | 1:15:A:MET:H     | 14       | 0.26          |
| (1,4016) | 1:15:A:MET:HA    | 1:15:A:MET:H     | 17       | 0.26          |
| (1,4006) | 1:42:A:GLU:HB3   | 1:41:A:ALA:H     | 8        | 0.26          |
| (1,3941) | 1:63:A:GLU:H     | 1:61:A:ALA:HB1   | 2        | 0.26          |
| (1,3861) | 1:110:A:VAL:HG21 | 1:91:A:GLY:H     | 7        | 0.26          |
| (1,3816) | 1:105:A:LEU:H    | 1:105:A:LEU:HD21 | 4        | 0.26          |
| (1,3816) | 1:105:A:LEU:H    | 1:105:A:LEU:HD22 | 5        | 0.26          |
| (1,3816) | 1:105:A:LEU:H    | 1:105:A:LEU:HD22 | 13       | 0.26          |
| (1,3783) | 1:117:A:LEU:HB3  | 1:117:A:LEU:H    | 11       | 0.26          |
| (1,3776) | 1:121:A:LYS:HA   | 1:122:A:ALA:H    | 5        | 0.26          |
| (1,3776) | 1:121:A:LYS:HA   | 1:122:A:ALA:H    | 8        | 0.26          |
| (1,3773) | 1:123:A:ARG:HA   | 1:124:A:VAL:H    | 3        | 0.26          |
| (1,3769) | 1:130:A:GLU:H    | 1:129:A:ALA:HB3  | 4        | 0.26          |
| (1,3733) | 1:27:A:VAL:HG13  | 1:26:A:GLU:H     | 8        | 0.26          |
| (1,3728) | 1:29:A:ALA:HA    | 1:30:A:PHE:H     | 9        | 0.26          |
| (1,3716) | 1:35:A:PHE:HE2   | 1:35:A:PHE:H     | 1        | 0.26          |
| (1,3610) | 1:121:A:LYS:HG3  | 1:117:A:LEU:HD11 | 5        | 0.26          |
| (1,3604) | 1:97:A:LEU:HB2   | 1:97:A:LEU:HA    | 1        | 0.26          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3604) | 1:97:A:LEU:HB2  | 1:97:A:LEU:HA    | 2        | 0.26          |
| (1,3604) | 1:97:A:LEU:HB2  | 1:97:A:LEU:HA    | 4        | 0.26          |
| (1,3604) | 1:97:A:LEU:HB2  | 1:97:A:LEU:HA    | 5        | 0.26          |
| (1,3604) | 1:97:A:LEU:HB2  | 1:97:A:LEU:HA    | 9        | 0.26          |
| (1,3604) | 1:97:A:LEU:HB2  | 1:97:A:LEU:HA    | 14       | 0.26          |
| (1,3604) | 1:97:A:LEU:HB2  | 1:97:A:LEU:HA    | 17       | 0.26          |
| (1,3592) | 1:109:A:HIS:HB2 | 1:110:A:VAL:HG11 | 1        | 0.26          |
| (1,3592) | 1:109:A:HIS:HB2 | 1:110:A:VAL:HG11 | 10       | 0.26          |
| (1,3588) | 1:105:A:LEU:HB3 | 1:110:A:VAL:HG21 | 4        | 0.26          |
| (1,3588) | 1:105:A:LEU:HB3 | 1:110:A:VAL:HG22 | 15       | 0.26          |
| (1,3583) | 1:112:A:HIS:H   | 1:109:A:HIS:HA   | 7        | 0.26          |
| (1,3583) | 1:112:A:HIS:H   | 1:109:A:HIS:HA   | 8        | 0.26          |
| (1,3583) | 1:112:A:HIS:H   | 1:109:A:HIS:HA   | 16       | 0.26          |
| (1,3565) | 1:105:A:LEU:HB3 | 1:105:A:LEU:HA   | 4        | 0.26          |
| (1,3565) | 1:105:A:LEU:HB3 | 1:105:A:LEU:HA   | 5        | 0.26          |
| (1,3565) | 1:105:A:LEU:HB3 | 1:105:A:LEU:HA   | 8        | 0.26          |
| (1,3565) | 1:105:A:LEU:HB3 | 1:105:A:LEU:HA   | 10       | 0.26          |
| (1,3565) | 1:105:A:LEU:HB3 | 1:105:A:LEU:HA   | 13       | 0.26          |
| (1,3565) | 1:105:A:LEU:HB3 | 1:105:A:LEU:HA   | 16       | 0.26          |
| (1,3565) | 1:105:A:LEU:HB3 | 1:105:A:LEU:HA   | 17       | 0.26          |
| (1,3534) | 1:122:A:ALA:HB2 | 1:121:A:LYS:HE3  | 4        | 0.26          |
| (1,3534) | 1:122:A:ALA:HB1 | 1:121:A:LYS:HE3  | 5        | 0.26          |
| (1,3534) | 1:122:A:ALA:HB1 | 1:121:A:LYS:HE3  | 10       | 0.26          |
| (1,3534) | 1:122:A:ALA:HB3 | 1:121:A:LYS:HE3  | 11       | 0.26          |
| (1,3531) | 1:65:A:ASN:H    | 1:65:A:ASN:HA    | 5        | 0.26          |
| (1,3531) | 1:65:A:ASN:H    | 1:65:A:ASN:HA    | 11       | 0.26          |
| (1,3508) | 1:113:A:ALA:HB3 | 1:88:A:VAL:HA    | 4        | 0.26          |
| (1,3508) | 1:113:A:ALA:HB1 | 1:88:A:VAL:HA    | 7        | 0.26          |
| (1,3503) | 1:27:A:VAL:HG23 | 1:31:A:LEU:H     | 5        | 0.26          |
| (1,3503) | 1:27:A:VAL:HG23 | 1:31:A:LEU:H     | 17       | 0.26          |
| (1,3501) | 1:27:A:VAL:HG22 | 1:28:A:ILE:HA    | 16       | 0.26          |
| (1,3498) | 1:70:A:GLN:HE21 | 1:27:A:VAL:HG11  | 15       | 0.26          |
| (1,3492) | 1:105:A:LEU:HB3 | 1:105:A:LEU:HD12 | 17       | 0.26          |
| (1,3491) | 1:86:A:TYR:HE1  | 1:85:A:LEU:HD22  | 2        | 0.26          |
| (1,3491) | 1:86:A:TYR:HE1  | 1:85:A:LEU:HD23  | 9        | 0.26          |
| (1,3491) | 1:86:A:TYR:HE1  | 1:85:A:LEU:HD23  | 11       | 0.26          |
| (1,3491) | 1:86:A:TYR:HE1  | 1:85:A:LEU:HD23  | 13       | 0.26          |
| (1,3481) | 1:83:A:ARG:HD3  | 1:45:A:ALA:HB1   | 9        | 0.26          |
| (1,3479) | 1:45:A:ALA:HB1  | 1:44:A:GLU:HB3   | 10       | 0.26          |
| (1,3479) | 1:45:A:ALA:HB2  | 1:44:A:GLU:HB3   | 15       | 0.26          |
| (1,3479) | 1:45:A:ALA:HB2  | 1:44:A:GLU:HB3   | 17       | 0.26          |
| (1,3476) | 1:107:A:GLU:HG2 | 1:108:A:GLN:H    | 1        | 0.26          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3465) | 1:88:A:VAL:HG22  | 1:85:A:LEU:HB3   | 8        | 0.26          |
| (1,3457) | 1:20:A:LYS:HE3   | 1:19:A:PRO:HA    | 17       | 0.26          |
| (1,3437) | 1:21:A:LEU:HB2   | 1:21:A:LEU:HD12  | 14       | 0.26          |
| (1,3437) | 1:21:A:LEU:HB2   | 1:21:A:LEU:HD11  | 15       | 0.26          |
| (1,3421) | 1:53:A:PHE:HA    | 1:75:A:LEU:HD21  | 8        | 0.26          |
| (1,3421) | 1:53:A:PHE:HA    | 1:75:A:LEU:HD23  | 10       | 0.26          |
| (1,3421) | 1:53:A:PHE:HA    | 1:75:A:LEU:HD21  | 12       | 0.26          |
| (1,3412) | 1:82:A:TRP:HZ3   | 1:117:A:LEU:HD13 | 6        | 0.26          |
| (1,3396) | 1:71:A:LEU:HA    | 1:74:A:ALA:HB3   | 1        | 0.26          |
| (1,3396) | 1:71:A:LEU:HA    | 1:74:A:ALA:HB2   | 16       | 0.26          |
| (1,3395) | 1:33:A:GLU:HB3   | 1:33:A:GLU:HA    | 8        | 0.26          |
| (1,3390) | 1:88:A:VAL:HG23  | 1:84:A:TYR:HA    | 17       | 0.26          |
| (1,3386) | 1:90:A:PRO:HA    | 1:92:A:ALA:HB2   | 15       | 0.26          |
| (1,3358) | 1:28:A:ILE:HB    | 1:29:A:ALA:HA    | 2        | 0.26          |
| (1,3358) | 1:28:A:ILE:HB    | 1:29:A:ALA:HA    | 4        | 0.26          |
| (1,3358) | 1:28:A:ILE:HB    | 1:29:A:ALA:HA    | 11       | 0.26          |
| (1,3345) | 1:29:A:ALA:HA    | 1:29:A:ALA:HB1   | 8        | 0.26          |
| (1,3345) | 1:29:A:ALA:HA    | 1:29:A:ALA:HB1   | 11       | 0.26          |
| (1,3345) | 1:29:A:ALA:HA    | 1:29:A:ALA:HB3   | 13       | 0.26          |
| (1,3345) | 1:29:A:ALA:HA    | 1:29:A:ALA:HB1   | 15       | 0.26          |
| (1,3336) | 1:71:A:LEU:HD21  | 1:74:A:ALA:H     | 7        | 0.26          |
| (1,3336) | 1:71:A:LEU:HD23  | 1:74:A:ALA:H     | 8        | 0.26          |
| (1,3336) | 1:71:A:LEU:HD21  | 1:74:A:ALA:H     | 10       | 0.26          |
| (1,3326) | 1:77:A:LEU:HG    | 1:77:A:LEU:HD12  | 4        | 0.26          |
| (1,3326) | 1:77:A:LEU:HG    | 1:77:A:LEU:HD11  | 9        | 0.26          |
| (1,3326) | 1:77:A:LEU:HG    | 1:77:A:LEU:HD11  | 12       | 0.26          |
| (1,3260) | 1:121:A:LYS:HG2  | 1:121:A:LYS:HB2  | 2        | 0.26          |
| (1,3260) | 1:121:A:LYS:HG2  | 1:121:A:LYS:HB2  | 11       | 0.26          |
| (1,3230) | 1:68:A:LYS:HB2   | 1:68:A:LYS:HA    | 11       | 0.26          |
| (1,3228) | 1:31:A:LEU:HB2   | 1:39:A:PHE:HE2   | 3        | 0.26          |
| (1,3228) | 1:31:A:LEU:HB2   | 1:39:A:PHE:HE2   | 11       | 0.26          |
| (1,3228) | 1:31:A:LEU:HB2   | 1:39:A:PHE:HE1   | 14       | 0.26          |
| (1,3223) | 1:84:A:TYR:HE1   | 1:79:A:THR:HA    | 13       | 0.26          |
| (1,3221) | 1:37:A:HIS:HB2   | 1:99:A:GLY:HA2   | 14       | 0.26          |
| (1,3221) | 1:37:A:HIS:HB2   | 1:99:A:GLY:HA2   | 17       | 0.26          |
| (1,3216) | 1:48:A:LEU:HG    | 1:84:A:TYR:HD2   | 1        | 0.26          |
| (1,3209) | 1:124:A:VAL:HG12 | 1:124:A:VAL:HB   | 8        | 0.26          |
| (1,3209) | 1:124:A:VAL:HG11 | 1:124:A:VAL:HB   | 10       | 0.26          |
| (1,3183) | 1:124:A:VAL:HG21 | 1:121:A:LYS:HA   | 1        | 0.26          |
| (1,3183) | 1:124:A:VAL:HG23 | 1:121:A:LYS:HA   | 14       | 0.26          |
| (1,3180) | 1:111:A:GLU:HG2  | 1:111:A:GLU:HA   | 3        | 0.26          |
| (1,3180) | 1:111:A:GLU:HG2  | 1:111:A:GLU:HA   | 6        | 0.26          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3180) | 1:111:A:GLU:HG2 | 1:111:A:GLU:HA   | 9        | 0.26          |
| (1,3180) | 1:111:A:GLU:HG2 | 1:111:A:GLU:HA   | 11       | 0.26          |
| (1,3132) | 1:68:A:LYS:HB2  | 1:53:A:PHE:HE1   | 6        | 0.26          |
| (1,3132) | 1:68:A:LYS:HB2  | 1:53:A:PHE:HE2   | 14       | 0.26          |
| (1,3132) | 1:68:A:LYS:HB2  | 1:53:A:PHE:HE2   | 16       | 0.26          |
| (1,3066) | 1:30:A:PHE:HB3  | 1:29:A:ALA:HB3   | 3        | 0.26          |
| (1,3066) | 1:30:A:PHE:HB3  | 1:29:A:ALA:HB3   | 12       | 0.26          |
| (1,3032) | 1:121:A:LYS:HG3 | 1:121:A:LYS:HE3  | 11       | 0.26          |
| (1,3032) | 1:121:A:LYS:HG3 | 1:121:A:LYS:HE3  | 13       | 0.26          |
| (1,3028) | 1:71:A:LEU:HD11 | 1:72:A:ARG:HA    | 10       | 0.26          |
| (1,3028) | 1:71:A:LEU:HD11 | 1:72:A:ARG:HA    | 12       | 0.26          |
| (1,3028) | 1:71:A:LEU:HD11 | 1:72:A:ARG:HA    | 16       | 0.26          |
| (1,3024) | 1:64:A:MET:HE1  | 1:65:A:ASN:HB3   | 16       | 0.26          |
| (1,3021) | 1:64:A:MET:HE1  | 1:63:A:GLU:H     | 3        | 0.26          |
| (1,2989) | 1:42:A:GLU:HA   | 1:42:A:GLU:HB2   | 6        | 0.26          |
| (1,2955) | 1:74:A:ALA:HB3  | 1:75:A:LEU:HD13  | 5        | 0.26          |
| (1,2945) | 1:110:A:VAL:HB  | 1:110:A:VAL:HG11 | 4        | 0.26          |
| (1,2945) | 1:110:A:VAL:HB  | 1:110:A:VAL:HG12 | 9        | 0.26          |
| (1,2945) | 1:110:A:VAL:HB  | 1:110:A:VAL:HG11 | 12       | 0.26          |
| (1,2945) | 1:110:A:VAL:HB  | 1:110:A:VAL:HG13 | 15       | 0.26          |
| (1,2942) | 1:57:A:VAL:HG23 | 1:57:A:VAL:HB    | 6        | 0.26          |
| (1,2933) | 1:95:A:VAL:HG22 | 1:99:A:GLY:H     | 13       | 0.26          |
| (1,2931) | 1:88:A:VAL:HG23 | 1:85:A:LEU:H     | 5        | 0.26          |
| (1,2930) | 1:31:A:LEU:HD22 | 1:60:A:VAL:HG11  | 2        | 0.26          |
| (1,2930) | 1:31:A:LEU:HD21 | 1:60:A:VAL:HG11  | 14       | 0.26          |
| (1,2891) | 1:32:A:ALA:HB2  | 1:28:A:ILE:HG23  | 4        | 0.26          |
| (1,2863) | 1:78:A:TYR:HE2  | 1:84:A:TYR:HD2   | 1        | 0.26          |
| (1,2832) | 1:97:A:LEU:HD21 | 1:97:A:LEU:H     | 6        | 0.26          |
| (1,2832) | 1:97:A:LEU:HD22 | 1:97:A:LEU:H     | 9        | 0.26          |
| (1,2832) | 1:97:A:LEU:HD22 | 1:97:A:LEU:H     | 13       | 0.26          |
| (1,2832) | 1:97:A:LEU:HD21 | 1:97:A:LEU:H     | 15       | 0.26          |
| (1,2831) | 1:97:A:LEU:HD22 | 1:35:A:PHE:HD2   | 14       | 0.26          |
| (1,2824) | 1:97:A:LEU:HD23 | 1:56:A:LEU:HA    | 4        | 0.26          |
| (1,2824) | 1:97:A:LEU:HD23 | 1:56:A:LEU:HA    | 8        | 0.26          |
| (1,2824) | 1:97:A:LEU:HD22 | 1:56:A:LEU:HA    | 12       | 0.26          |
| (1,2769) | 1:43:A:GLY:HA2  | 1:42:A:GLU:HB2   | 4        | 0.26          |
| (1,2729) | 1:17:A:ASN:HB3  | 1:17:A:ASN:HB2   | 4        | 0.26          |
| (1,2720) | 1:86:A:TYR:HB3  | 1:117:A:LEU:HD13 | 3        | 0.26          |
| (1,2713) | 1:53:A:PHE:HB3  | 1:75:A:LEU:HD11  | 17       | 0.26          |
| (1,2675) | 1:85:A:LEU:HB2  | 1:86:A:TYR:HD1   | 6        | 0.26          |
| (1,2675) | 1:85:A:LEU:HB2  | 1:86:A:TYR:HD1   | 8        | 0.26          |
| (1,2675) | 1:85:A:LEU:HB2  | 1:86:A:TYR:HD1   | 13       | 0.26          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2675) | 1:85:A:LEU:HB2   | 1:86:A:TYR:HD2   | 16       | 0.26          |
| (1,2605) | 1:31:A:LEU:HD22  | 1:30:A:PHE:HD2   | 2        | 0.26          |
| (1,2598) | 1:27:A:VAL:HG23  | 1:27:A:VAL:HG13  | 1        | 0.26          |
| (1,2598) | 1:27:A:VAL:HG21  | 1:27:A:VAL:HG11  | 2        | 0.26          |
| (1,2598) | 1:27:A:VAL:HG23  | 1:27:A:VAL:HG11  | 13       | 0.26          |
| (1,2598) | 1:27:A:VAL:HG23  | 1:27:A:VAL:HG11  | 14       | 0.26          |
| (1,2598) | 1:27:A:VAL:HG21  | 1:27:A:VAL:HG12  | 17       | 0.26          |
| (1,2596) | 1:74:A:ALA:HB2   | 1:27:A:VAL:HG11  | 3        | 0.26          |
| (1,2596) | 1:74:A:ALA:HB2   | 1:27:A:VAL:HG11  | 11       | 0.26          |
| (1,2596) | 1:74:A:ALA:HB3   | 1:27:A:VAL:HG13  | 16       | 0.26          |
| (1,2583) | 1:60:A:VAL:HG13  | 1:34:A:ARG:HG2   | 10       | 0.26          |
| (1,2576) | 1:124:A:VAL:HG22 | 1:120:A:ALA:HA   | 11       | 0.26          |
| (1,2560) | 1:86:A:TYR:HE2   | 1:86:A:TYR:HD2   | 5        | 0.26          |
| (1,2560) | 1:86:A:TYR:HE1   | 1:86:A:TYR:HD1   | 8        | 0.26          |
| (1,2560) | 1:86:A:TYR:HE1   | 1:86:A:TYR:HD1   | 10       | 0.26          |
| (1,2546) | 1:73:A:SER:HA    | 1:73:A:SER:HB3   | 3        | 0.26          |
| (1,2546) | 1:73:A:SER:HA    | 1:73:A:SER:HB3   | 4        | 0.26          |
| (1,2546) | 1:73:A:SER:HA    | 1:73:A:SER:HB3   | 5        | 0.26          |
| (1,2546) | 1:73:A:SER:HA    | 1:73:A:SER:HB3   | 7        | 0.26          |
| (1,2546) | 1:73:A:SER:HA    | 1:73:A:SER:HB3   | 13       | 0.26          |
| (1,2542) | 1:21:A:LEU:HD13  | 1:30:A:PHE:HA    | 13       | 0.26          |
| (1,2529) | 1:79:A:THR:HG22  | 1:75:A:LEU:HA    | 8        | 0.26          |
| (1,2502) | 1:42:A:GLU:HA    | 1:43:A:GLY:H     | 3        | 0.26          |
| (1,2468) | 1:53:A:PHE:HE1   | 1:72:A:ARG:HG3   | 1        | 0.26          |
| (1,2468) | 1:53:A:PHE:HE2   | 1:72:A:ARG:HG3   | 12       | 0.26          |
| (1,2411) | 1:45:A:ALA:HB3   | 1:84:A:TYR:HB3   | 1        | 0.26          |
| (1,2404) | 1:28:A:ILE:HD11  | 1:74:A:ALA:HA    | 11       | 0.26          |
| (1,2404) | 1:28:A:ILE:HD13  | 1:74:A:ALA:HA    | 17       | 0.26          |
| (1,2369) | 1:52:A:ILE:HD13  | 1:56:A:LEU:H     | 3        | 0.26          |
| (1,2358) | 1:107:A:GLU:HA   | 1:111:A:GLU:H    | 14       | 0.26          |
| (1,2346) | 1:105:A:LEU:HD13 | 1:107:A:GLU:HA   | 6        | 0.26          |
| (1,2344) | 1:104:A:GLU:HG2  | 1:105:A:LEU:HD23 | 17       | 0.26          |
| (1,2341) | 1:66:A:LEU:HD21  | 1:70:A:GLN:H     | 9        | 0.26          |
| (1,2341) | 1:66:A:LEU:HD23  | 1:70:A:GLN:H     | 11       | 0.26          |
| (1,2307) | 1:117:A:LEU:HD11 | 1:86:A:TYR:HB2   | 4        | 0.26          |
| (1,2307) | 1:117:A:LEU:HD11 | 1:86:A:TYR:HB2   | 11       | 0.26          |
| (1,2307) | 1:117:A:LEU:HD11 | 1:86:A:TYR:HB2   | 13       | 0.26          |
| (1,2307) | 1:117:A:LEU:HD11 | 1:86:A:TYR:HB2   | 16       | 0.26          |
| (1,2253) | 1:44:A:GLU:HB3   | 1:44:A:GLU:H     | 15       | 0.26          |
| (1,2221) | 1:31:A:LEU:HA    | 1:60:A:VAL:HB    | 3        | 0.26          |
| (1,2210) | 1:105:A:LEU:HG   | 1:110:A:VAL:HG13 | 6        | 0.26          |
| (1,2210) | 1:105:A:LEU:HG   | 1:110:A:VAL:HG13 | 12       | 0.26          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2149) | 1:21:A:LEU:HD23  | 1:30:A:PHE:HD2   | 15       | 0.26          |
| (1,2116) | 1:45:A:ALA:HB2   | 1:84:A:TYR:HA    | 6        | 0.26          |
| (1,2036) | 1:97:A:LEU:HD21  | 1:97:A:LEU:HB2   | 1        | 0.26          |
| (1,2028) | 1:97:A:LEU:HD22  | 1:97:A:LEU:H     | 8        | 0.26          |
| (1,2021) | 1:53:A:PHE:HE2   | 1:57:A:VAL:HG12  | 17       | 0.26          |
| (1,1994) | 1:91:A:GLY:HA2   | 1:91:A:GLY:H     | 4        | 0.26          |
| (1,1994) | 1:91:A:GLY:HA2   | 1:91:A:GLY:H     | 7        | 0.26          |
| (1,1955) | 1:92:A:ALA:HB3   | 1:113:A:ALA:HB1  | 7        | 0.26          |
| (1,1947) | 1:93:A:THR:HB    | 1:88:A:VAL:HG13  | 1        | 0.26          |
| (1,1947) | 1:93:A:THR:HB    | 1:88:A:VAL:HG12  | 3        | 0.26          |
| (1,1947) | 1:93:A:THR:HB    | 1:88:A:VAL:HG12  | 5        | 0.26          |
| (1,1940) | 1:111:A:GLU:HB2  | 1:109:A:HIS:HA   | 2        | 0.26          |
| (1,1940) | 1:111:A:GLU:HB2  | 1:109:A:HIS:HA   | 5        | 0.26          |
| (1,1940) | 1:111:A:GLU:HB2  | 1:109:A:HIS:HA   | 15       | 0.26          |
| (1,1904) | 1:74:A:ALA:HB3   | 1:28:A:ILE:HA    | 3        | 0.26          |
| (1,1904) | 1:74:A:ALA:HB1   | 1:28:A:ILE:HA    | 7        | 0.26          |
| (1,1904) | 1:74:A:ALA:HB2   | 1:28:A:ILE:HA    | 9        | 0.26          |
| (1,1904) | 1:74:A:ALA:HB1   | 1:28:A:ILE:HA    | 17       | 0.26          |
| (1,1903) | 1:122:A:ALA:HB3  | 1:121:A:LYS:HE3  | 1        | 0.26          |
| (1,1886) | 1:102:A:CYS:HB3  | 1:49:A:LYS:HA    | 4        | 0.26          |
| (1,1886) | 1:102:A:CYS:HB3  | 1:49:A:LYS:HA    | 6        | 0.26          |
| (1,1881) | 1:113:A:ALA:HB1  | 1:88:A:VAL:HA    | 9        | 0.26          |
| (1,1872) | 1:56:A:LEU:HD21  | 1:55:A:ASP:HB3   | 8        | 0.26          |
| (1,1872) | 1:56:A:LEU:HD21  | 1:55:A:ASP:HB3   | 12       | 0.26          |
| (1,1865) | 1:45:A:ALA:HB1   | 1:44:A:GLU:HB3   | 7        | 0.26          |
| (1,1752) | 1:41:A:ALA:HB3   | 1:28:A:ILE:HG21  | 2        | 0.26          |
| (1,1752) | 1:41:A:ALA:HB2   | 1:28:A:ILE:HG23  | 8        | 0.26          |
| (1,1737) | 1:77:A:LEU:HG    | 1:77:A:LEU:HD12  | 3        | 0.26          |
| (1,1737) | 1:77:A:LEU:HG    | 1:77:A:LEU:HD11  | 10       | 0.26          |
| (1,1736) | 1:77:A:LEU:HB3   | 1:77:A:LEU:HD12  | 8        | 0.26          |
| (1,1733) | 1:30:A:PHE:HD1   | 1:66:A:LEU:HD23  | 14       | 0.26          |
| (1,1723) | 1:68:A:LYS:HD3   | 1:57:A:VAL:HG13  | 1        | 0.26          |
| (1,1723) | 1:68:A:LYS:HD3   | 1:57:A:VAL:HG12  | 7        | 0.26          |
| (1,1723) | 1:68:A:LYS:HD3   | 1:57:A:VAL:HG13  | 15       | 0.26          |
| (1,1723) | 1:68:A:LYS:HD3   | 1:57:A:VAL:HG13  | 16       | 0.26          |
| (1,1690) | 1:42:A:GLU:HG2   | 1:41:A:ALA:HB2   | 12       | 0.26          |
| (1,1681) | 1:40:A:SER:HA    | 1:41:A:ALA:HB3   | 7        | 0.26          |
| (1,1629) | 1:116:A:GLN:HG3  | 1:113:A:ALA:HB3  | 17       | 0.26          |
| (1,1618) | 1:109:A:HIS:HB2  | 1:110:A:VAL:HG11 | 10       | 0.26          |
| (1,1613) | 1:124:A:VAL:HG22 | 1:121:A:LYS:HA   | 6        | 0.26          |
| (1,1613) | 1:124:A:VAL:HG22 | 1:121:A:LYS:HA   | 13       | 0.26          |
| (1,1613) | 1:124:A:VAL:HG22 | 1:121:A:LYS:HA   | 15       | 0.26          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1592) | 1:126:A:ALA:HB3  | 1:125:A:GLN:HG3 | 14       | 0.26          |
| (1,1553) | 1:57:A:VAL:HG13  | 1:61:A:ALA:H    | 8        | 0.26          |
| (1,1521) | 1:30:A:PHE:HB3   | 1:29:A:ALA:HB1  | 5        | 0.26          |
| (1,1521) | 1:30:A:PHE:HB3   | 1:29:A:ALA:HB1  | 6        | 0.26          |
| (1,1510) | 1:52:A:ILE:HG23  | 1:50:A:ILE:H    | 12       | 0.26          |
| (1,1485) | 1:71:A:LEU:HD13  | 1:72:A:ARG:HA   | 1        | 0.26          |
| (1,1482) | 1:64:A:MET:HE2   | 1:27:A:VAL:HA   | 7        | 0.26          |
| (1,1480) | 1:64:A:MET:HE3   | 1:63:A:GLU:H    | 10       | 0.26          |
| (1,1480) | 1:64:A:MET:HE3   | 1:63:A:GLU:H    | 17       | 0.26          |
| (1,1478) | 1:64:A:MET:HE1   | 1:66:A:LEU:H    | 9        | 0.26          |
| (1,1428) | 1:93:A:THR:HG22  | 1:101:A:PRO:HB3 | 15       | 0.26          |
| (1,1419) | 1:77:A:LEU:HD12  | 1:25:A:LYS:HA   | 14       | 0.26          |
| (1,1403) | 1:95:A:VAL:HG23  | 1:95:A:VAL:HG11 | 5        | 0.26          |
| (1,1395) | 1:31:A:LEU:HD21  | 1:39:A:PHE:HD2  | 7        | 0.26          |
| (1,1363) | 1:29:A:ALA:HA    | 1:32:A:ALA:HB3  | 6        | 0.26          |
| (1,1357) | 1:74:A:ALA:HB2   | 1:31:A:LEU:HD11 | 12       | 0.26          |
| (1,1309) | 1:97:A:LEU:HD22  | 1:97:A:LEU:H    | 8        | 0.26          |
| (1,1308) | 1:97:A:LEU:HD21  | 1:35:A:PHE:HD1  | 16       | 0.26          |
| (1,1307) | 1:97:A:LEU:HD22  | 1:97:A:LEU:HB2  | 2        | 0.26          |
| (1,1307) | 1:97:A:LEU:HD22  | 1:97:A:LEU:HB2  | 5        | 0.26          |
| (1,1307) | 1:97:A:LEU:HD22  | 1:97:A:LEU:HB2  | 14       | 0.26          |
| (1,1307) | 1:97:A:LEU:HD21  | 1:97:A:LEU:HB2  | 16       | 0.26          |
| (1,1304) | 1:97:A:LEU:HD21  | 1:56:A:LEU:HA   | 1        | 0.26          |
| (1,1124) | 1:97:A:LEU:HD13  | 1:57:A:VAL:H    | 11       | 0.26          |
| (1,1081) | 1:71:A:LEU:HD13  | 1:57:A:VAL:H    | 4        | 0.26          |
| (1,1081) | 1:71:A:LEU:HD11  | 1:57:A:VAL:H    | 7        | 0.26          |
| (1,1048) | 1:124:A:VAL:HG23 | 1:120:A:ALA:HA  | 3        | 0.26          |
| (1,993)  | 1:79:A:THR:HG23  | 1:75:A:LEU:HA   | 16       | 0.26          |
| (1,895)  | 1:129:A:ALA:HB3  | 1:129:A:ALA:HA  | 5        | 0.26          |
| (1,894)  | 1:133:A:ALA:HA   | 1:133:A:ALA:HB3 | 2        | 0.26          |
| (1,894)  | 1:133:A:ALA:HA   | 1:133:A:ALA:HB3 | 3        | 0.26          |
| (1,894)  | 1:133:A:ALA:HA   | 1:133:A:ALA:HB1 | 4        | 0.26          |
| (1,894)  | 1:133:A:ALA:HA   | 1:133:A:ALA:HB1 | 5        | 0.26          |
| (1,894)  | 1:133:A:ALA:HA   | 1:133:A:ALA:HB3 | 6        | 0.26          |
| (1,894)  | 1:133:A:ALA:HA   | 1:133:A:ALA:HB1 | 8        | 0.26          |
| (1,894)  | 1:133:A:ALA:HA   | 1:133:A:ALA:HB1 | 11       | 0.26          |
| (1,894)  | 1:133:A:ALA:HA   | 1:133:A:ALA:HB1 | 13       | 0.26          |
| (1,894)  | 1:133:A:ALA:HA   | 1:133:A:ALA:HB3 | 15       | 0.26          |
| (1,894)  | 1:133:A:ALA:HA   | 1:133:A:ALA:HB3 | 16       | 0.26          |
| (1,894)  | 1:133:A:ALA:HA   | 1:133:A:ALA:HB2 | 17       | 0.26          |
| (1,853)  | 1:65:A:ASN:HB2   | 1:65:A:ASN:HD21 | 6        | 0.26          |
| (1,852)  | 1:65:A:ASN:HB3   | 1:65:A:ASN:HD21 | 13       | 0.26          |

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| Key     | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,852) | 1:65:A:ASN:HB3  | 1:65:A:ASN:HD21  | 16       | 0.26          |
| (1,850) | 1:86:A:TYR:HB2  | 1:117:A:LEU:HB3  | 1        | 0.26          |
| (1,850) | 1:86:A:TYR:HB2  | 1:117:A:LEU:HB3  | 2        | 0.26          |
| (1,850) | 1:86:A:TYR:HB2  | 1:117:A:LEU:HB3  | 3        | 0.26          |
| (1,850) | 1:86:A:TYR:HB2  | 1:117:A:LEU:HB3  | 9        | 0.26          |
| (1,850) | 1:86:A:TYR:HB2  | 1:117:A:LEU:HB3  | 11       | 0.26          |
| (1,850) | 1:86:A:TYR:HB2  | 1:117:A:LEU:HB3  | 12       | 0.26          |
| (1,829) | 1:41:A:ALA:HB1  | 1:41:A:ALA:H     | 7        | 0.26          |
| (1,819) | 1:28:A:ILE:HD11 | 1:74:A:ALA:HA    | 10       | 0.26          |
| (1,819) | 1:28:A:ILE:HD12 | 1:74:A:ALA:HA    | 16       | 0.26          |
| (1,691) | 1:75:A:LEU:HD23 | 1:54:A:GLN:H     | 3        | 0.26          |
| (1,691) | 1:75:A:LEU:HD23 | 1:54:A:GLN:H     | 9        | 0.26          |
| (1,635) | 1:127:A:GLN:H   | 1:127:A:GLN:HB3  | 17       | 0.26          |
| (1,580) | 1:98:A:ASP:HB2  | 1:100:A:ASN:HD21 | 5        | 0.26          |
| (1,580) | 1:98:A:ASP:HB2  | 1:100:A:ASN:HD21 | 15       | 0.26          |
| (1,570) | 1:60:A:VAL:HG12 | 1:34:A:ARG:HE    | 17       | 0.26          |
| (1,564) | 1:59:A:ARG:HE   | 1:97:A:LEU:HD11  | 11       | 0.26          |
| (1,557) | 1:66:A:LEU:HB2  | 1:70:A:GLN:HE22  | 11       | 0.26          |
| (1,552) | 1:65:A:ASN:H    | 1:65:A:ASN:HD21  | 4        | 0.26          |
| (1,552) | 1:65:A:ASN:H    | 1:65:A:ASN:HD21  | 14       | 0.26          |
| (1,528) | 1:65:A:ASN:HB2  | 1:65:A:ASN:HD21  | 10       | 0.26          |
| (1,528) | 1:65:A:ASN:HB2  | 1:65:A:ASN:HD21  | 12       | 0.26          |
| (1,528) | 1:65:A:ASN:HB2  | 1:65:A:ASN:HD21  | 17       | 0.26          |
| (1,524) | 1:20:A:LYS:HB3  | 1:22:A:ASN:HD22  | 17       | 0.26          |
| (1,478) | 1:27:A:VAL:HG23 | 1:29:A:ALA:H     | 7        | 0.26          |
| (1,441) | 1:42:A:GLU:HB3  | 1:41:A:ALA:H     | 11       | 0.26          |
| (1,441) | 1:42:A:GLU:HB3  | 1:41:A:ALA:H     | 15       | 0.26          |
| (1,441) | 1:42:A:GLU:HB3  | 1:41:A:ALA:H     | 17       | 0.26          |
| (1,300) | 1:100:A:ASN:HB3 | 1:100:A:ASN:HD21 | 2        | 0.26          |
| (1,300) | 1:100:A:ASN:HB3 | 1:100:A:ASN:HD21 | 3        | 0.26          |
| (1,300) | 1:100:A:ASN:HB3 | 1:100:A:ASN:HD21 | 4        | 0.26          |
| (1,300) | 1:100:A:ASN:HB3 | 1:100:A:ASN:HD21 | 8        | 0.26          |
| (1,300) | 1:100:A:ASN:HB3 | 1:100:A:ASN:HD21 | 9        | 0.26          |
| (1,300) | 1:100:A:ASN:HB3 | 1:100:A:ASN:HD21 | 14       | 0.26          |
| (1,300) | 1:100:A:ASN:HB3 | 1:100:A:ASN:HD21 | 15       | 0.26          |
| (1,234) | 1:95:A:VAL:HG22 | 1:99:A:GLY:H     | 6        | 0.26          |
| (1,172) | 1:27:A:VAL:HG11 | 1:21:A:LEU:H     | 9        | 0.26          |
| (1,154) | 1:130:A:GLU:H   | 1:129:A:ALA:HB3  | 2        | 0.26          |
| (1,154) | 1:130:A:GLU:H   | 1:129:A:ALA:HB1  | 8        | 0.26          |
| (1,128) | 1:35:A:PHE:HD1  | 1:39:A:PHE:H     | 6        | 0.26          |
| (1,125) | 1:28:A:ILE:HG13 | 1:28:A:ILE:H     | 1        | 0.26          |
| (1,125) | 1:28:A:ILE:HG13 | 1:28:A:ILE:H     | 2        | 0.26          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,125)  | 1:28:A:ILE:HG13 | 1:28:A:ILE:H     | 5        | 0.26          |
| (1,125)  | 1:28:A:ILE:HG13 | 1:28:A:ILE:H     | 8        | 0.26          |
| (1,125)  | 1:28:A:ILE:HG13 | 1:28:A:ILE:H     | 9        | 0.26          |
| (1,125)  | 1:28:A:ILE:HG13 | 1:28:A:ILE:H     | 12       | 0.26          |
| (1,125)  | 1:28:A:ILE:HG13 | 1:28:A:ILE:H     | 13       | 0.26          |
| (1,125)  | 1:28:A:ILE:HG13 | 1:28:A:ILE:H     | 14       | 0.26          |
| (1,125)  | 1:28:A:ILE:HG13 | 1:28:A:ILE:H     | 16       | 0.26          |
| (1,125)  | 1:28:A:ILE:HG13 | 1:28:A:ILE:H     | 17       | 0.26          |
| (1,117)  | 1:27:A:VAL:HG13 | 1:26:A:GLU:H     | 1        | 0.26          |
| (1,117)  | 1:27:A:VAL:HG11 | 1:26:A:GLU:H     | 5        | 0.26          |
| (1,117)  | 1:27:A:VAL:HG13 | 1:26:A:GLU:H     | 9        | 0.26          |
| (1,117)  | 1:27:A:VAL:HG11 | 1:26:A:GLU:H     | 14       | 0.26          |
| (1,116)  | 1:21:A:LEU:HD13 | 1:30:A:PHE:H     | 10       | 0.26          |
| (1,116)  | 1:21:A:LEU:HD12 | 1:30:A:PHE:H     | 17       | 0.26          |
| (1,56)   | 1:84:A:TYR:H    | 1:84:A:TYR:HD2   | 6        | 0.26          |
| (3,148)  | 1:22:A:ASN:H    | 1:22:A:ASN:HB2   | 14       | 0.25          |
| (3,129)  | 1:71:A:LEU:HD13 | 1:60:A:VAL:HB    | 13       | 0.25          |
| (3,117)  | 1:48:A:LEU:HD22 | 1:39:A:PHE:HD1   | 4        | 0.25          |
| (3,111)  | 1:111:A:GLU:HG2 | 1:112:A:HIS:HA   | 1        | 0.25          |
| (3,109)  | 1:92:A:ALA:H    | 1:110:A:VAL:HB   | 10       | 0.25          |
| (3,92)   | 1:88:A:VAL:HG22 | 1:87:A:GLY:HA2   | 3        | 0.25          |
| (3,92)   | 1:88:A:VAL:HG23 | 1:87:A:GLY:HA2   | 13       | 0.25          |
| (3,59)   | 1:117:A:LEU:HA  | 1:85:A:LEU:HD23  | 6        | 0.25          |
| (3,34)   | 1:97:A:LEU:HD22 | 1:31:A:LEU:HD13  | 1        | 0.25          |
| (3,31)   | 1:22:A:ASN:HD21 | 1:22:A:ASN:HB2   | 1        | 0.25          |
| (3,22)   | 1:48:A:LEU:H    | 1:48:A:LEU:HD11  | 1        | 0.25          |
| (3,18)   | 1:58:A:ASP:HB3  | 1:60:A:VAL:HG12  | 11       | 0.25          |
| (3,16)   | 1:90:A:PRO:HA   | 1:110:A:VAL:HG11 | 4        | 0.25          |
| (3,15)   | 1:85:A:LEU:HB3  | 1:82:A:TRP:HA    | 3        | 0.25          |
| (3,15)   | 1:85:A:LEU:HB3  | 1:82:A:TRP:HA    | 9        | 0.25          |
| (3,15)   | 1:85:A:LEU:HB3  | 1:82:A:TRP:HA    | 12       | 0.25          |
| (3,15)   | 1:85:A:LEU:HB3  | 1:82:A:TRP:HA    | 13       | 0.25          |
| (3,14)   | 1:82:A:TRP:HA   | 1:85:A:LEU:HB2   | 4        | 0.25          |
| (3,14)   | 1:82:A:TRP:HA   | 1:85:A:LEU:HB2   | 5        | 0.25          |
| (3,14)   | 1:82:A:TRP:HA   | 1:85:A:LEU:HB2   | 8        | 0.25          |
| (1,4342) | 1:38:A:CYS:H    | 1:95:A:VAL:HG12  | 10       | 0.25          |
| (1,4310) | 1:64:A:MET:HA   | 1:65:A:ASN:H     | 4        | 0.25          |
| (1,4310) | 1:64:A:MET:HA   | 1:65:A:ASN:H     | 11       | 0.25          |
| (1,4310) | 1:64:A:MET:HA   | 1:65:A:ASN:H     | 13       | 0.25          |
| (1,4300) | 1:92:A:ALA:H    | 1:105:A:LEU:HD23 | 10       | 0.25          |
| (1,4299) | 1:65:A:ASN:HD22 | 1:65:A:ASN:HD21  | 1        | 0.25          |
| (1,4299) | 1:65:A:ASN:HD22 | 1:65:A:ASN:HD21  | 2        | 0.25          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,4299) | 1:65:A:ASN:HD22  | 1:65:A:ASN:HD21  | 3        | 0.25          |
| (1,4299) | 1:65:A:ASN:HD22  | 1:65:A:ASN:HD21  | 6        | 0.25          |
| (1,4299) | 1:65:A:ASN:HD22  | 1:65:A:ASN:HD21  | 10       | 0.25          |
| (1,4299) | 1:65:A:ASN:HD22  | 1:65:A:ASN:HD21  | 11       | 0.25          |
| (1,4299) | 1:65:A:ASN:HD22  | 1:65:A:ASN:HD21  | 14       | 0.25          |
| (1,4299) | 1:65:A:ASN:HD22  | 1:65:A:ASN:HD21  | 17       | 0.25          |
| (1,4280) | 1:112:A:HIS:HA   | 1:116:A:GLN:H    | 9        | 0.25          |
| (1,4230) | 1:128:A:ARG:HA   | 1:128:A:ARG:H    | 13       | 0.25          |
| (1,4172) | 1:105:A:LEU:H    | 1:92:A:ALA:H     | 5        | 0.25          |
| (1,4172) | 1:105:A:LEU:H    | 1:92:A:ALA:H     | 14       | 0.25          |
| (1,4153) | 1:18:A:GLN:HB3   | 1:18:A:GLN:H     | 7        | 0.25          |
| (1,4141) | 1:98:A:ASP:HB2   | 1:100:A:ASN:HD21 | 8        | 0.25          |
| (1,4141) | 1:98:A:ASP:HB2   | 1:100:A:ASN:HD21 | 10       | 0.25          |
| (1,4126) | 1:59:A:ARG:HE    | 1:97:A:LEU:HD11  | 15       | 0.25          |
| (1,4109) | 1:97:A:LEU:HD12  | 1:98:A:ASP:H     | 11       | 0.25          |
| (1,4069) | 1:13:A:ASP:HB2   | 1:13:A:ASP:H     | 15       | 0.25          |
| (1,4037) | 1:27:A:VAL:HG23  | 1:29:A:ALA:H     | 11       | 0.25          |
| (1,4036) | 1:31:A:LEU:H     | 1:31:A:LEU:HD11  | 5        | 0.25          |
| (1,3941) | 1:63:A:GLU:H     | 1:61:A:ALA:HB3   | 15       | 0.25          |
| (1,3874) | 1:85:A:LEU:HB3   | 1:86:A:TYR:H     | 3        | 0.25          |
| (1,3874) | 1:85:A:LEU:HB3   | 1:86:A:TYR:H     | 9        | 0.25          |
| (1,3874) | 1:85:A:LEU:HB3   | 1:86:A:TYR:H     | 12       | 0.25          |
| (1,3874) | 1:85:A:LEU:HB3   | 1:86:A:TYR:H     | 15       | 0.25          |
| (1,3874) | 1:85:A:LEU:HB3   | 1:86:A:TYR:H     | 17       | 0.25          |
| (1,3861) | 1:110:A:VAL:HG21 | 1:91:A:GLY:H     | 5        | 0.25          |
| (1,3839) | 1:65:A:ASN:HB3   | 1:65:A:ASN:HD21  | 6        | 0.25          |
| (1,3816) | 1:105:A:LEU:H    | 1:105:A:LEU:HD22 | 14       | 0.25          |
| (1,3816) | 1:105:A:LEU:H    | 1:105:A:LEU:HD21 | 16       | 0.25          |
| (1,3786) | 1:27:A:VAL:HG12  | 1:21:A:LEU:H     | 7        | 0.25          |
| (1,3783) | 1:117:A:LEU:HB3  | 1:117:A:LEU:H    | 2        | 0.25          |
| (1,3776) | 1:121:A:LYS:HA   | 1:122:A:ALA:H    | 6        | 0.25          |
| (1,3776) | 1:121:A:LYS:HA   | 1:122:A:ALA:H    | 10       | 0.25          |
| (1,3775) | 1:124:A:VAL:HA   | 1:125:A:GLN:H    | 1        | 0.25          |
| (1,3775) | 1:124:A:VAL:HA   | 1:125:A:GLN:H    | 9        | 0.25          |
| (1,3775) | 1:124:A:VAL:HA   | 1:125:A:GLN:H    | 14       | 0.25          |
| (1,3773) | 1:123:A:ARG:HA   | 1:124:A:VAL:H    | 5        | 0.25          |
| (1,3773) | 1:123:A:ARG:HA   | 1:124:A:VAL:H    | 6        | 0.25          |
| (1,3773) | 1:123:A:ARG:HA   | 1:124:A:VAL:H    | 7        | 0.25          |
| (1,3773) | 1:123:A:ARG:HA   | 1:124:A:VAL:H    | 9        | 0.25          |
| (1,3773) | 1:123:A:ARG:HA   | 1:124:A:VAL:H    | 12       | 0.25          |
| (1,3773) | 1:123:A:ARG:HA   | 1:124:A:VAL:H    | 14       | 0.25          |
| (1,3773) | 1:123:A:ARG:HA   | 1:124:A:VAL:H    | 17       | 0.25          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3732) | 1:21:A:LEU:HD13  | 1:30:A:PHE:H     | 7        | 0.25          |
| (1,3716) | 1:35:A:PHE:HE2   | 1:35:A:PHE:H     | 5        | 0.25          |
| (1,3716) | 1:35:A:PHE:HE1   | 1:35:A:PHE:H     | 16       | 0.25          |
| (1,3678) | 1:95:A:VAL:H     | 1:96:A:ASP:H     | 3        | 0.25          |
| (1,3668) | 1:84:A:TYR:H     | 1:84:A:TYR:HD2   | 13       | 0.25          |
| (1,3662) | 1:83:A:ARG:H     | 1:82:A:TRP:HD1   | 14       | 0.25          |
| (1,3610) | 1:121:A:LYS:HG3  | 1:117:A:LEU:HD13 | 6        | 0.25          |
| (1,3600) | 1:113:A:ALA:HB1  | 1:92:A:ALA:HA    | 5        | 0.25          |
| (1,3592) | 1:109:A:HIS:HB2  | 1:110:A:VAL:HG13 | 4        | 0.25          |
| (1,3592) | 1:109:A:HIS:HB2  | 1:110:A:VAL:HG12 | 15       | 0.25          |
| (1,3591) | 1:93:A:THR:HB    | 1:88:A:VAL:HG13  | 2        | 0.25          |
| (1,3588) | 1:105:A:LEU:HB3  | 1:110:A:VAL:HG22 | 2        | 0.25          |
| (1,3588) | 1:105:A:LEU:HB3  | 1:110:A:VAL:HG21 | 3        | 0.25          |
| (1,3588) | 1:105:A:LEU:HB3  | 1:110:A:VAL:HG23 | 7        | 0.25          |
| (1,3588) | 1:105:A:LEU:HB3  | 1:110:A:VAL:HG21 | 9        | 0.25          |
| (1,3588) | 1:105:A:LEU:HB3  | 1:110:A:VAL:HG22 | 13       | 0.25          |
| (1,3588) | 1:105:A:LEU:HB3  | 1:110:A:VAL:HG21 | 16       | 0.25          |
| (1,3588) | 1:105:A:LEU:HB3  | 1:110:A:VAL:HG21 | 17       | 0.25          |
| (1,3583) | 1:112:A:HIS:H    | 1:109:A:HIS:HA   | 3        | 0.25          |
| (1,3583) | 1:112:A:HIS:H    | 1:109:A:HIS:HA   | 6        | 0.25          |
| (1,3583) | 1:112:A:HIS:H    | 1:109:A:HIS:HA   | 9        | 0.25          |
| (1,3583) | 1:112:A:HIS:H    | 1:109:A:HIS:HA   | 10       | 0.25          |
| (1,3580) | 1:111:A:GLU:HB2  | 1:109:A:HIS:HA   | 14       | 0.25          |
| (1,3536) | 1:66:A:LEU:HB3   | 1:62:A:GLY:HA3   | 7        | 0.25          |
| (1,3534) | 1:122:A:ALA:HB1  | 1:121:A:LYS:HE3  | 2        | 0.25          |
| (1,3534) | 1:122:A:ALA:HB3  | 1:121:A:LYS:HE3  | 3        | 0.25          |
| (1,3534) | 1:122:A:ALA:HB3  | 1:121:A:LYS:HE3  | 7        | 0.25          |
| (1,3534) | 1:122:A:ALA:HB2  | 1:121:A:LYS:HE3  | 12       | 0.25          |
| (1,3534) | 1:122:A:ALA:HB1  | 1:121:A:LYS:HE3  | 17       | 0.25          |
| (1,3531) | 1:65:A:ASN:H     | 1:65:A:ASN:HA    | 6        | 0.25          |
| (1,3513) | 1:72:A:ARG:HG3   | 1:73:A:SER:HB3   | 11       | 0.25          |
| (1,3508) | 1:113:A:ALA:HB3  | 1:88:A:VAL:HA    | 15       | 0.25          |
| (1,3506) | 1:60:A:VAL:HG12  | 1:35:A:PHE:HZ    | 11       | 0.25          |
| (1,3505) | 1:124:A:VAL:HG12 | 1:124:A:VAL:HG21 | 2        | 0.25          |
| (1,3503) | 1:27:A:VAL:HG23  | 1:31:A:LEU:H     | 9        | 0.25          |
| (1,3503) | 1:27:A:VAL:HG22  | 1:31:A:LEU:H     | 13       | 0.25          |
| (1,3501) | 1:27:A:VAL:HG22  | 1:28:A:ILE:HA    | 8        | 0.25          |
| (1,3492) | 1:105:A:LEU:HB3  | 1:105:A:LEU:HD11 | 2        | 0.25          |
| (1,3492) | 1:105:A:LEU:HB3  | 1:105:A:LEU:HD11 | 10       | 0.25          |
| (1,3491) | 1:86:A:TYR:HE1   | 1:85:A:LEU:HD23  | 10       | 0.25          |
| (1,3491) | 1:86:A:TYR:HE2   | 1:85:A:LEU:HD21  | 12       | 0.25          |
| (1,3491) | 1:86:A:TYR:HE2   | 1:85:A:LEU:HD22  | 17       | 0.25          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3479) | 1:45:A:ALA:HB3   | 1:44:A:GLU:HB3   | 12       | 0.25          |
| (1,3476) | 1:107:A:GLU:HG2  | 1:108:A:GLN:H    | 4        | 0.25          |
| (1,3465) | 1:88:A:VAL:HG22  | 1:85:A:LEU:HB3   | 14       | 0.25          |
| (1,3437) | 1:21:A:LEU:HB2   | 1:21:A:LEU:HD11  | 5        | 0.25          |
| (1,3437) | 1:21:A:LEU:HB2   | 1:21:A:LEU:HD11  | 13       | 0.25          |
| (1,3437) | 1:21:A:LEU:HB2   | 1:21:A:LEU:HD13  | 16       | 0.25          |
| (1,3417) | 1:117:A:LEU:HG   | 1:117:A:LEU:HD13 | 12       | 0.25          |
| (1,3412) | 1:82:A:TRP:HZ3   | 1:117:A:LEU:HD11 | 5        | 0.25          |
| (1,3401) | 1:86:A:TYR:HE1   | 1:86:A:TYR:HA    | 11       | 0.25          |
| (1,3396) | 1:71:A:LEU:HA    | 1:74:A:ALA:HB2   | 4        | 0.25          |
| (1,3396) | 1:71:A:LEU:HA    | 1:74:A:ALA:HB2   | 10       | 0.25          |
| (1,3358) | 1:28:A:ILE:HB    | 1:29:A:ALA:HA    | 3        | 0.25          |
| (1,3358) | 1:28:A:ILE:HB    | 1:29:A:ALA:HA    | 6        | 0.25          |
| (1,3358) | 1:28:A:ILE:HB    | 1:29:A:ALA:HA    | 9        | 0.25          |
| (1,3345) | 1:29:A:ALA:HA    | 1:29:A:ALA:HB1   | 12       | 0.25          |
| (1,3341) | 1:41:A:ALA:HB1   | 1:28:A:ILE:HG23  | 4        | 0.25          |
| (1,3336) | 1:71:A:LEU:HD23  | 1:74:A:ALA:H     | 6        | 0.25          |
| (1,3336) | 1:71:A:LEU:HD23  | 1:74:A:ALA:H     | 16       | 0.25          |
| (1,3326) | 1:77:A:LEU:HG    | 1:77:A:LEU:HD11  | 7        | 0.25          |
| (1,3326) | 1:77:A:LEU:HG    | 1:77:A:LEU:HD12  | 11       | 0.25          |
| (1,3326) | 1:77:A:LEU:HG    | 1:77:A:LEU:HD12  | 15       | 0.25          |
| (1,3266) | 1:85:A:LEU:HD11  | 1:85:A:LEU:HD22  | 3        | 0.25          |
| (1,3264) | 1:121:A:LYS:HG2  | 1:121:A:LYS:H    | 14       | 0.25          |
| (1,3253) | 1:92:A:ALA:HB3   | 1:91:A:GLY:H     | 14       | 0.25          |
| (1,3228) | 1:31:A:LEU:HB2   | 1:39:A:PHE:HE2   | 1        | 0.25          |
| (1,3228) | 1:31:A:LEU:HB2   | 1:39:A:PHE:HE1   | 5        | 0.25          |
| (1,3228) | 1:31:A:LEU:HB2   | 1:39:A:PHE:HE1   | 13       | 0.25          |
| (1,3228) | 1:31:A:LEU:HB2   | 1:39:A:PHE:HE1   | 15       | 0.25          |
| (1,3223) | 1:84:A:TYR:HE2   | 1:79:A:THR:HA    | 1        | 0.25          |
| (1,3223) | 1:84:A:TYR:HE1   | 1:79:A:THR:HA    | 6        | 0.25          |
| (1,3221) | 1:37:A:HIS:HB2   | 1:99:A:GLY:HA2   | 2        | 0.25          |
| (1,3221) | 1:37:A:HIS:HB2   | 1:99:A:GLY:HA2   | 8        | 0.25          |
| (1,3221) | 1:37:A:HIS:HB2   | 1:99:A:GLY:HA2   | 13       | 0.25          |
| (1,3209) | 1:124:A:VAL:HG12 | 1:124:A:VAL:HB   | 4        | 0.25          |
| (1,3209) | 1:124:A:VAL:HG11 | 1:124:A:VAL:HB   | 16       | 0.25          |
| (1,3180) | 1:111:A:GLU:HG2  | 1:111:A:GLU:HA   | 15       | 0.25          |
| (1,3166) | 1:75:A:LEU:HD22  | 1:53:A:PHE:HD1   | 2        | 0.25          |
| (1,3135) | 1:68:A:LYS:HD3   | 1:68:A:LYS:HB2   | 5        | 0.25          |
| (1,3132) | 1:68:A:LYS:HB2   | 1:53:A:PHE:HE1   | 3        | 0.25          |
| (1,3123) | 1:59:A:ARG:HB2   | 1:59:A:ARG:HA    | 3        | 0.25          |
| (1,3123) | 1:59:A:ARG:HB2   | 1:59:A:ARG:HA    | 5        | 0.25          |
| (1,3123) | 1:59:A:ARG:HB2   | 1:59:A:ARG:HA    | 7        | 0.25          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3123) | 1:59:A:ARG:HB2   | 1:59:A:ARG:HA    | 11       | 0.25          |
| (1,3114) | 1:57:A:VAL:HG22  | 1:57:A:VAL:HG13  | 14       | 0.25          |
| (1,3113) | 1:57:A:VAL:HG13  | 1:61:A:ALA:H     | 10       | 0.25          |
| (1,3103) | 1:56:A:LEU:HD12  | 1:60:A:VAL:HB    | 7        | 0.25          |
| (1,3080) | 1:125:A:GLN:HB2  | 1:125:A:GLN:HA   | 3        | 0.25          |
| (1,3080) | 1:125:A:GLN:HB2  | 1:125:A:GLN:HA   | 9        | 0.25          |
| (1,3080) | 1:125:A:GLN:HB2  | 1:125:A:GLN:HA   | 14       | 0.25          |
| (1,3066) | 1:30:A:PHE:HB3   | 1:29:A:ALA:HB3   | 17       | 0.25          |
| (1,3061) | 1:31:A:LEU:HD11  | 1:28:A:ILE:HG22  | 5        | 0.25          |
| (1,3061) | 1:31:A:LEU:HD11  | 1:28:A:ILE:HG21  | 9        | 0.25          |
| (1,3045) | 1:52:A:ILE:HG13  | 1:54:A:GLN:HE21  | 16       | 0.25          |
| (1,3036) | 1:78:A:TYR:HH    | 1:45:A:ALA:HB2   | 6        | 0.25          |
| (1,3032) | 1:121:A:LYS:HG3  | 1:121:A:LYS:HE3  | 2        | 0.25          |
| (1,3032) | 1:121:A:LYS:HG3  | 1:121:A:LYS:HE3  | 8        | 0.25          |
| (1,3032) | 1:121:A:LYS:HG3  | 1:121:A:LYS:HE3  | 14       | 0.25          |
| (1,3028) | 1:71:A:LEU:HD12  | 1:72:A:ARG:HA    | 2        | 0.25          |
| (1,3028) | 1:71:A:LEU:HD13  | 1:72:A:ARG:HA    | 6        | 0.25          |
| (1,3025) | 1:21:A:LEU:HG    | 1:64:A:MET:HE1   | 4        | 0.25          |
| (1,3021) | 1:64:A:MET:HE2   | 1:63:A:GLU:H     | 6        | 0.25          |
| (1,2992) | 1:20:A:LYS:HB3   | 1:20:A:LYS:H     | 7        | 0.25          |
| (1,2992) | 1:20:A:LYS:HB3   | 1:20:A:LYS:H     | 16       | 0.25          |
| (1,2989) | 1:42:A:GLU:HA    | 1:42:A:GLU:HB2   | 3        | 0.25          |
| (1,2989) | 1:42:A:GLU:HA    | 1:42:A:GLU:HB2   | 4        | 0.25          |
| (1,2989) | 1:42:A:GLU:HA    | 1:42:A:GLU:HB2   | 5        | 0.25          |
| (1,2989) | 1:42:A:GLU:HA    | 1:42:A:GLU:HB2   | 8        | 0.25          |
| (1,2989) | 1:42:A:GLU:HA    | 1:42:A:GLU:HB2   | 11       | 0.25          |
| (1,2960) | 1:77:A:LEU:HD13  | 1:25:A:LYS:HA    | 1        | 0.25          |
| (1,2960) | 1:77:A:LEU:HD13  | 1:25:A:LYS:HA    | 2        | 0.25          |
| (1,2955) | 1:74:A:ALA:HB2   | 1:75:A:LEU:HD11  | 6        | 0.25          |
| (1,2955) | 1:74:A:ALA:HB3   | 1:75:A:LEU:HD11  | 14       | 0.25          |
| (1,2950) | 1:75:A:LEU:HD11  | 1:75:A:LEU:H     | 9        | 0.25          |
| (1,2945) | 1:110:A:VAL:HB   | 1:110:A:VAL:HG13 | 2        | 0.25          |
| (1,2945) | 1:110:A:VAL:HB   | 1:110:A:VAL:HG11 | 6        | 0.25          |
| (1,2945) | 1:110:A:VAL:HB   | 1:110:A:VAL:HG12 | 10       | 0.25          |
| (1,2945) | 1:110:A:VAL:HB   | 1:110:A:VAL:HG13 | 16       | 0.25          |
| (1,2945) | 1:110:A:VAL:HB   | 1:110:A:VAL:HG11 | 17       | 0.25          |
| (1,2930) | 1:31:A:LEU:HD21  | 1:60:A:VAL:HG11  | 16       | 0.25          |
| (1,2909) | 1:110:A:VAL:HG13 | 1:91:A:GLY:HA2   | 5        | 0.25          |
| (1,2909) | 1:110:A:VAL:HG12 | 1:91:A:GLY:HA2   | 6        | 0.25          |
| (1,2909) | 1:110:A:VAL:HG13 | 1:91:A:GLY:HA2   | 14       | 0.25          |
| (1,2891) | 1:32:A:ALA:HB3   | 1:28:A:ILE:HG22  | 1        | 0.25          |
| (1,2891) | 1:32:A:ALA:HB1   | 1:28:A:ILE:HG23  | 6        | 0.25          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2891) | 1:32:A:ALA:HB2   | 1:28:A:ILE:HG22  | 11       | 0.25          |
| (1,2888) | 1:29:A:ALA:HA    | 1:32:A:ALA:HB2   | 15       | 0.25          |
| (1,2881) | 1:74:A:ALA:HB3   | 1:31:A:LEU:HD12  | 9        | 0.25          |
| (1,2877) | 1:61:A:ALA:HB2   | 1:61:A:ALA:HA    | 11       | 0.25          |
| (1,2852) | 1:81:A:SER:HB3   | 1:84:A:TYR:HD1   | 4        | 0.25          |
| (1,2832) | 1:97:A:LEU:HD21  | 1:97:A:LEU:H     | 10       | 0.25          |
| (1,2832) | 1:97:A:LEU:HD22  | 1:97:A:LEU:H     | 11       | 0.25          |
| (1,2832) | 1:97:A:LEU:HD21  | 1:97:A:LEU:H     | 17       | 0.25          |
| (1,2824) | 1:97:A:LEU:HD22  | 1:56:A:LEU:HA    | 2        | 0.25          |
| (1,2819) | 1:97:A:LEU:HD12  | 1:35:A:PHE:HE1   | 8        | 0.25          |
| (1,2769) | 1:43:A:GLY:HA2   | 1:42:A:GLU:HB2   | 14       | 0.25          |
| (1,2753) | 1:97:A:LEU:HD11  | 1:59:A:ARG:HD3   | 10       | 0.25          |
| (1,2745) | 1:34:A:ARG:HD3   | 1:34:A:ARG:HG3   | 2        | 0.25          |
| (1,2745) | 1:34:A:ARG:HD3   | 1:34:A:ARG:HG3   | 3        | 0.25          |
| (1,2729) | 1:17:A:ASN:HB3   | 1:17:A:ASN:HB2   | 1        | 0.25          |
| (1,2729) | 1:17:A:ASN:HB3   | 1:17:A:ASN:HB2   | 7        | 0.25          |
| (1,2720) | 1:86:A:TYR:HB3   | 1:117:A:LEU:HD11 | 7        | 0.25          |
| (1,2713) | 1:53:A:PHE:HB3   | 1:75:A:LEU:HD11  | 4        | 0.25          |
| (1,2713) | 1:53:A:PHE:HB3   | 1:75:A:LEU:HD12  | 11       | 0.25          |
| (1,2713) | 1:53:A:PHE:HB3   | 1:75:A:LEU:HD11  | 16       | 0.25          |
| (1,2679) | 1:53:A:PHE:HA    | 1:53:A:PHE:HE2   | 9        | 0.25          |
| (1,2679) | 1:53:A:PHE:HA    | 1:53:A:PHE:HE2   | 12       | 0.25          |
| (1,2679) | 1:53:A:PHE:HA    | 1:53:A:PHE:HE1   | 15       | 0.25          |
| (1,2675) | 1:85:A:LEU:HB2   | 1:86:A:TYR:HD2   | 5        | 0.25          |
| (1,2672) | 1:31:A:LEU:HD13  | 1:35:A:PHE:HD2   | 1        | 0.25          |
| (1,2662) | 1:97:A:LEU:HD12  | 1:57:A:VAL:H     | 4        | 0.25          |
| (1,2662) | 1:97:A:LEU:HD12  | 1:57:A:VAL:H     | 5        | 0.25          |
| (1,2622) | 1:71:A:LEU:HD13  | 1:57:A:VAL:H     | 16       | 0.25          |
| (1,2618) | 1:34:A:ARG:HG3   | 1:34:A:ARG:H     | 1        | 0.25          |
| (1,2618) | 1:34:A:ARG:HG3   | 1:34:A:ARG:H     | 2        | 0.25          |
| (1,2618) | 1:34:A:ARG:HG3   | 1:34:A:ARG:H     | 10       | 0.25          |
| (1,2618) | 1:34:A:ARG:HG3   | 1:34:A:ARG:H     | 13       | 0.25          |
| (1,2618) | 1:34:A:ARG:HG3   | 1:34:A:ARG:H     | 14       | 0.25          |
| (1,2598) | 1:27:A:VAL:HG21  | 1:27:A:VAL:HG13  | 6        | 0.25          |
| (1,2598) | 1:27:A:VAL:HG23  | 1:27:A:VAL:HG13  | 8        | 0.25          |
| (1,2596) | 1:74:A:ALA:HB1   | 1:27:A:VAL:HG13  | 1        | 0.25          |
| (1,2596) | 1:74:A:ALA:HB2   | 1:27:A:VAL:HG11  | 10       | 0.25          |
| (1,2596) | 1:74:A:ALA:HB3   | 1:27:A:VAL:HG12  | 15       | 0.25          |
| (1,2583) | 1:60:A:VAL:HG11  | 1:34:A:ARG:HG2   | 2        | 0.25          |
| (1,2583) | 1:60:A:VAL:HG11  | 1:34:A:ARG:HG2   | 6        | 0.25          |
| (1,2576) | 1:124:A:VAL:HG22 | 1:120:A:ALA:HA   | 4        | 0.25          |
| (1,2576) | 1:124:A:VAL:HG22 | 1:120:A:ALA:HA   | 7        | 0.25          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2576) | 1:124:A:VAL:HG21 | 1:120:A:ALA:HA   | 16       | 0.25          |
| (1,2560) | 1:86:A:TYR:HE1   | 1:86:A:TYR:HD1   | 2        | 0.25          |
| (1,2560) | 1:86:A:TYR:HE1   | 1:86:A:TYR:HD1   | 6        | 0.25          |
| (1,2560) | 1:86:A:TYR:HE1   | 1:86:A:TYR:HD1   | 11       | 0.25          |
| (1,2560) | 1:86:A:TYR:HE1   | 1:86:A:TYR:HD1   | 13       | 0.25          |
| (1,2560) | 1:86:A:TYR:HE2   | 1:86:A:TYR:HD2   | 16       | 0.25          |
| (1,2547) | 1:11:A:SER:HA    | 1:12:A:GLN:HG3   | 4        | 0.25          |
| (1,2547) | 1:11:A:SER:HA    | 1:12:A:GLN:HG3   | 8        | 0.25          |
| (1,2546) | 1:73:A:SER:HA    | 1:73:A:SER:HB3   | 15       | 0.25          |
| (1,2502) | 1:42:A:GLU:HA    | 1:43:A:GLY:H     | 6        | 0.25          |
| (1,2502) | 1:42:A:GLU:HA    | 1:43:A:GLY:H     | 14       | 0.25          |
| (1,2476) | 1:50:A:ILE:HD12  | 1:50:A:ILE:HB    | 17       | 0.25          |
| (1,2418) | 1:113:A:ALA:HB2  | 1:110:A:VAL:HG12 | 1        | 0.25          |
| (1,2415) | 1:45:A:ALA:HB3   | 1:84:A:TYR:HD2   | 1        | 0.25          |
| (1,2404) | 1:28:A:ILE:HD11  | 1:74:A:ALA:HA    | 2        | 0.25          |
| (1,2404) | 1:28:A:ILE:HD12  | 1:74:A:ALA:HA    | 4        | 0.25          |
| (1,2404) | 1:28:A:ILE:HD11  | 1:74:A:ALA:HA    | 9        | 0.25          |
| (1,2404) | 1:28:A:ILE:HD11  | 1:74:A:ALA:HA    | 12       | 0.25          |
| (1,2404) | 1:28:A:ILE:HD11  | 1:74:A:ALA:HA    | 15       | 0.25          |
| (1,2369) | 1:52:A:ILE:HD13  | 1:56:A:LEU:H     | 11       | 0.25          |
| (1,2358) | 1:107:A:GLU:HA   | 1:111:A:GLU:H    | 3        | 0.25          |
| (1,2358) | 1:107:A:GLU:HA   | 1:111:A:GLU:H    | 4        | 0.25          |
| (1,2358) | 1:107:A:GLU:HA   | 1:111:A:GLU:H    | 6        | 0.25          |
| (1,2358) | 1:107:A:GLU:HA   | 1:111:A:GLU:H    | 9        | 0.25          |
| (1,2358) | 1:107:A:GLU:HA   | 1:111:A:GLU:H    | 11       | 0.25          |
| (1,2358) | 1:107:A:GLU:HA   | 1:111:A:GLU:H    | 16       | 0.25          |
| (1,2346) | 1:105:A:LEU:HD11 | 1:107:A:GLU:HA   | 4        | 0.25          |
| (1,2346) | 1:105:A:LEU:HD11 | 1:107:A:GLU:HA   | 11       | 0.25          |
| (1,2341) | 1:66:A:LEU:HD22  | 1:70:A:GLN:H     | 2        | 0.25          |
| (1,2341) | 1:66:A:LEU:HD23  | 1:70:A:GLN:H     | 4        | 0.25          |
| (1,2341) | 1:66:A:LEU:HD23  | 1:70:A:GLN:H     | 7        | 0.25          |
| (1,2307) | 1:117:A:LEU:HD13 | 1:86:A:TYR:HB2   | 2        | 0.25          |
| (1,2307) | 1:117:A:LEU:HD12 | 1:86:A:TYR:HB2   | 5        | 0.25          |
| (1,2307) | 1:117:A:LEU:HD13 | 1:86:A:TYR:HB2   | 9        | 0.25          |
| (1,2307) | 1:117:A:LEU:HD11 | 1:86:A:TYR:HB2   | 10       | 0.25          |
| (1,2307) | 1:117:A:LEU:HD12 | 1:86:A:TYR:HB2   | 14       | 0.25          |
| (1,2221) | 1:31:A:LEU:HA    | 1:60:A:VAL:HB    | 5        | 0.25          |
| (1,2210) | 1:105:A:LEU:HG   | 1:110:A:VAL:HG11 | 5        | 0.25          |
| (1,2149) | 1:21:A:LEU:HD23  | 1:30:A:PHE:HD1   | 1        | 0.25          |
| (1,2149) | 1:21:A:LEU:HD23  | 1:30:A:PHE:HD1   | 5        | 0.25          |
| (1,1945) | 1:105:A:LEU:HB3  | 1:110:A:VAL:HG23 | 6        | 0.25          |
| (1,1904) | 1:74:A:ALA:HB1   | 1:28:A:ILE:HA    | 12       | 0.25          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1904) | 1:74:A:ALA:HB2  | 1:28:A:ILE:HA    | 13       | 0.25          |
| (1,1904) | 1:74:A:ALA:HB2  | 1:28:A:ILE:HA    | 14       | 0.25          |
| (1,1889) | 1:65:A:ASN:H    | 1:65:A:ASN:HB3   | 15       | 0.25          |
| (1,1872) | 1:56:A:LEU:HD23 | 1:55:A:ASP:HB3   | 10       | 0.25          |
| (1,1872) | 1:56:A:LEU:HD23 | 1:55:A:ASP:HB3   | 17       | 0.25          |
| (1,1865) | 1:45:A:ALA:HB2  | 1:44:A:GLU:HB3   | 8        | 0.25          |
| (1,1865) | 1:45:A:ALA:HB1  | 1:44:A:GLU:HB3   | 11       | 0.25          |
| (1,1826) | 1:64:A:MET:HE2  | 1:21:A:LEU:HD13  | 7        | 0.25          |
| (1,1817) | 1:77:A:LEU:HG   | 1:77:A:LEU:HD23  | 9        | 0.25          |
| (1,1817) | 1:77:A:LEU:HG   | 1:77:A:LEU:HD23  | 11       | 0.25          |
| (1,1817) | 1:77:A:LEU:HG   | 1:77:A:LEU:HD23  | 12       | 0.25          |
| (1,1812) | 1:117:A:LEU:HA  | 1:117:A:LEU:HD13 | 7        | 0.25          |
| (1,1812) | 1:117:A:LEU:HA  | 1:117:A:LEU:HD13 | 15       | 0.25          |
| (1,1799) | 1:71:A:LEU:HA   | 1:74:A:ALA:HB3   | 9        | 0.25          |
| (1,1752) | 1:41:A:ALA:HB2  | 1:28:A:ILE:HG22  | 1        | 0.25          |
| (1,1752) | 1:41:A:ALA:HB2  | 1:28:A:ILE:HG23  | 13       | 0.25          |
| (1,1752) | 1:41:A:ALA:HB2  | 1:28:A:ILE:HG23  | 16       | 0.25          |
| (1,1746) | 1:71:A:LEU:HD21 | 1:74:A:ALA:H     | 5        | 0.25          |
| (1,1746) | 1:71:A:LEU:HD23 | 1:74:A:ALA:H     | 9        | 0.25          |
| (1,1746) | 1:71:A:LEU:HD21 | 1:74:A:ALA:H     | 15       | 0.25          |
| (1,1741) | 1:55:A:ASP:HB2  | 1:56:A:LEU:HD21  | 8        | 0.25          |
| (1,1741) | 1:55:A:ASP:HB2  | 1:56:A:LEU:HD21  | 15       | 0.25          |
| (1,1741) | 1:55:A:ASP:HB2  | 1:56:A:LEU:HD23  | 17       | 0.25          |
| (1,1737) | 1:77:A:LEU:HG   | 1:77:A:LEU:HD11  | 8        | 0.25          |
| (1,1736) | 1:77:A:LEU:HB3  | 1:77:A:LEU:HD12  | 9        | 0.25          |
| (1,1736) | 1:77:A:LEU:HB3  | 1:77:A:LEU:HD12  | 10       | 0.25          |
| (1,1736) | 1:77:A:LEU:HB3  | 1:77:A:LEU:HD12  | 17       | 0.25          |
| (1,1730) | 1:27:A:VAL:HA   | 1:66:A:LEU:HD21  | 4        | 0.25          |
| (1,1730) | 1:27:A:VAL:HA   | 1:66:A:LEU:HD21  | 7        | 0.25          |
| (1,1730) | 1:27:A:VAL:HA   | 1:66:A:LEU:HD22  | 9        | 0.25          |
| (1,1730) | 1:27:A:VAL:HA   | 1:66:A:LEU:HD21  | 11       | 0.25          |
| (1,1730) | 1:27:A:VAL:HA   | 1:66:A:LEU:HD23  | 14       | 0.25          |
| (1,1730) | 1:27:A:VAL:HA   | 1:66:A:LEU:HD22  | 17       | 0.25          |
| (1,1723) | 1:68:A:LYS:HD3  | 1:57:A:VAL:HG12  | 14       | 0.25          |
| (1,1686) | 1:85:A:LEU:HD11 | 1:85:A:LEU:HD22  | 15       | 0.25          |
| (1,1683) | 1:48:A:LEU:HD12 | 1:38:A:CYS:HA    | 1        | 0.25          |
| (1,1683) | 1:48:A:LEU:HD13 | 1:38:A:CYS:HA    | 9        | 0.25          |
| (1,1618) | 1:109:A:HIS:HB2 | 1:110:A:VAL:HG12 | 2        | 0.25          |
| (1,1618) | 1:109:A:HIS:HB2 | 1:110:A:VAL:HG13 | 3        | 0.25          |
| (1,1618) | 1:109:A:HIS:HB2 | 1:110:A:VAL:HG13 | 4        | 0.25          |
| (1,1618) | 1:109:A:HIS:HB2 | 1:110:A:VAL:HG11 | 7        | 0.25          |
| (1,1618) | 1:109:A:HIS:HB2 | 1:110:A:VAL:HG12 | 8        | 0.25          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1618) | 1:109:A:HIS:HB2  | 1:110:A:VAL:HG13 | 13       | 0.25          |
| (1,1618) | 1:109:A:HIS:HB2  | 1:110:A:VAL:HG12 | 15       | 0.25          |
| (1,1618) | 1:109:A:HIS:HB2  | 1:110:A:VAL:HG13 | 17       | 0.25          |
| (1,1613) | 1:124:A:VAL:HG22 | 1:121:A:LYS:HA   | 7        | 0.25          |
| (1,1613) | 1:124:A:VAL:HG21 | 1:121:A:LYS:HA   | 8        | 0.25          |
| (1,1592) | 1:126:A:ALA:HB3  | 1:125:A:GLN:HG3  | 8        | 0.25          |
| (1,1592) | 1:126:A:ALA:HB3  | 1:125:A:GLN:HG3  | 9        | 0.25          |
| (1,1553) | 1:57:A:VAL:HG11  | 1:61:A:ALA:H     | 7        | 0.25          |
| (1,1552) | 1:124:A:VAL:HG12 | 1:124:A:VAL:HB   | 8        | 0.25          |
| (1,1521) | 1:30:A:PHE:HB3   | 1:29:A:ALA:HB1   | 1        | 0.25          |
| (1,1513) | 1:52:A:ILE:HG22  | 1:53:A:PHE:HB3   | 12       | 0.25          |
| (1,1428) | 1:93:A:THR:HG21  | 1:101:A:PRO:HB3  | 5        | 0.25          |
| (1,1428) | 1:93:A:THR:HG22  | 1:101:A:PRO:HB3  | 12       | 0.25          |
| (1,1419) | 1:77:A:LEU:HD13  | 1:25:A:LYS:HA    | 15       | 0.25          |
| (1,1403) | 1:95:A:VAL:HG23  | 1:95:A:VAL:HG13  | 10       | 0.25          |
| (1,1399) | 1:95:A:VAL:HG21  | 1:95:A:VAL:H     | 1        | 0.25          |
| (1,1395) | 1:31:A:LEU:HD21  | 1:39:A:PHE:HD2   | 1        | 0.25          |
| (1,1395) | 1:31:A:LEU:HD22  | 1:39:A:PHE:HD1   | 5        | 0.25          |
| (1,1395) | 1:31:A:LEU:HD23  | 1:39:A:PHE:HD2   | 9        | 0.25          |
| (1,1371) | 1:28:A:ILE:HD11  | 1:75:A:LEU:H     | 1        | 0.25          |
| (1,1363) | 1:29:A:ALA:HA    | 1:32:A:ALA:HB3   | 5        | 0.25          |
| (1,1337) | 1:78:A:TYR:HD2   | 1:28:A:ILE:HD12  | 6        | 0.25          |
| (1,1337) | 1:78:A:TYR:HD1   | 1:28:A:ILE:HD11  | 12       | 0.25          |
| (1,1331) | 1:78:A:TYR:HE2   | 1:84:A:TYR:HD1   | 5        | 0.25          |
| (1,1307) | 1:97:A:LEU:HD21  | 1:97:A:LEU:HB2   | 1        | 0.25          |
| (1,1303) | 1:97:A:LEU:HD12  | 1:35:A:PHE:HE2   | 9        | 0.25          |
| (1,1232) | 1:60:A:VAL:HG13  | 1:59:A:ARG:HD3   | 15       | 0.25          |
| (1,1210) | 1:86:A:TYR:HB3   | 1:86:A:TYR:H     | 8        | 0.25          |
| (1,1210) | 1:86:A:TYR:HB3   | 1:86:A:TYR:H     | 9        | 0.25          |
| (1,1210) | 1:86:A:TYR:HB3   | 1:86:A:TYR:H     | 14       | 0.25          |
| (1,1210) | 1:86:A:TYR:HB3   | 1:86:A:TYR:H     | 16       | 0.25          |
| (1,1082) | 1:71:A:LEU:HD13  | 1:72:A:ARG:H     | 1        | 0.25          |
| (1,1081) | 1:71:A:LEU:HD12  | 1:57:A:VAL:H     | 1        | 0.25          |
| (1,1081) | 1:71:A:LEU:HD13  | 1:57:A:VAL:H     | 12       | 0.25          |
| (1,1030) | 1:86:A:TYR:HE1   | 1:86:A:TYR:HB2   | 6        | 0.25          |
| (1,1030) | 1:86:A:TYR:HE1   | 1:86:A:TYR:HB2   | 10       | 0.25          |
| (1,895)  | 1:129:A:ALA:HB1  | 1:129:A:ALA:HA   | 15       | 0.25          |
| (1,895)  | 1:129:A:ALA:HB3  | 1:129:A:ALA:HA   | 16       | 0.25          |
| (1,894)  | 1:133:A:ALA:HA   | 1:133:A:ALA:HB2  | 7        | 0.25          |
| (1,894)  | 1:133:A:ALA:HA   | 1:133:A:ALA:HB3  | 9        | 0.25          |
| (1,894)  | 1:133:A:ALA:HA   | 1:133:A:ALA:HB3  | 12       | 0.25          |
| (1,894)  | 1:133:A:ALA:HA   | 1:133:A:ALA:HB3  | 14       | 0.25          |

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| Key     | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,838) | 1:64:A:MET:HE1  | 1:30:A:PHE:HD2   | 12       | 0.25          |
| (1,829) | 1:41:A:ALA:HB2  | 1:41:A:ALA:H     | 13       | 0.25          |
| (1,822) | 1:49:A:LYS:H    | 1:52:A:ILE:HD11  | 1        | 0.25          |
| (1,822) | 1:49:A:LYS:H    | 1:52:A:ILE:HD11  | 12       | 0.25          |
| (1,819) | 1:28:A:ILE:HD12 | 1:74:A:ALA:HA    | 3        | 0.25          |
| (1,819) | 1:28:A:ILE:HD13 | 1:74:A:ALA:HA    | 8        | 0.25          |
| (1,819) | 1:28:A:ILE:HD13 | 1:74:A:ALA:HA    | 13       | 0.25          |
| (1,753) | 1:92:A:ALA:HB2  | 1:91:A:GLY:H     | 2        | 0.25          |
| (1,753) | 1:92:A:ALA:HB1  | 1:91:A:GLY:H     | 9        | 0.25          |
| (1,691) | 1:75:A:LEU:HD22 | 1:54:A:GLN:H     | 4        | 0.25          |
| (1,691) | 1:75:A:LEU:HD22 | 1:54:A:GLN:H     | 7        | 0.25          |
| (1,691) | 1:75:A:LEU:HD21 | 1:54:A:GLN:H     | 16       | 0.25          |
| (1,610) | 1:48:A:LEU:HD23 | 1:49:A:LYS:H     | 2        | 0.25          |
| (1,610) | 1:48:A:LEU:HD23 | 1:49:A:LYS:H     | 17       | 0.25          |
| (1,580) | 1:98:A:ASP:HB2  | 1:100:A:ASN:HD21 | 1        | 0.25          |
| (1,580) | 1:98:A:ASP:HB2  | 1:100:A:ASN:HD21 | 3        | 0.25          |
| (1,580) | 1:98:A:ASP:HB2  | 1:100:A:ASN:HD21 | 4        | 0.25          |
| (1,580) | 1:98:A:ASP:HB2  | 1:100:A:ASN:HD21 | 6        | 0.25          |
| (1,580) | 1:98:A:ASP:HB2  | 1:100:A:ASN:HD21 | 9        | 0.25          |
| (1,552) | 1:65:A:ASN:H    | 1:65:A:ASN:HD21  | 3        | 0.25          |
| (1,552) | 1:65:A:ASN:H    | 1:65:A:ASN:HD21  | 5        | 0.25          |
| (1,552) | 1:65:A:ASN:H    | 1:65:A:ASN:HD21  | 6        | 0.25          |
| (1,527) | 1:65:A:ASN:HB3  | 1:65:A:ASN:HD21  | 4        | 0.25          |
| (1,441) | 1:42:A:GLU:HB3  | 1:41:A:ALA:H     | 1        | 0.25          |
| (1,441) | 1:42:A:GLU:HB3  | 1:41:A:ALA:H     | 13       | 0.25          |
| (1,410) | 1:53:A:PHE:H    | 1:56:A:LEU:HB3   | 12       | 0.25          |
| (1,300) | 1:100:A:ASN:HB3 | 1:100:A:ASN:HD21 | 1        | 0.25          |
| (1,300) | 1:100:A:ASN:HB3 | 1:100:A:ASN:HD21 | 7        | 0.25          |
| (1,300) | 1:100:A:ASN:HB3 | 1:100:A:ASN:HD21 | 10       | 0.25          |
| (1,300) | 1:100:A:ASN:HB3 | 1:100:A:ASN:HD21 | 12       | 0.25          |
| (1,241) | 1:95:A:VAL:HG13 | 1:96:A:ASP:H     | 17       | 0.25          |
| (1,234) | 1:95:A:VAL:HG21 | 1:99:A:GLY:H     | 5        | 0.25          |
| (1,156) | 1:126:A:ALA:HB3 | 1:126:A:ALA:H    | 13       | 0.25          |
| (1,154) | 1:130:A:GLU:H   | 1:129:A:ALA:HB3  | 3        | 0.25          |
| (1,154) | 1:130:A:GLU:H   | 1:129:A:ALA:HB1  | 5        | 0.25          |
| (1,154) | 1:130:A:GLU:H   | 1:129:A:ALA:HB2  | 7        | 0.25          |
| (1,154) | 1:130:A:GLU:H   | 1:129:A:ALA:HB1  | 11       | 0.25          |
| (1,128) | 1:35:A:PHE:HD1  | 1:39:A:PHE:H     | 11       | 0.25          |
| (1,125) | 1:28:A:ILE:HG13 | 1:28:A:ILE:H     | 3        | 0.25          |
| (1,125) | 1:28:A:ILE:HG13 | 1:28:A:ILE:H     | 10       | 0.25          |
| (1,125) | 1:28:A:ILE:HG13 | 1:28:A:ILE:H     | 15       | 0.25          |
| (1,117) | 1:27:A:VAL:HG13 | 1:26:A:GLU:H     | 6        | 0.25          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,12)   | 1:100:A:ASN:H   | 1:100:A:ASN:HD21 | 8        | 0.25          |
| (1,12)   | 1:100:A:ASN:H   | 1:100:A:ASN:HD21 | 13       | 0.25          |
| (3,152)  | 1:27:A:VAL:H    | 1:74:A:ALA:HB3   | 6        | 0.24          |
| (3,129)  | 1:71:A:LEU:HD11 | 1:60:A:VAL:HB    | 2        | 0.24          |
| (3,129)  | 1:71:A:LEU:HD13 | 1:60:A:VAL:HB    | 10       | 0.24          |
| (3,109)  | 1:92:A:ALA:H    | 1:110:A:VAL:HB   | 3        | 0.24          |
| (3,109)  | 1:92:A:ALA:H    | 1:110:A:VAL:HB   | 4        | 0.24          |
| (3,106)  | 1:68:A:LYS:HD2  | 1:68:A:LYS:HA    | 2        | 0.24          |
| (3,95)   | 1:75:A:LEU:HD11 | 1:50:A:ILE:H     | 8        | 0.24          |
| (3,93)   | 1:21:A:LEU:HB3  | 1:21:A:LEU:HD13  | 4        | 0.24          |
| (3,83)   | 1:114:A:ARG:HB2 | 1:113:A:ALA:HB1  | 6        | 0.24          |
| (3,64)   | 1:55:A:ASP:HB2  | 1:52:A:ILE:HG22  | 16       | 0.24          |
| (3,34)   | 1:97:A:LEU:HD23 | 1:31:A:LEU:HD13  | 10       | 0.24          |
| (3,34)   | 1:97:A:LEU:HD23 | 1:31:A:LEU:HD11  | 17       | 0.24          |
| (3,31)   | 1:22:A:ASN:HD21 | 1:22:A:ASN:HB2   | 15       | 0.24          |
| (3,29)   | 1:48:A:LEU:HD21 | 1:39:A:PHE:HD2   | 13       | 0.24          |
| (3,16)   | 1:90:A:PRO:HA   | 1:110:A:VAL:HG13 | 8        | 0.24          |
| (3,16)   | 1:90:A:PRO:HA   | 1:110:A:VAL:HG12 | 10       | 0.24          |
| (3,16)   | 1:90:A:PRO:HA   | 1:110:A:VAL:HG13 | 16       | 0.24          |
| (3,15)   | 1:85:A:LEU:HB3  | 1:82:A:TRP:HA    | 11       | 0.24          |
| (3,14)   | 1:82:A:TRP:HA   | 1:85:A:LEU:HB2   | 2        | 0.24          |
| (3,14)   | 1:82:A:TRP:HA   | 1:85:A:LEU:HB2   | 6        | 0.24          |
| (3,14)   | 1:82:A:TRP:HA   | 1:85:A:LEU:HB2   | 13       | 0.24          |
| (3,14)   | 1:82:A:TRP:HA   | 1:85:A:LEU:HB2   | 16       | 0.24          |
| (3,14)   | 1:82:A:TRP:HA   | 1:85:A:LEU:HB2   | 17       | 0.24          |
| (1,4310) | 1:64:A:MET:HA   | 1:65:A:ASN:H     | 7        | 0.24          |
| (1,4310) | 1:64:A:MET:HA   | 1:65:A:ASN:H     | 9        | 0.24          |
| (1,4310) | 1:64:A:MET:HA   | 1:65:A:ASN:H     | 12       | 0.24          |
| (1,4299) | 1:65:A:ASN:HD22 | 1:65:A:ASN:HD21  | 12       | 0.24          |
| (1,4197) | 1:66:A:LEU:HD23 | 1:67:A:SER:H     | 15       | 0.24          |
| (1,4172) | 1:105:A:LEU:H   | 1:92:A:ALA:H     | 2        | 0.24          |
| (1,4172) | 1:105:A:LEU:H   | 1:92:A:ALA:H     | 6        | 0.24          |
| (1,4172) | 1:105:A:LEU:H   | 1:92:A:ALA:H     | 8        | 0.24          |
| (1,4172) | 1:105:A:LEU:H   | 1:92:A:ALA:H     | 9        | 0.24          |
| (1,4172) | 1:105:A:LEU:H   | 1:92:A:ALA:H     | 11       | 0.24          |
| (1,4172) | 1:105:A:LEU:H   | 1:92:A:ALA:H     | 12       | 0.24          |
| (1,4172) | 1:105:A:LEU:H   | 1:92:A:ALA:H     | 15       | 0.24          |
| (1,4172) | 1:105:A:LEU:H   | 1:92:A:ALA:H     | 16       | 0.24          |
| (1,4172) | 1:105:A:LEU:H   | 1:92:A:ALA:H     | 17       | 0.24          |
| (1,4153) | 1:18:A:GLN:HB3  | 1:18:A:GLN:H     | 1        | 0.24          |
| (1,4150) | 1:17:A:ASN:HB3  | 1:18:A:GLN:H     | 14       | 0.24          |
| (1,4141) | 1:98:A:ASP:HB2  | 1:100:A:ASN:HD21 | 2        | 0.24          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,4141) | 1:98:A:ASP:HB2  | 1:100:A:ASN:HD21 | 12       | 0.24          |
| (1,4141) | 1:98:A:ASP:HB2  | 1:100:A:ASN:HD21 | 13       | 0.24          |
| (1,4113) | 1:22:A:ASN:H    | 1:22:A:ASN:HD22  | 9        | 0.24          |
| (1,4069) | 1:13:A:ASP:HB2  | 1:13:A:ASP:H     | 6        | 0.24          |
| (1,4037) | 1:27:A:VAL:HG22 | 1:29:A:ALA:H     | 4        | 0.24          |
| (1,4037) | 1:27:A:VAL:HG23 | 1:29:A:ALA:H     | 16       | 0.24          |
| (1,4036) | 1:31:A:LEU:H    | 1:31:A:LEU:HD13  | 7        | 0.24          |
| (1,4006) | 1:42:A:GLU:HB3  | 1:41:A:ALA:H     | 7        | 0.24          |
| (1,3961) | 1:57:A:VAL:H    | 1:56:A:LEU:HB3   | 10       | 0.24          |
| (1,3941) | 1:63:A:GLU:H    | 1:61:A:ALA:HB3   | 12       | 0.24          |
| (1,3898) | 1:79:A:THR:HG21 | 1:80:A:SER:H     | 17       | 0.24          |
| (1,3874) | 1:85:A:LEU:HB3  | 1:86:A:TYR:H     | 7        | 0.24          |
| (1,3874) | 1:85:A:LEU:HB3  | 1:86:A:TYR:H     | 10       | 0.24          |
| (1,3874) | 1:85:A:LEU:HB3  | 1:86:A:TYR:H     | 11       | 0.24          |
| (1,3874) | 1:85:A:LEU:HB3  | 1:86:A:TYR:H     | 16       | 0.24          |
| (1,3845) | 1:95:A:VAL:HG13 | 1:96:A:ASP:H     | 5        | 0.24          |
| (1,3816) | 1:105:A:LEU:H   | 1:105:A:LEU:HD23 | 2        | 0.24          |
| (1,3816) | 1:105:A:LEU:H   | 1:105:A:LEU:HD23 | 6        | 0.24          |
| (1,3816) | 1:105:A:LEU:H   | 1:105:A:LEU:HD22 | 7        | 0.24          |
| (1,3816) | 1:105:A:LEU:H   | 1:105:A:LEU:HD23 | 9        | 0.24          |
| (1,3776) | 1:121:A:LYS:HA  | 1:122:A:ALA:H    | 12       | 0.24          |
| (1,3776) | 1:121:A:LYS:HA  | 1:122:A:ALA:H    | 14       | 0.24          |
| (1,3776) | 1:121:A:LYS:HA  | 1:122:A:ALA:H    | 16       | 0.24          |
| (1,3776) | 1:121:A:LYS:HA  | 1:122:A:ALA:H    | 17       | 0.24          |
| (1,3775) | 1:124:A:VAL:HA  | 1:125:A:GLN:H    | 8        | 0.24          |
| (1,3773) | 1:123:A:ARG:HA  | 1:124:A:VAL:H    | 1        | 0.24          |
| (1,3773) | 1:123:A:ARG:HA  | 1:124:A:VAL:H    | 11       | 0.24          |
| (1,3773) | 1:123:A:ARG:HA  | 1:124:A:VAL:H    | 15       | 0.24          |
| (1,3768) | 1:130:A:GLU:H   | 1:130:A:GLU:HA   | 4        | 0.24          |
| (1,3744) | 1:35:A:PHE:HD1  | 1:39:A:PHE:H     | 13       | 0.24          |
| (1,3716) | 1:35:A:PHE:HE2  | 1:35:A:PHE:H     | 3        | 0.24          |
| (1,3716) | 1:35:A:PHE:HE1  | 1:35:A:PHE:H     | 6        | 0.24          |
| (1,3716) | 1:35:A:PHE:HE1  | 1:35:A:PHE:H     | 11       | 0.24          |
| (1,3716) | 1:35:A:PHE:HE2  | 1:35:A:PHE:H     | 15       | 0.24          |
| (1,3662) | 1:83:A:ARG:H    | 1:82:A:TRP:HD1   | 2        | 0.24          |
| (1,3662) | 1:83:A:ARG:H    | 1:82:A:TRP:HD1   | 10       | 0.24          |
| (1,3662) | 1:83:A:ARG:H    | 1:82:A:TRP:HD1   | 12       | 0.24          |
| (1,3599) | 1:92:A:ALA:HB3  | 1:113:A:ALA:HB1  | 7        | 0.24          |
| (1,3599) | 1:92:A:ALA:HB1  | 1:113:A:ALA:HB1  | 9        | 0.24          |
| (1,3592) | 1:109:A:HIS:HB2 | 1:110:A:VAL:HG12 | 2        | 0.24          |
| (1,3592) | 1:109:A:HIS:HB2 | 1:110:A:VAL:HG13 | 3        | 0.24          |
| (1,3592) | 1:109:A:HIS:HB2 | 1:110:A:VAL:HG11 | 7        | 0.24          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3592) | 1:109:A:HIS:HB2 | 1:110:A:VAL:HG12 | 8        | 0.24          |
| (1,3592) | 1:109:A:HIS:HB2 | 1:110:A:VAL:HG11 | 9        | 0.24          |
| (1,3592) | 1:109:A:HIS:HB2 | 1:110:A:VAL:HG12 | 11       | 0.24          |
| (1,3592) | 1:109:A:HIS:HB2 | 1:110:A:VAL:HG13 | 13       | 0.24          |
| (1,3592) | 1:109:A:HIS:HB2 | 1:110:A:VAL:HG12 | 16       | 0.24          |
| (1,3592) | 1:109:A:HIS:HB2 | 1:110:A:VAL:HG13 | 17       | 0.24          |
| (1,3591) | 1:93:A:THR:HB   | 1:88:A:VAL:HG13  | 11       | 0.24          |
| (1,3591) | 1:93:A:THR:HB   | 1:88:A:VAL:HG12  | 17       | 0.24          |
| (1,3588) | 1:105:A:LEU:HB3 | 1:110:A:VAL:HG23 | 8        | 0.24          |
| (1,3583) | 1:112:A:HIS:H   | 1:109:A:HIS:HA   | 12       | 0.24          |
| (1,3583) | 1:112:A:HIS:H   | 1:109:A:HIS:HA   | 17       | 0.24          |
| (1,3580) | 1:111:A:GLU:HB2 | 1:109:A:HIS:HA   | 1        | 0.24          |
| (1,3580) | 1:111:A:GLU:HB2 | 1:109:A:HIS:HA   | 11       | 0.24          |
| (1,3580) | 1:111:A:GLU:HB2 | 1:109:A:HIS:HA   | 12       | 0.24          |
| (1,3536) | 1:66:A:LEU:HB3  | 1:62:A:GLY:HA3   | 10       | 0.24          |
| (1,3536) | 1:66:A:LEU:HB3  | 1:62:A:GLY:HA3   | 12       | 0.24          |
| (1,3536) | 1:66:A:LEU:HB3  | 1:62:A:GLY:HA3   | 13       | 0.24          |
| (1,3536) | 1:66:A:LEU:HB3  | 1:62:A:GLY:HA3   | 14       | 0.24          |
| (1,3534) | 1:122:A:ALA:HB2 | 1:121:A:LYS:HE3  | 9        | 0.24          |
| (1,3534) | 1:122:A:ALA:HB1 | 1:121:A:LYS:HE3  | 14       | 0.24          |
| (1,3531) | 1:65:A:ASN:H    | 1:65:A:ASN:HA    | 15       | 0.24          |
| (1,3511) | 1:50:A:ILE:HG13 | 1:49:A:LYS:HA    | 17       | 0.24          |
| (1,3508) | 1:113:A:ALA:HB3 | 1:88:A:VAL:HA    | 17       | 0.24          |
| (1,3503) | 1:27:A:VAL:HG22 | 1:31:A:LEU:H     | 1        | 0.24          |
| (1,3503) | 1:27:A:VAL:HG23 | 1:31:A:LEU:H     | 2        | 0.24          |
| (1,3503) | 1:27:A:VAL:HG22 | 1:31:A:LEU:H     | 4        | 0.24          |
| (1,3503) | 1:27:A:VAL:HG23 | 1:31:A:LEU:H     | 6        | 0.24          |
| (1,3503) | 1:27:A:VAL:HG23 | 1:31:A:LEU:H     | 10       | 0.24          |
| (1,3503) | 1:27:A:VAL:HG22 | 1:31:A:LEU:H     | 16       | 0.24          |
| (1,3501) | 1:27:A:VAL:HG22 | 1:28:A:ILE:HA    | 4        | 0.24          |
| (1,3501) | 1:27:A:VAL:HG23 | 1:28:A:ILE:HA    | 6        | 0.24          |
| (1,3501) | 1:27:A:VAL:HG23 | 1:28:A:ILE:HA    | 7        | 0.24          |
| (1,3498) | 1:70:A:GLN:HE21 | 1:27:A:VAL:HG13  | 13       | 0.24          |
| (1,3492) | 1:105:A:LEU:HB3 | 1:105:A:LEU:HD12 | 3        | 0.24          |
| (1,3492) | 1:105:A:LEU:HB3 | 1:105:A:LEU:HD12 | 4        | 0.24          |
| (1,3492) | 1:105:A:LEU:HB3 | 1:105:A:LEU:HD13 | 8        | 0.24          |
| (1,3492) | 1:105:A:LEU:HB3 | 1:105:A:LEU:HD11 | 12       | 0.24          |
| (1,3492) | 1:105:A:LEU:HB3 | 1:105:A:LEU:HD13 | 13       | 0.24          |
| (1,3481) | 1:83:A:ARG:HD3  | 1:45:A:ALA:HB1   | 13       | 0.24          |
| (1,3479) | 1:45:A:ALA:HB1  | 1:44:A:GLU:HB3   | 13       | 0.24          |
| (1,3476) | 1:107:A:GLU:HG2 | 1:108:A:GLN:H    | 6        | 0.24          |
| (1,3476) | 1:107:A:GLU:HG2 | 1:108:A:GLN:H    | 14       | 0.24          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3465) | 1:88:A:VAL:HG22  | 1:85:A:LEU:HB3   | 9        | 0.24          |
| (1,3465) | 1:88:A:VAL:HG22  | 1:85:A:LEU:HB3   | 13       | 0.24          |
| (1,3437) | 1:21:A:LEU:HB2   | 1:21:A:LEU:HD11  | 10       | 0.24          |
| (1,3430) | 1:45:A:ALA:HB1   | 1:84:A:TYR:HA    | 8        | 0.24          |
| (1,3417) | 1:117:A:LEU:HG   | 1:117:A:LEU:HD11 | 11       | 0.24          |
| (1,3417) | 1:117:A:LEU:HG   | 1:117:A:LEU:HD12 | 16       | 0.24          |
| (1,3412) | 1:82:A:TRP:HZ3   | 1:117:A:LEU:HD11 | 14       | 0.24          |
| (1,3401) | 1:86:A:TYR:HE2   | 1:86:A:TYR:HA    | 1        | 0.24          |
| (1,3401) | 1:86:A:TYR:HE1   | 1:86:A:TYR:HA    | 2        | 0.24          |
| (1,3395) | 1:33:A:GLU:HB3   | 1:33:A:GLU:HA    | 5        | 0.24          |
| (1,3358) | 1:28:A:ILE:HB    | 1:29:A:ALA:HA    | 7        | 0.24          |
| (1,3358) | 1:28:A:ILE:HB    | 1:29:A:ALA:HA    | 8        | 0.24          |
| (1,3358) | 1:28:A:ILE:HB    | 1:29:A:ALA:HA    | 10       | 0.24          |
| (1,3358) | 1:28:A:ILE:HB    | 1:29:A:ALA:HA    | 15       | 0.24          |
| (1,3358) | 1:28:A:ILE:HB    | 1:29:A:ALA:HA    | 17       | 0.24          |
| (1,3345) | 1:29:A:ALA:HA    | 1:29:A:ALA:HB3   | 7        | 0.24          |
| (1,3345) | 1:29:A:ALA:HA    | 1:29:A:ALA:HB1   | 9        | 0.24          |
| (1,3342) | 1:92:A:ALA:HB2   | 1:88:A:VAL:H     | 1        | 0.24          |
| (1,3341) | 1:41:A:ALA:HB2   | 1:28:A:ILE:HG23  | 6        | 0.24          |
| (1,3341) | 1:41:A:ALA:HB1   | 1:28:A:ILE:HG21  | 7        | 0.24          |
| (1,3341) | 1:41:A:ALA:HB2   | 1:28:A:ILE:HG22  | 9        | 0.24          |
| (1,3341) | 1:41:A:ALA:HB2   | 1:28:A:ILE:HG22  | 14       | 0.24          |
| (1,3341) | 1:41:A:ALA:HB2   | 1:28:A:ILE:HG23  | 15       | 0.24          |
| (1,3336) | 1:71:A:LEU:HD22  | 1:74:A:ALA:H     | 2        | 0.24          |
| (1,3336) | 1:71:A:LEU:HD22  | 1:74:A:ALA:H     | 12       | 0.24          |
| (1,3336) | 1:71:A:LEU:HD21  | 1:74:A:ALA:H     | 14       | 0.24          |
| (1,3326) | 1:77:A:LEU:HG    | 1:77:A:LEU:HD12  | 3        | 0.24          |
| (1,3326) | 1:77:A:LEU:HG    | 1:77:A:LEU:HD11  | 10       | 0.24          |
| (1,3326) | 1:77:A:LEU:HG    | 1:77:A:LEU:HD11  | 14       | 0.24          |
| (1,3326) | 1:77:A:LEU:HG    | 1:77:A:LEU:HD11  | 17       | 0.24          |
| (1,3311) | 1:68:A:LYS:HD3   | 1:57:A:VAL:HG13  | 9        | 0.24          |
| (1,3311) | 1:68:A:LYS:HD3   | 1:57:A:VAL:HG11  | 11       | 0.24          |
| (1,3282) | 1:44:A:GLU:HG2   | 1:45:A:ALA:HB1   | 11       | 0.24          |
| (1,3260) | 1:121:A:LYS:HG2  | 1:121:A:LYS:HB2  | 9        | 0.24          |
| (1,3250) | 1:41:A:ALA:HA    | 1:41:A:ALA:HB2   | 1        | 0.24          |
| (1,3250) | 1:41:A:ALA:HA    | 1:41:A:ALA:HB2   | 15       | 0.24          |
| (1,3223) | 1:84:A:TYR:HE2   | 1:79:A:THR:HA    | 17       | 0.24          |
| (1,3221) | 1:37:A:HIS:HB2   | 1:99:A:GLY:HA2   | 12       | 0.24          |
| (1,3221) | 1:37:A:HIS:HB2   | 1:99:A:GLY:HA2   | 16       | 0.24          |
| (1,3209) | 1:124:A:VAL:HG12 | 1:124:A:VAL:HB   | 1        | 0.24          |
| (1,3209) | 1:124:A:VAL:HG13 | 1:124:A:VAL:HB   | 5        | 0.24          |
| (1,3209) | 1:124:A:VAL:HG12 | 1:124:A:VAL:HB   | 6        | 0.24          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3209) | 1:124:A:VAL:HG13 | 1:124:A:VAL:HB   | 13       | 0.24          |
| (1,3209) | 1:124:A:VAL:HG11 | 1:124:A:VAL:HB   | 15       | 0.24          |
| (1,3209) | 1:124:A:VAL:HG11 | 1:124:A:VAL:HB   | 17       | 0.24          |
| (1,3200) | 1:116:A:GLN:HG3  | 1:113:A:ALA:HB1  | 7        | 0.24          |
| (1,3183) | 1:124:A:VAL:HG23 | 1:121:A:LYS:HA   | 5        | 0.24          |
| (1,3180) | 1:111:A:GLU:HG2  | 1:111:A:GLU:HA   | 1        | 0.24          |
| (1,3166) | 1:75:A:LEU:HD23  | 1:53:A:PHE:HD2   | 3        | 0.24          |
| (1,3166) | 1:75:A:LEU:HD22  | 1:53:A:PHE:HD2   | 7        | 0.24          |
| (1,3161) | 1:82:A:TRP:HH2   | 1:120:A:ALA:HB3  | 2        | 0.24          |
| (1,3132) | 1:68:A:LYS:HB2   | 1:53:A:PHE:HE2   | 2        | 0.24          |
| (1,3113) | 1:57:A:VAL:HG11  | 1:61:A:ALA:H     | 14       | 0.24          |
| (1,3081) | 1:97:A:LEU:HD13  | 1:55:A:ASP:HA    | 7        | 0.24          |
| (1,3080) | 1:125:A:GLN:HB2  | 1:125:A:GLN:HA   | 2        | 0.24          |
| (1,3080) | 1:125:A:GLN:HB2  | 1:125:A:GLN:HA   | 10       | 0.24          |
| (1,3080) | 1:125:A:GLN:HB2  | 1:125:A:GLN:HA   | 12       | 0.24          |
| (1,3080) | 1:125:A:GLN:HB2  | 1:125:A:GLN:HA   | 16       | 0.24          |
| (1,3066) | 1:30:A:PHE:HB3   | 1:29:A:ALA:HB2   | 2        | 0.24          |
| (1,3066) | 1:30:A:PHE:HB3   | 1:29:A:ALA:HB3   | 8        | 0.24          |
| (1,3066) | 1:30:A:PHE:HB3   | 1:29:A:ALA:HB2   | 13       | 0.24          |
| (1,3028) | 1:71:A:LEU:HD12  | 1:72:A:ARG:HA    | 7        | 0.24          |
| (1,3028) | 1:71:A:LEU:HD11  | 1:72:A:ARG:HA    | 9        | 0.24          |
| (1,3028) | 1:71:A:LEU:HD11  | 1:72:A:ARG:HA    | 13       | 0.24          |
| (1,3028) | 1:71:A:LEU:HD13  | 1:72:A:ARG:HA    | 14       | 0.24          |
| (1,3022) | 1:64:A:MET:HE2   | 1:30:A:PHE:HA    | 7        | 0.24          |
| (1,2992) | 1:20:A:LYS:HB3   | 1:20:A:LYS:H     | 10       | 0.24          |
| (1,2991) | 1:54:A:GLN:HE22  | 1:54:A:GLN:HG2   | 16       | 0.24          |
| (1,2989) | 1:42:A:GLU:HA    | 1:42:A:GLU:HB2   | 1        | 0.24          |
| (1,2989) | 1:42:A:GLU:HA    | 1:42:A:GLU:HB2   | 7        | 0.24          |
| (1,2989) | 1:42:A:GLU:HA    | 1:42:A:GLU:HB2   | 9        | 0.24          |
| (1,2989) | 1:42:A:GLU:HA    | 1:42:A:GLU:HB2   | 10       | 0.24          |
| (1,2945) | 1:110:A:VAL:HB   | 1:110:A:VAL:HG12 | 7        | 0.24          |
| (1,2945) | 1:110:A:VAL:HB   | 1:110:A:VAL:HG13 | 8        | 0.24          |
| (1,2945) | 1:110:A:VAL:HB   | 1:110:A:VAL:HG13 | 11       | 0.24          |
| (1,2937) | 1:95:A:VAL:HG23  | 1:95:A:VAL:HG11  | 5        | 0.24          |
| (1,2933) | 1:95:A:VAL:HG21  | 1:99:A:GLY:H     | 16       | 0.24          |
| (1,2909) | 1:110:A:VAL:HG11 | 1:91:A:GLY:HA2   | 11       | 0.24          |
| (1,2888) | 1:29:A:ALA:HA    | 1:32:A:ALA:HB2   | 1        | 0.24          |
| (1,2888) | 1:29:A:ALA:HA    | 1:32:A:ALA:HB1   | 4        | 0.24          |
| (1,2832) | 1:97:A:LEU:HD21  | 1:97:A:LEU:H     | 12       | 0.24          |
| (1,2829) | 1:97:A:LEU:HD22  | 1:97:A:LEU:HB2   | 5        | 0.24          |
| (1,2829) | 1:97:A:LEU:HD22  | 1:97:A:LEU:HB2   | 7        | 0.24          |
| (1,2829) | 1:97:A:LEU:HD21  | 1:97:A:LEU:HB2   | 16       | 0.24          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2769) | 1:43:A:GLY:HA2   | 1:42:A:GLU:HB2  | 9        | 0.24          |
| (1,2753) | 1:97:A:LEU:HD13  | 1:59:A:ARG:HD3  | 1        | 0.24          |
| (1,2753) | 1:97:A:LEU:HD11  | 1:59:A:ARG:HD3  | 11       | 0.24          |
| (1,2745) | 1:34:A:ARG:HD3   | 1:34:A:ARG:HG3  | 5        | 0.24          |
| (1,2745) | 1:34:A:ARG:HD3   | 1:34:A:ARG:HG3  | 9        | 0.24          |
| (1,2745) | 1:34:A:ARG:HD3   | 1:34:A:ARG:HG3  | 15       | 0.24          |
| (1,2729) | 1:17:A:ASN:HB3   | 1:17:A:ASN:HB2  | 5        | 0.24          |
| (1,2729) | 1:17:A:ASN:HB3   | 1:17:A:ASN:HB2  | 13       | 0.24          |
| (1,2713) | 1:53:A:PHE:HB3   | 1:75:A:LEU:HD12 | 5        | 0.24          |
| (1,2713) | 1:53:A:PHE:HB3   | 1:75:A:LEU:HD13 | 6        | 0.24          |
| (1,2713) | 1:53:A:PHE:HB3   | 1:75:A:LEU:HD12 | 7        | 0.24          |
| (1,2713) | 1:53:A:PHE:HB3   | 1:75:A:LEU:HD12 | 10       | 0.24          |
| (1,2713) | 1:53:A:PHE:HB3   | 1:75:A:LEU:HD12 | 12       | 0.24          |
| (1,2713) | 1:53:A:PHE:HB3   | 1:75:A:LEU:HD11 | 13       | 0.24          |
| (1,2713) | 1:53:A:PHE:HB3   | 1:75:A:LEU:HD13 | 14       | 0.24          |
| (1,2679) | 1:53:A:PHE:HA    | 1:53:A:PHE:HE2  | 17       | 0.24          |
| (1,2675) | 1:85:A:LEU:HB2   | 1:86:A:TYR:HD1  | 4        | 0.24          |
| (1,2675) | 1:85:A:LEU:HB2   | 1:86:A:TYR:HD1  | 10       | 0.24          |
| (1,2622) | 1:71:A:LEU:HD12  | 1:57:A:VAL:H    | 15       | 0.24          |
| (1,2618) | 1:34:A:ARG:HG3   | 1:34:A:ARG:H    | 9        | 0.24          |
| (1,2605) | 1:31:A:LEU:HD21  | 1:30:A:PHE:HD2  | 4        | 0.24          |
| (1,2605) | 1:31:A:LEU:HD23  | 1:30:A:PHE:HD1  | 7        | 0.24          |
| (1,2605) | 1:31:A:LEU:HD22  | 1:30:A:PHE:HD2  | 8        | 0.24          |
| (1,2605) | 1:31:A:LEU:HD22  | 1:30:A:PHE:HD2  | 15       | 0.24          |
| (1,2605) | 1:31:A:LEU:HD21  | 1:30:A:PHE:HD1  | 16       | 0.24          |
| (1,2605) | 1:31:A:LEU:HD21  | 1:30:A:PHE:HD1  | 17       | 0.24          |
| (1,2596) | 1:74:A:ALA:HB3   | 1:27:A:VAL:HG12 | 17       | 0.24          |
| (1,2576) | 1:124:A:VAL:HG21 | 1:120:A:ALA:HA  | 1        | 0.24          |
| (1,2576) | 1:124:A:VAL:HG22 | 1:120:A:ALA:HA  | 10       | 0.24          |
| (1,2576) | 1:124:A:VAL:HG22 | 1:120:A:ALA:HA  | 15       | 0.24          |
| (1,2576) | 1:124:A:VAL:HG23 | 1:120:A:ALA:HA  | 17       | 0.24          |
| (1,2560) | 1:86:A:TYR:HE1   | 1:86:A:TYR:HD1  | 9        | 0.24          |
| (1,2545) | 1:76:A:ARG:HB2   | 1:73:A:SER:HA   | 11       | 0.24          |
| (1,2529) | 1:79:A:THR:HG23  | 1:75:A:LEU:HA   | 10       | 0.24          |
| (1,2527) | 1:123:A:ARG:H    | 1:123:A:ARG:HA  | 4        | 0.24          |
| (1,2527) | 1:123:A:ARG:H    | 1:123:A:ARG:HA  | 15       | 0.24          |
| (1,2515) | 1:122:A:ALA:HA   | 1:122:A:ALA:H   | 8        | 0.24          |
| (1,2515) | 1:122:A:ALA:HA   | 1:122:A:ALA:H   | 13       | 0.24          |
| (1,2505) | 1:126:A:ALA:HA   | 1:126:A:ALA:H   | 4        | 0.24          |
| (1,2444) | 1:53:A:PHE:HE2   | 1:53:A:PHE:HB2  | 3        | 0.24          |
| (1,2444) | 1:53:A:PHE:HE1   | 1:53:A:PHE:HB2  | 5        | 0.24          |
| (1,2444) | 1:53:A:PHE:HE2   | 1:53:A:PHE:HB2  | 6        | 0.24          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2444) | 1:53:A:PHE:HE2   | 1:53:A:PHE:HB2   | 7        | 0.24          |
| (1,2434) | 1:86:A:TYR:HB2   | 1:117:A:LEU:HB3  | 4        | 0.24          |
| (1,2434) | 1:86:A:TYR:HB2   | 1:117:A:LEU:HB3  | 13       | 0.24          |
| (1,2409) | 1:49:A:LYS:H     | 1:52:A:ILE:HD13  | 8        | 0.24          |
| (1,2409) | 1:49:A:LYS:H     | 1:52:A:ILE:HD11  | 15       | 0.24          |
| (1,2404) | 1:28:A:ILE:HD11  | 1:74:A:ALA:HA    | 7        | 0.24          |
| (1,2397) | 1:50:A:ILE:HD11  | 1:50:A:ILE:HA    | 4        | 0.24          |
| (1,2358) | 1:107:A:GLU:HA   | 1:111:A:GLU:H    | 17       | 0.24          |
| (1,2346) | 1:105:A:LEU:HD11 | 1:107:A:GLU:HA   | 17       | 0.24          |
| (1,2341) | 1:66:A:LEU:HD21  | 1:70:A:GLN:H     | 17       | 0.24          |
| (1,2307) | 1:117:A:LEU:HD13 | 1:86:A:TYR:HB2   | 1        | 0.24          |
| (1,2307) | 1:117:A:LEU:HD11 | 1:86:A:TYR:HB2   | 6        | 0.24          |
| (1,2283) | 1:33:A:GLU:HG2   | 1:33:A:GLU:HA    | 15       | 0.24          |
| (1,2253) | 1:44:A:GLU:HB3   | 1:44:A:GLU:H     | 9        | 0.24          |
| (1,2210) | 1:105:A:LEU:HG   | 1:110:A:VAL:HG13 | 4        | 0.24          |
| (1,2210) | 1:105:A:LEU:HG   | 1:110:A:VAL:HG11 | 10       | 0.24          |
| (1,2210) | 1:105:A:LEU:HG   | 1:110:A:VAL:HG12 | 16       | 0.24          |
| (1,2210) | 1:105:A:LEU:HG   | 1:110:A:VAL:HG13 | 17       | 0.24          |
| (1,2178) | 1:48:A:LEU:HB2   | 1:52:A:ILE:HG22  | 8        | 0.24          |
| (1,2116) | 1:45:A:ALA:HB1   | 1:84:A:TYR:HA    | 14       | 0.24          |
| (1,2094) | 1:95:A:VAL:HG23  | 1:97:A:LEU:HD22  | 9        | 0.24          |
| (1,2075) | 1:61:A:ALA:HB2   | 1:62:A:GLY:H     | 5        | 0.24          |
| (1,2024) | 1:95:A:VAL:HA    | 1:95:A:VAL:HG11  | 4        | 0.24          |
| (1,1947) | 1:93:A:THR:HB    | 1:88:A:VAL:HG13  | 9        | 0.24          |
| (1,1947) | 1:93:A:THR:HB    | 1:88:A:VAL:HG12  | 10       | 0.24          |
| (1,1947) | 1:93:A:THR:HB    | 1:88:A:VAL:HG12  | 14       | 0.24          |
| (1,1945) | 1:105:A:LEU:HB3  | 1:110:A:VAL:HG21 | 12       | 0.24          |
| (1,1904) | 1:74:A:ALA:HB2   | 1:28:A:ILE:HA    | 1        | 0.24          |
| (1,1904) | 1:74:A:ALA:HB2   | 1:28:A:ILE:HA    | 2        | 0.24          |
| (1,1904) | 1:74:A:ALA:HB1   | 1:28:A:ILE:HA    | 6        | 0.24          |
| (1,1904) | 1:74:A:ALA:HB2   | 1:28:A:ILE:HA    | 8        | 0.24          |
| (1,1881) | 1:113:A:ALA:HB1  | 1:88:A:VAL:HA    | 12       | 0.24          |
| (1,1881) | 1:113:A:ALA:HB3  | 1:88:A:VAL:HA    | 16       | 0.24          |
| (1,1865) | 1:45:A:ALA:HB1   | 1:44:A:GLU:HB3   | 1        | 0.24          |
| (1,1865) | 1:45:A:ALA:HB1   | 1:44:A:GLU:HB3   | 4        | 0.24          |
| (1,1865) | 1:45:A:ALA:HB1   | 1:44:A:GLU:HB3   | 5        | 0.24          |
| (1,1865) | 1:45:A:ALA:HB3   | 1:44:A:GLU:HB3   | 6        | 0.24          |
| (1,1831) | 1:21:A:LEU:HG    | 1:21:A:LEU:HB3   | 2        | 0.24          |
| (1,1831) | 1:21:A:LEU:HG    | 1:21:A:LEU:HB3   | 6        | 0.24          |
| (1,1831) | 1:21:A:LEU:HG    | 1:21:A:LEU:HB3   | 8        | 0.24          |
| (1,1831) | 1:21:A:LEU:HG    | 1:21:A:LEU:HB3   | 13       | 0.24          |
| (1,1826) | 1:64:A:MET:HE1   | 1:21:A:LEU:HD12  | 4        | 0.24          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1817) | 1:77:A:LEU:HG    | 1:77:A:LEU:HD23  | 8        | 0.24          |
| (1,1817) | 1:77:A:LEU:HG    | 1:77:A:LEU:HD23  | 10       | 0.24          |
| (1,1812) | 1:117:A:LEU:HA   | 1:117:A:LEU:HD12 | 3        | 0.24          |
| (1,1799) | 1:71:A:LEU:HA    | 1:74:A:ALA:HB1   | 2        | 0.24          |
| (1,1773) | 1:24:A:SER:HA    | 1:27:A:VAL:HG21  | 5        | 0.24          |
| (1,1753) | 1:113:A:ALA:HB1  | 1:89:A:LYS:H     | 7        | 0.24          |
| (1,1752) | 1:41:A:ALA:HB2   | 1:28:A:ILE:HG23  | 10       | 0.24          |
| (1,1746) | 1:71:A:LEU:HD23  | 1:74:A:ALA:H     | 1        | 0.24          |
| (1,1746) | 1:71:A:LEU:HD23  | 1:74:A:ALA:H     | 4        | 0.24          |
| (1,1746) | 1:71:A:LEU:HD23  | 1:74:A:ALA:H     | 13       | 0.24          |
| (1,1736) | 1:77:A:LEU:HB3   | 1:77:A:LEU:HD13  | 1        | 0.24          |
| (1,1736) | 1:77:A:LEU:HB3   | 1:77:A:LEU:HD13  | 2        | 0.24          |
| (1,1736) | 1:77:A:LEU:HB3   | 1:77:A:LEU:HD12  | 7        | 0.24          |
| (1,1736) | 1:77:A:LEU:HB3   | 1:77:A:LEU:HD13  | 11       | 0.24          |
| (1,1736) | 1:77:A:LEU:HB3   | 1:77:A:LEU:HD12  | 12       | 0.24          |
| (1,1736) | 1:77:A:LEU:HB3   | 1:77:A:LEU:HD12  | 14       | 0.24          |
| (1,1733) | 1:30:A:PHE:HD2   | 1:66:A:LEU:HD22  | 9        | 0.24          |
| (1,1733) | 1:30:A:PHE:HD1   | 1:66:A:LEU:HD22  | 12       | 0.24          |
| (1,1730) | 1:27:A:VAL:HA    | 1:66:A:LEU:HD21  | 1        | 0.24          |
| (1,1730) | 1:27:A:VAL:HA    | 1:66:A:LEU:HD23  | 3        | 0.24          |
| (1,1730) | 1:27:A:VAL:HA    | 1:66:A:LEU:HD21  | 6        | 0.24          |
| (1,1730) | 1:27:A:VAL:HA    | 1:66:A:LEU:HD21  | 10       | 0.24          |
| (1,1686) | 1:85:A:LEU:HD13  | 1:85:A:LEU:HD23  | 4        | 0.24          |
| (1,1684) | 1:48:A:LEU:HD13  | 1:50:A:ILE:HA    | 11       | 0.24          |
| (1,1668) | 1:52:A:ILE:HG13  | 1:48:A:LEU:HD12  | 5        | 0.24          |
| (1,1629) | 1:116:A:GLN:HG3  | 1:113:A:ALA:HB1  | 9        | 0.24          |
| (1,1618) | 1:109:A:HIS:HB2  | 1:110:A:VAL:HG11 | 9        | 0.24          |
| (1,1618) | 1:109:A:HIS:HB2  | 1:110:A:VAL:HG12 | 11       | 0.24          |
| (1,1618) | 1:109:A:HIS:HB2  | 1:110:A:VAL:HG11 | 14       | 0.24          |
| (1,1618) | 1:109:A:HIS:HB2  | 1:110:A:VAL:HG12 | 16       | 0.24          |
| (1,1613) | 1:124:A:VAL:HG22 | 1:121:A:LYS:HA   | 2        | 0.24          |
| (1,1568) | 1:68:A:LYS:HB2   | 1:57:A:VAL:HG12  | 17       | 0.24          |
| (1,1552) | 1:124:A:VAL:HG12 | 1:124:A:VAL:HB   | 4        | 0.24          |
| (1,1552) | 1:124:A:VAL:HG11 | 1:124:A:VAL:HB   | 10       | 0.24          |
| (1,1552) | 1:124:A:VAL:HG11 | 1:124:A:VAL:HB   | 16       | 0.24          |
| (1,1480) | 1:64:A:MET:HE1   | 1:63:A:GLU:H     | 13       | 0.24          |
| (1,1428) | 1:93:A:THR:HG22  | 1:101:A:PRO:HB3  | 7        | 0.24          |
| (1,1428) | 1:93:A:THR:HG23  | 1:101:A:PRO:HB3  | 10       | 0.24          |
| (1,1428) | 1:93:A:THR:HG23  | 1:101:A:PRO:HB3  | 11       | 0.24          |
| (1,1403) | 1:95:A:VAL:HG23  | 1:95:A:VAL:HG12  | 16       | 0.24          |
| (1,1399) | 1:95:A:VAL:HG23  | 1:95:A:VAL:H     | 6        | 0.24          |
| (1,1395) | 1:31:A:LEU:HD23  | 1:39:A:PHE:HD2   | 2        | 0.24          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1395) | 1:31:A:LEU:HD22  | 1:39:A:PHE:HD2   | 4        | 0.24          |
| (1,1395) | 1:31:A:LEU:HD22  | 1:39:A:PHE:HD1   | 16       | 0.24          |
| (1,1393) | 1:21:A:LEU:HD23  | 1:21:A:LEU:H     | 7        | 0.24          |
| (1,1382) | 1:57:A:VAL:HG23  | 1:53:A:PHE:HE2   | 1        | 0.24          |
| (1,1371) | 1:28:A:ILE:HD13  | 1:75:A:LEU:H     | 8        | 0.24          |
| (1,1365) | 1:32:A:ALA:HB3   | 1:28:A:ILE:HG23  | 10       | 0.24          |
| (1,1363) | 1:29:A:ALA:HA    | 1:32:A:ALA:HB1   | 11       | 0.24          |
| (1,1357) | 1:74:A:ALA:HB3   | 1:31:A:LEU:HD11  | 14       | 0.24          |
| (1,1353) | 1:61:A:ALA:HB3   | 1:62:A:GLY:H     | 11       | 0.24          |
| (1,1315) | 1:95:A:VAL:HG21  | 1:97:A:LEU:HD22  | 13       | 0.24          |
| (1,1232) | 1:60:A:VAL:HG13  | 1:59:A:ARG:HD3   | 16       | 0.24          |
| (1,1210) | 1:86:A:TYR:HB3   | 1:86:A:TYR:H     | 3        | 0.24          |
| (1,1210) | 1:86:A:TYR:HB3   | 1:86:A:TYR:H     | 4        | 0.24          |
| (1,1210) | 1:86:A:TYR:HB3   | 1:86:A:TYR:H     | 5        | 0.24          |
| (1,1210) | 1:86:A:TYR:HB3   | 1:86:A:TYR:H     | 10       | 0.24          |
| (1,1210) | 1:86:A:TYR:HB3   | 1:86:A:TYR:H     | 11       | 0.24          |
| (1,1210) | 1:86:A:TYR:HB3   | 1:86:A:TYR:H     | 12       | 0.24          |
| (1,1210) | 1:86:A:TYR:HB3   | 1:86:A:TYR:H     | 13       | 0.24          |
| (1,1210) | 1:86:A:TYR:HB3   | 1:86:A:TYR:H     | 17       | 0.24          |
| (1,1206) | 1:117:A:LEU:HD11 | 1:86:A:TYR:HB2   | 8        | 0.24          |
| (1,1194) | 1:39:A:PHE:HB3   | 1:35:A:PHE:HB3   | 7        | 0.24          |
| (1,1081) | 1:71:A:LEU:HD11  | 1:57:A:VAL:H     | 3        | 0.24          |
| (1,1081) | 1:71:A:LEU:HD13  | 1:57:A:VAL:H     | 13       | 0.24          |
| (1,1062) | 1:27:A:VAL:HG21  | 1:27:A:VAL:HG12  | 15       | 0.24          |
| (1,1060) | 1:74:A:ALA:HB1   | 1:27:A:VAL:HG11  | 14       | 0.24          |
| (1,1030) | 1:86:A:TYR:HE1   | 1:86:A:TYR:HB2   | 13       | 0.24          |
| (1,993)  | 1:79:A:THR:HG23  | 1:75:A:LEU:HA    | 9        | 0.24          |
| (1,895)  | 1:129:A:ALA:HB2  | 1:129:A:ALA:HA   | 7        | 0.24          |
| (1,853)  | 1:65:A:ASN:HB2   | 1:65:A:ASN:HD21  | 3        | 0.24          |
| (1,852)  | 1:65:A:ASN:HB3   | 1:65:A:ASN:HD21  | 9        | 0.24          |
| (1,829)  | 1:41:A:ALA:HB2   | 1:41:A:ALA:H     | 8        | 0.24          |
| (1,827)  | 1:45:A:ALA:HB1   | 1:45:A:ALA:H     | 1        | 0.24          |
| (1,827)  | 1:45:A:ALA:HB3   | 1:45:A:ALA:H     | 6        | 0.24          |
| (1,753)  | 1:92:A:ALA:HB1   | 1:91:A:GLY:H     | 17       | 0.24          |
| (1,691)  | 1:75:A:LEU:HD21  | 1:54:A:GLN:H     | 8        | 0.24          |
| (1,691)  | 1:75:A:LEU:HD23  | 1:54:A:GLN:H     | 10       | 0.24          |
| (1,691)  | 1:75:A:LEU:HD21  | 1:54:A:GLN:H     | 12       | 0.24          |
| (1,691)  | 1:75:A:LEU:HD21  | 1:54:A:GLN:H     | 15       | 0.24          |
| (1,691)  | 1:75:A:LEU:HD22  | 1:54:A:GLN:H     | 17       | 0.24          |
| (1,580)  | 1:98:A:ASP:HB2   | 1:100:A:ASN:HD21 | 7        | 0.24          |
| (1,580)  | 1:98:A:ASP:HB2   | 1:100:A:ASN:HD21 | 11       | 0.24          |
| (1,580)  | 1:98:A:ASP:HB2   | 1:100:A:ASN:HD21 | 17       | 0.24          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,564)  | 1:59:A:ARG:HE   | 1:97:A:LEU:HD11  | 6        | 0.24          |
| (1,527)  | 1:65:A:ASN:HB3  | 1:65:A:ASN:HD21  | 13       | 0.24          |
| (1,527)  | 1:65:A:ASN:HB3  | 1:65:A:ASN:HD21  | 16       | 0.24          |
| (1,451)  | 1:32:A:ALA:HB2  | 1:35:A:PHE:H     | 6        | 0.24          |
| (1,441)  | 1:42:A:GLU:HB3  | 1:41:A:ALA:H     | 4        | 0.24          |
| (1,441)  | 1:42:A:GLU:HB3  | 1:41:A:ALA:H     | 16       | 0.24          |
| (1,300)  | 1:100:A:ASN:HB3 | 1:100:A:ASN:HD21 | 16       | 0.24          |
| (1,234)  | 1:95:A:VAL:HG22 | 1:99:A:GLY:H     | 15       | 0.24          |
| (1,172)  | 1:27:A:VAL:HG12 | 1:21:A:LEU:H     | 13       | 0.24          |
| (1,117)  | 1:27:A:VAL:HG11 | 1:26:A:GLU:H     | 4        | 0.24          |
| (1,116)  | 1:21:A:LEU:HD13 | 1:30:A:PHE:H     | 12       | 0.24          |
| (1,56)   | 1:84:A:TYR:H    | 1:84:A:TYR:HD1   | 2        | 0.24          |
| (1,56)   | 1:84:A:TYR:H    | 1:84:A:TYR:HD1   | 16       | 0.24          |
| (1,12)   | 1:100:A:ASN:H   | 1:100:A:ASN:HD21 | 1        | 0.24          |
| (3,143)  | 1:25:A:LYS:H    | 1:77:A:LEU:HD22  | 1        | 0.23          |
| (3,143)  | 1:25:A:LYS:H    | 1:77:A:LEU:HD23  | 3        | 0.23          |
| (3,143)  | 1:25:A:LYS:H    | 1:77:A:LEU:HD21  | 11       | 0.23          |
| (3,129)  | 1:71:A:LEU:HD13 | 1:60:A:VAL:HB    | 4        | 0.23          |
| (3,129)  | 1:71:A:LEU:HD11 | 1:60:A:VAL:HB    | 5        | 0.23          |
| (3,129)  | 1:71:A:LEU:HD11 | 1:60:A:VAL:HB    | 8        | 0.23          |
| (3,129)  | 1:71:A:LEU:HD12 | 1:60:A:VAL:HB    | 11       | 0.23          |
| (3,129)  | 1:71:A:LEU:HD13 | 1:60:A:VAL:HB    | 12       | 0.23          |
| (3,129)  | 1:71:A:LEU:HD12 | 1:60:A:VAL:HB    | 15       | 0.23          |
| (3,129)  | 1:71:A:LEU:HD11 | 1:60:A:VAL:HB    | 17       | 0.23          |
| (3,126)  | 1:21:A:LEU:HD23 | 1:22:A:ASN:H     | 9        | 0.23          |
| (3,111)  | 1:111:A:GLU:HG2 | 1:112:A:HIS:HA   | 11       | 0.23          |
| (3,94)   | 1:56:A:LEU:HB2  | 1:75:A:LEU:HD13  | 1        | 0.23          |
| (3,94)   | 1:56:A:LEU:HB2  | 1:75:A:LEU:HD13  | 9        | 0.23          |
| (3,83)   | 1:114:A:ARG:HB2 | 1:113:A:ALA:HB3  | 3        | 0.23          |
| (3,22)   | 1:48:A:LEU:HD12 | 1:97:A:LEU:H     | 10       | 0.23          |
| (3,14)   | 1:82:A:TRP:HA   | 1:85:A:LEU:HB2   | 9        | 0.23          |
| (3,14)   | 1:82:A:TRP:HA   | 1:85:A:LEU:HB2   | 11       | 0.23          |
| (1,4344) | 1:120:A:ALA:H   | 1:119:A:GLU:HG2  | 9        | 0.23          |
| (1,4342) | 1:38:A:CYS:H    | 1:95:A:VAL:HG11  | 1        | 0.23          |
| (1,4342) | 1:38:A:CYS:H    | 1:95:A:VAL:HG11  | 6        | 0.23          |
| (1,4342) | 1:38:A:CYS:H    | 1:95:A:VAL:HG11  | 17       | 0.23          |
| (1,4310) | 1:64:A:MET:HA   | 1:65:A:ASN:H     | 10       | 0.23          |
| (1,4310) | 1:64:A:MET:HA   | 1:65:A:ASN:H     | 17       | 0.23          |
| (1,4299) | 1:65:A:ASN:HD22 | 1:65:A:ASN:HD21  | 16       | 0.23          |
| (1,4202) | 1:127:A:GLN:H   | 1:127:A:GLN:HB3  | 15       | 0.23          |
| (1,4172) | 1:105:A:LEU:H   | 1:92:A:ALA:H     | 4        | 0.23          |
| (1,4172) | 1:105:A:LEU:H   | 1:92:A:ALA:H     | 10       | 0.23          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,4172) | 1:105:A:LEU:H    | 1:92:A:ALA:H     | 13       | 0.23          |
| (1,4153) | 1:18:A:GLN:HB3   | 1:18:A:GLN:H     | 6        | 0.23          |
| (1,4153) | 1:18:A:GLN:HB3   | 1:18:A:GLN:H     | 9        | 0.23          |
| (1,4153) | 1:18:A:GLN:HB3   | 1:18:A:GLN:H     | 13       | 0.23          |
| (1,4150) | 1:17:A:ASN:HB3   | 1:18:A:GLN:H     | 15       | 0.23          |
| (1,4119) | 1:66:A:LEU:HB2   | 1:70:A:GLN:HE22  | 15       | 0.23          |
| (1,4119) | 1:66:A:LEU:HB2   | 1:70:A:GLN:HE22  | 16       | 0.23          |
| (1,4109) | 1:97:A:LEU:HD12  | 1:98:A:ASP:H     | 17       | 0.23          |
| (1,4083) | 1:21:A:LEU:HA    | 1:22:A:ASN:HD22  | 1        | 0.23          |
| (1,4069) | 1:13:A:ASP:HB2   | 1:13:A:ASP:H     | 10       | 0.23          |
| (1,4069) | 1:13:A:ASP:HB2   | 1:13:A:ASP:H     | 11       | 0.23          |
| (1,4069) | 1:13:A:ASP:HB2   | 1:13:A:ASP:H     | 13       | 0.23          |
| (1,4036) | 1:31:A:LEU:H     | 1:31:A:LEU:HD11  | 1        | 0.23          |
| (1,4036) | 1:31:A:LEU:H     | 1:31:A:LEU:HD12  | 8        | 0.23          |
| (1,4017) | 1:32:A:ALA:HB1   | 1:35:A:PHE:H     | 1        | 0.23          |
| (1,4017) | 1:32:A:ALA:HB2   | 1:35:A:PHE:H     | 3        | 0.23          |
| (1,3961) | 1:57:A:VAL:H     | 1:56:A:LEU:HB3   | 8        | 0.23          |
| (1,3961) | 1:57:A:VAL:H     | 1:56:A:LEU:HB3   | 12       | 0.23          |
| (1,3961) | 1:57:A:VAL:H     | 1:56:A:LEU:HB3   | 17       | 0.23          |
| (1,3941) | 1:63:A:GLU:H     | 1:61:A:ALA:HB2   | 14       | 0.23          |
| (1,3901) | 1:79:A:THR:H     | 1:77:A:LEU:HB2   | 14       | 0.23          |
| (1,3874) | 1:85:A:LEU:HB3   | 1:86:A:TYR:H     | 2        | 0.23          |
| (1,3874) | 1:85:A:LEU:HB3   | 1:86:A:TYR:H     | 6        | 0.23          |
| (1,3874) | 1:85:A:LEU:HB3   | 1:86:A:TYR:H     | 13       | 0.23          |
| (1,3874) | 1:85:A:LEU:HB3   | 1:86:A:TYR:H     | 14       | 0.23          |
| (1,3861) | 1:110:A:VAL:HG22 | 1:91:A:GLY:H     | 11       | 0.23          |
| (1,3861) | 1:110:A:VAL:HG23 | 1:91:A:GLY:H     | 14       | 0.23          |
| (1,3816) | 1:105:A:LEU:H    | 1:105:A:LEU:HD21 | 1        | 0.23          |
| (1,3816) | 1:105:A:LEU:H    | 1:105:A:LEU:HD22 | 3        | 0.23          |
| (1,3816) | 1:105:A:LEU:H    | 1:105:A:LEU:HD21 | 12       | 0.23          |
| (1,3784) | 1:21:A:LEU:HG    | 1:21:A:LEU:H     | 4        | 0.23          |
| (1,3776) | 1:121:A:LYS:HA   | 1:122:A:ALA:H    | 2        | 0.23          |
| (1,3776) | 1:121:A:LYS:HA   | 1:122:A:ALA:H    | 3        | 0.23          |
| (1,3776) | 1:121:A:LYS:HA   | 1:122:A:ALA:H    | 4        | 0.23          |
| (1,3776) | 1:121:A:LYS:HA   | 1:122:A:ALA:H    | 7        | 0.23          |
| (1,3776) | 1:121:A:LYS:HA   | 1:122:A:ALA:H    | 9        | 0.23          |
| (1,3776) | 1:121:A:LYS:HA   | 1:122:A:ALA:H    | 15       | 0.23          |
| (1,3775) | 1:124:A:VAL:HA   | 1:125:A:GLN:H    | 4        | 0.23          |
| (1,3773) | 1:123:A:ARG:HA   | 1:124:A:VAL:H    | 4        | 0.23          |
| (1,3773) | 1:123:A:ARG:HA   | 1:124:A:VAL:H    | 8        | 0.23          |
| (1,3773) | 1:123:A:ARG:HA   | 1:124:A:VAL:H    | 16       | 0.23          |
| (1,3769) | 1:130:A:GLU:H    | 1:129:A:ALA:HB2  | 13       | 0.23          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3766) | 1:128:A:ARG:HB3 | 1:129:A:ALA:H    | 10       | 0.23          |
| (1,3716) | 1:35:A:PHE:HE1  | 1:35:A:PHE:H     | 8        | 0.23          |
| (1,3716) | 1:35:A:PHE:HE1  | 1:35:A:PHE:H     | 13       | 0.23          |
| (1,3698) | 1:30:A:PHE:HD2  | 1:30:A:PHE:H     | 5        | 0.23          |
| (1,3668) | 1:84:A:TYR:H    | 1:84:A:TYR:HD2   | 5        | 0.23          |
| (1,3668) | 1:84:A:TYR:H    | 1:84:A:TYR:HD1   | 7        | 0.23          |
| (1,3668) | 1:84:A:TYR:H    | 1:84:A:TYR:HD2   | 11       | 0.23          |
| (1,3668) | 1:84:A:TYR:H    | 1:84:A:TYR:HD1   | 15       | 0.23          |
| (1,3592) | 1:109:A:HIS:HB2 | 1:110:A:VAL:HG13 | 6        | 0.23          |
| (1,3592) | 1:109:A:HIS:HB2 | 1:110:A:VAL:HG11 | 14       | 0.23          |
| (1,3591) | 1:93:A:THR:HB   | 1:88:A:VAL:HG12  | 6        | 0.23          |
| (1,3583) | 1:112:A:HIS:H   | 1:109:A:HIS:HA   | 4        | 0.23          |
| (1,3583) | 1:112:A:HIS:H   | 1:109:A:HIS:HA   | 14       | 0.23          |
| (1,3580) | 1:111:A:GLU:HB2 | 1:109:A:HIS:HA   | 4        | 0.23          |
| (1,3580) | 1:111:A:GLU:HB2 | 1:109:A:HIS:HA   | 7        | 0.23          |
| (1,3580) | 1:111:A:GLU:HB2 | 1:109:A:HIS:HA   | 8        | 0.23          |
| (1,3580) | 1:111:A:GLU:HB2 | 1:109:A:HIS:HA   | 9        | 0.23          |
| (1,3580) | 1:111:A:GLU:HB2 | 1:109:A:HIS:HA   | 16       | 0.23          |
| (1,3562) | 1:104:A:GLU:HB3 | 1:91:A:GLY:HA3   | 15       | 0.23          |
| (1,3562) | 1:104:A:GLU:HB3 | 1:91:A:GLY:HA3   | 17       | 0.23          |
| (1,3536) | 1:66:A:LEU:HB3  | 1:62:A:GLY:HA3   | 4        | 0.23          |
| (1,3536) | 1:66:A:LEU:HB3  | 1:62:A:GLY:HA3   | 6        | 0.23          |
| (1,3536) | 1:66:A:LEU:HB3  | 1:62:A:GLY:HA3   | 9        | 0.23          |
| (1,3535) | 1:74:A:ALA:HB1  | 1:28:A:ILE:HA    | 4        | 0.23          |
| (1,3535) | 1:74:A:ALA:HB2  | 1:28:A:ILE:HA    | 5        | 0.23          |
| (1,3535) | 1:74:A:ALA:HB3  | 1:28:A:ILE:HA    | 10       | 0.23          |
| (1,3535) | 1:74:A:ALA:HB1  | 1:28:A:ILE:HA    | 15       | 0.23          |
| (1,3535) | 1:74:A:ALA:HB1  | 1:28:A:ILE:HA    | 16       | 0.23          |
| (1,3534) | 1:122:A:ALA:HB1 | 1:121:A:LYS:HE3  | 6        | 0.23          |
| (1,3534) | 1:122:A:ALA:HB2 | 1:121:A:LYS:HE3  | 8        | 0.23          |
| (1,3519) | 1:65:A:ASN:H    | 1:65:A:ASN:HB3   | 1        | 0.23          |
| (1,3519) | 1:65:A:ASN:H    | 1:65:A:ASN:HB3   | 6        | 0.23          |
| (1,3503) | 1:27:A:VAL:HG22 | 1:31:A:LEU:H     | 11       | 0.23          |
| (1,3492) | 1:105:A:LEU:HB3 | 1:105:A:LEU:HD11 | 6        | 0.23          |
| (1,3479) | 1:45:A:ALA:HB1  | 1:44:A:GLU:HB3   | 3        | 0.23          |
| (1,3476) | 1:107:A:GLU:HG2 | 1:108:A:GLN:H    | 3        | 0.23          |
| (1,3476) | 1:107:A:GLU:HG2 | 1:108:A:GLN:H    | 9        | 0.23          |
| (1,3476) | 1:107:A:GLU:HG2 | 1:108:A:GLN:H    | 16       | 0.23          |
| (1,3430) | 1:45:A:ALA:HB3  | 1:84:A:TYR:HA    | 4        | 0.23          |
| (1,3417) | 1:117:A:LEU:HG  | 1:117:A:LEU:HD13 | 5        | 0.23          |
| (1,3417) | 1:117:A:LEU:HG  | 1:117:A:LEU:HD13 | 9        | 0.23          |
| (1,3395) | 1:33:A:GLU:HB3  | 1:33:A:GLU:HA    | 2        | 0.23          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3395) | 1:33:A:GLU:HB3   | 1:33:A:GLU:HA   | 6        | 0.23          |
| (1,3395) | 1:33:A:GLU:HB3   | 1:33:A:GLU:HA   | 12       | 0.23          |
| (1,3395) | 1:33:A:GLU:HB3   | 1:33:A:GLU:HA   | 14       | 0.23          |
| (1,3395) | 1:33:A:GLU:HB3   | 1:33:A:GLU:HA   | 15       | 0.23          |
| (1,3358) | 1:28:A:ILE:HB    | 1:29:A:ALA:HA   | 1        | 0.23          |
| (1,3358) | 1:28:A:ILE:HB    | 1:29:A:ALA:HA   | 5        | 0.23          |
| (1,3358) | 1:28:A:ILE:HB    | 1:29:A:ALA:HA   | 12       | 0.23          |
| (1,3358) | 1:28:A:ILE:HB    | 1:29:A:ALA:HA   | 13       | 0.23          |
| (1,3358) | 1:28:A:ILE:HB    | 1:29:A:ALA:HA   | 16       | 0.23          |
| (1,3341) | 1:41:A:ALA:HB3   | 1:28:A:ILE:HG23 | 3        | 0.23          |
| (1,3341) | 1:41:A:ALA:HB3   | 1:28:A:ILE:HG23 | 5        | 0.23          |
| (1,3325) | 1:77:A:LEU:HB3   | 1:77:A:LEU:HD12 | 8        | 0.23          |
| (1,3311) | 1:68:A:LYS:HD3   | 1:57:A:VAL:HG13 | 2        | 0.23          |
| (1,3311) | 1:68:A:LYS:HD3   | 1:57:A:VAL:HG13 | 4        | 0.23          |
| (1,3311) | 1:68:A:LYS:HD3   | 1:57:A:VAL:HG13 | 6        | 0.23          |
| (1,3311) | 1:68:A:LYS:HD3   | 1:57:A:VAL:HG13 | 13       | 0.23          |
| (1,3311) | 1:68:A:LYS:HD3   | 1:57:A:VAL:HG13 | 16       | 0.23          |
| (1,3311) | 1:68:A:LYS:HD3   | 1:57:A:VAL:HG12 | 17       | 0.23          |
| (1,3282) | 1:44:A:GLU:HG2   | 1:45:A:ALA:HB2  | 17       | 0.23          |
| (1,3250) | 1:41:A:ALA:HA    | 1:41:A:ALA:HB2  | 6        | 0.23          |
| (1,3228) | 1:31:A:LEU:HB2   | 1:39:A:PHE:HE1  | 8        | 0.23          |
| (1,3221) | 1:37:A:HIS:HB2   | 1:99:A:GLY:HA2  | 10       | 0.23          |
| (1,3216) | 1:48:A:LEU:HG    | 1:84:A:TYR:HD1  | 6        | 0.23          |
| (1,3209) | 1:124:A:VAL:HG11 | 1:124:A:VAL:HB  | 2        | 0.23          |
| (1,3209) | 1:124:A:VAL:HG13 | 1:124:A:VAL:HB  | 9        | 0.23          |
| (1,3209) | 1:124:A:VAL:HG13 | 1:124:A:VAL:HB  | 12       | 0.23          |
| (1,3209) | 1:124:A:VAL:HG11 | 1:124:A:VAL:HB  | 14       | 0.23          |
| (1,3200) | 1:116:A:GLN:HG3  | 1:113:A:ALA:HB3 | 6        | 0.23          |
| (1,3195) | 1:113:A:ALA:HA   | 1:113:A:ALA:H   | 5        | 0.23          |
| (1,3195) | 1:113:A:ALA:HA   | 1:113:A:ALA:H   | 7        | 0.23          |
| (1,3195) | 1:113:A:ALA:HA   | 1:113:A:ALA:H   | 8        | 0.23          |
| (1,3195) | 1:113:A:ALA:HA   | 1:113:A:ALA:H   | 10       | 0.23          |
| (1,3195) | 1:113:A:ALA:HA   | 1:113:A:ALA:H   | 13       | 0.23          |
| (1,3195) | 1:113:A:ALA:HA   | 1:113:A:ALA:H   | 16       | 0.23          |
| (1,3195) | 1:113:A:ALA:HA   | 1:113:A:ALA:H   | 17       | 0.23          |
| (1,3183) | 1:124:A:VAL:HG22 | 1:121:A:LYS:HA  | 4        | 0.23          |
| (1,3183) | 1:124:A:VAL:HG22 | 1:121:A:LYS:HA  | 11       | 0.23          |
| (1,3183) | 1:124:A:VAL:HG22 | 1:121:A:LYS:HA  | 13       | 0.23          |
| (1,3181) | 1:108:A:GLN:HG3  | 1:108:A:GLN:HA  | 14       | 0.23          |
| (1,3172) | 1:25:A:LYS:HE3   | 1:25:A:LYS:HA   | 1        | 0.23          |
| (1,3172) | 1:25:A:LYS:HE3   | 1:25:A:LYS:HA   | 2        | 0.23          |
| (1,3166) | 1:75:A:LEU:HD23  | 1:53:A:PHE:HD1  | 1        | 0.23          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3166) | 1:75:A:LEU:HD22 | 1:53:A:PHE:HD2  | 4        | 0.23          |
| (1,3166) | 1:75:A:LEU:HD21 | 1:53:A:PHE:HD1  | 8        | 0.23          |
| (1,3166) | 1:75:A:LEU:HD23 | 1:53:A:PHE:HD2  | 10       | 0.23          |
| (1,3166) | 1:75:A:LEU:HD22 | 1:53:A:PHE:HD2  | 13       | 0.23          |
| (1,3165) | 1:126:A:ALA:HB3 | 1:125:A:GLN:HG3 | 14       | 0.23          |
| (1,3161) | 1:82:A:TRP:HH2  | 1:120:A:ALA:HB3 | 11       | 0.23          |
| (1,3132) | 1:68:A:LYS:HB2  | 1:53:A:PHE:HE1  | 10       | 0.23          |
| (1,3132) | 1:68:A:LYS:HB2  | 1:53:A:PHE:HE1  | 12       | 0.23          |
| (1,3132) | 1:68:A:LYS:HB2  | 1:53:A:PHE:HE1  | 13       | 0.23          |
| (1,3132) | 1:68:A:LYS:HB2  | 1:53:A:PHE:HE2  | 15       | 0.23          |
| (1,3103) | 1:56:A:LEU:HD13 | 1:60:A:VAL:HB   | 16       | 0.23          |
| (1,3080) | 1:125:A:GLN:HB2 | 1:125:A:GLN:HA  | 7        | 0.23          |
| (1,3080) | 1:125:A:GLN:HB2 | 1:125:A:GLN:HA  | 8        | 0.23          |
| (1,3080) | 1:125:A:GLN:HB2 | 1:125:A:GLN:HA  | 15       | 0.23          |
| (1,3067) | 1:52:A:ILE:HG22 | 1:53:A:PHE:HB3  | 5        | 0.23          |
| (1,3067) | 1:52:A:ILE:HG21 | 1:53:A:PHE:HB3  | 14       | 0.23          |
| (1,3066) | 1:30:A:PHE:HB3  | 1:29:A:ALA:HB2  | 10       | 0.23          |
| (1,3052) | 1:39:A:PHE:HZ   | 1:52:A:ILE:HG23 | 6        | 0.23          |
| (1,3036) | 1:78:A:TYR:HH   | 1:45:A:ALA:HB1  | 17       | 0.23          |
| (1,3035) | 1:25:A:LYS:H    | 1:25:A:LYS:HG2  | 14       | 0.23          |
| (1,3032) | 1:121:A:LYS:HG3 | 1:121:A:LYS:HE3 | 1        | 0.23          |
| (1,3028) | 1:71:A:LEU:HD11 | 1:72:A:ARG:HA   | 4        | 0.23          |
| (1,3028) | 1:71:A:LEU:HD13 | 1:72:A:ARG:HA   | 15       | 0.23          |
| (1,2992) | 1:20:A:LYS:HB3  | 1:20:A:LYS:H    | 1        | 0.23          |
| (1,2989) | 1:42:A:GLU:HA   | 1:42:A:GLU:HB2  | 13       | 0.23          |
| (1,2989) | 1:42:A:GLU:HA   | 1:42:A:GLU:HB2  | 16       | 0.23          |
| (1,2969) | 1:93:A:THR:HG22 | 1:101:A:PRO:HB3 | 15       | 0.23          |
| (1,2960) | 1:77:A:LEU:HD12 | 1:25:A:LYS:HA   | 14       | 0.23          |
| (1,2950) | 1:75:A:LEU:HD11 | 1:75:A:LEU:H    | 6        | 0.23          |
| (1,2932) | 1:95:A:VAL:HG23 | 1:95:A:VAL:H    | 3        | 0.23          |
| (1,2888) | 1:29:A:ALA:HA   | 1:32:A:ALA:HB3  | 6        | 0.23          |
| (1,2861) | 1:84:A:TYR:HE2  | 1:84:A:TYR:HA   | 2        | 0.23          |
| (1,2851) | 1:50:A:ILE:HG22 | 1:50:A:ILE:HA   | 4        | 0.23          |
| (1,2851) | 1:50:A:ILE:HG22 | 1:50:A:ILE:HA   | 17       | 0.23          |
| (1,2831) | 1:97:A:LEU:HD21 | 1:35:A:PHE:HD1  | 16       | 0.23          |
| (1,2829) | 1:97:A:LEU:HD22 | 1:97:A:LEU:HB2  | 2        | 0.23          |
| (1,2829) | 1:97:A:LEU:HD22 | 1:97:A:LEU:HB2  | 14       | 0.23          |
| (1,2745) | 1:34:A:ARG:HD3  | 1:34:A:ARG:HG3  | 1        | 0.23          |
| (1,2745) | 1:34:A:ARG:HD3  | 1:34:A:ARG:HG3  | 4        | 0.23          |
| (1,2745) | 1:34:A:ARG:HD3  | 1:34:A:ARG:HG3  | 6        | 0.23          |
| (1,2745) | 1:34:A:ARG:HD3  | 1:34:A:ARG:HG3  | 8        | 0.23          |
| (1,2745) | 1:34:A:ARG:HD3  | 1:34:A:ARG:HG3  | 10       | 0.23          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2745) | 1:34:A:ARG:HD3   | 1:34:A:ARG:HG3  | 13       | 0.23          |
| (1,2745) | 1:34:A:ARG:HD3   | 1:34:A:ARG:HG3  | 14       | 0.23          |
| (1,2729) | 1:17:A:ASN:HB3   | 1:17:A:ASN:HB2  | 2        | 0.23          |
| (1,2729) | 1:17:A:ASN:HB3   | 1:17:A:ASN:HB2  | 8        | 0.23          |
| (1,2729) | 1:17:A:ASN:HB3   | 1:17:A:ASN:HB2  | 9        | 0.23          |
| (1,2729) | 1:17:A:ASN:HB3   | 1:17:A:ASN:HB2  | 11       | 0.23          |
| (1,2729) | 1:17:A:ASN:HB3   | 1:17:A:ASN:HB2  | 14       | 0.23          |
| (1,2729) | 1:17:A:ASN:HB3   | 1:17:A:ASN:HB2  | 15       | 0.23          |
| (1,2729) | 1:17:A:ASN:HB3   | 1:17:A:ASN:HB2  | 16       | 0.23          |
| (1,2729) | 1:17:A:ASN:HB3   | 1:17:A:ASN:HB2  | 17       | 0.23          |
| (1,2713) | 1:53:A:PHE:HB3   | 1:75:A:LEU:HD13 | 3        | 0.23          |
| (1,2713) | 1:53:A:PHE:HB3   | 1:75:A:LEU:HD13 | 9        | 0.23          |
| (1,2713) | 1:53:A:PHE:HB3   | 1:75:A:LEU:HD11 | 15       | 0.23          |
| (1,2694) | 1:73:A:SER:HB2   | 1:74:A:ALA:H    | 2        | 0.23          |
| (1,2679) | 1:53:A:PHE:HA    | 1:53:A:PHE:HE1  | 8        | 0.23          |
| (1,2672) | 1:31:A:LEU:HD13  | 1:35:A:PHE:HD2  | 9        | 0.23          |
| (1,2622) | 1:71:A:LEU:HD13  | 1:57:A:VAL:H    | 10       | 0.23          |
| (1,2618) | 1:34:A:ARG:HG3   | 1:34:A:ARG:H    | 4        | 0.23          |
| (1,2618) | 1:34:A:ARG:HG3   | 1:34:A:ARG:H    | 5        | 0.23          |
| (1,2618) | 1:34:A:ARG:HG3   | 1:34:A:ARG:H    | 6        | 0.23          |
| (1,2618) | 1:34:A:ARG:HG3   | 1:34:A:ARG:H    | 15       | 0.23          |
| (1,2618) | 1:34:A:ARG:HG3   | 1:34:A:ARG:H    | 17       | 0.23          |
| (1,2605) | 1:31:A:LEU:HD22  | 1:30:A:PHE:HD2  | 9        | 0.23          |
| (1,2576) | 1:124:A:VAL:HG21 | 1:120:A:ALA:HA  | 9        | 0.23          |
| (1,2560) | 1:86:A:TYR:HE1   | 1:86:A:TYR:HD1  | 4        | 0.23          |
| (1,2559) | 1:86:A:TYR:HE2   | 1:86:A:TYR:HB2  | 5        | 0.23          |
| (1,2547) | 1:11:A:SER:HA    | 1:12:A:GLN:HG3  | 13       | 0.23          |
| (1,2529) | 1:79:A:THR:HG23  | 1:75:A:LEU:HA   | 16       | 0.23          |
| (1,2527) | 1:123:A:ARG:H    | 1:123:A:ARG:HA  | 1        | 0.23          |
| (1,2527) | 1:123:A:ARG:H    | 1:123:A:ARG:HA  | 5        | 0.23          |
| (1,2527) | 1:123:A:ARG:H    | 1:123:A:ARG:HA  | 6        | 0.23          |
| (1,2527) | 1:123:A:ARG:H    | 1:123:A:ARG:HA  | 7        | 0.23          |
| (1,2527) | 1:123:A:ARG:H    | 1:123:A:ARG:HA  | 8        | 0.23          |
| (1,2527) | 1:123:A:ARG:H    | 1:123:A:ARG:HA  | 9        | 0.23          |
| (1,2527) | 1:123:A:ARG:H    | 1:123:A:ARG:HA  | 10       | 0.23          |
| (1,2527) | 1:123:A:ARG:H    | 1:123:A:ARG:HA  | 11       | 0.23          |
| (1,2527) | 1:123:A:ARG:H    | 1:123:A:ARG:HA  | 12       | 0.23          |
| (1,2527) | 1:123:A:ARG:H    | 1:123:A:ARG:HA  | 16       | 0.23          |
| (1,2527) | 1:123:A:ARG:H    | 1:123:A:ARG:HA  | 17       | 0.23          |
| (1,2515) | 1:122:A:ALA:HA   | 1:122:A:ALA:H   | 11       | 0.23          |
| (1,2515) | 1:122:A:ALA:HA   | 1:122:A:ALA:H   | 12       | 0.23          |
| (1,2515) | 1:122:A:ALA:HA   | 1:122:A:ALA:H   | 16       | 0.23          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2505) | 1:126:A:ALA:HA   | 1:126:A:ALA:H    | 5        | 0.23          |
| (1,2505) | 1:126:A:ALA:HA   | 1:126:A:ALA:H    | 12       | 0.23          |
| (1,2505) | 1:126:A:ALA:HA   | 1:126:A:ALA:H    | 15       | 0.23          |
| (1,2444) | 1:53:A:PHE:HE1   | 1:53:A:PHE:HB2   | 2        | 0.23          |
| (1,2444) | 1:53:A:PHE:HE2   | 1:53:A:PHE:HB2   | 9        | 0.23          |
| (1,2444) | 1:53:A:PHE:HE1   | 1:53:A:PHE:HB2   | 14       | 0.23          |
| (1,2434) | 1:86:A:TYR:HB2   | 1:117:A:LEU:HB3  | 5        | 0.23          |
| (1,2434) | 1:86:A:TYR:HB2   | 1:117:A:LEU:HB3  | 8        | 0.23          |
| (1,2434) | 1:86:A:TYR:HB2   | 1:117:A:LEU:HB3  | 10       | 0.23          |
| (1,2434) | 1:86:A:TYR:HB2   | 1:117:A:LEU:HB3  | 16       | 0.23          |
| (1,2434) | 1:86:A:TYR:HB2   | 1:117:A:LEU:HB3  | 17       | 0.23          |
| (1,2415) | 1:45:A:ALA:HB3   | 1:84:A:TYR:HD1   | 9        | 0.23          |
| (1,2404) | 1:28:A:ILE:HD11  | 1:74:A:ALA:HA    | 1        | 0.23          |
| (1,2404) | 1:28:A:ILE:HD13  | 1:74:A:ALA:HA    | 5        | 0.23          |
| (1,2404) | 1:28:A:ILE:HD12  | 1:74:A:ALA:HA    | 6        | 0.23          |
| (1,2404) | 1:28:A:ILE:HD13  | 1:74:A:ALA:HA    | 14       | 0.23          |
| (1,2404) | 1:28:A:ILE:HD12  | 1:74:A:ALA:HA    | 16       | 0.23          |
| (1,2358) | 1:107:A:GLU:HA   | 1:111:A:GLU:H    | 2        | 0.23          |
| (1,2358) | 1:107:A:GLU:HA   | 1:111:A:GLU:H    | 12       | 0.23          |
| (1,2358) | 1:107:A:GLU:HA   | 1:111:A:GLU:H    | 13       | 0.23          |
| (1,2348) | 1:30:A:PHE:HD1   | 1:21:A:LEU:HD13  | 7        | 0.23          |
| (1,2346) | 1:105:A:LEU:HD11 | 1:107:A:GLU:HA   | 3        | 0.23          |
| (1,2346) | 1:105:A:LEU:HD12 | 1:107:A:GLU:HA   | 13       | 0.23          |
| (1,2299) | 1:55:A:ASP:HB3   | 1:96:A:ASP:HA    | 16       | 0.23          |
| (1,2210) | 1:105:A:LEU:HG   | 1:110:A:VAL:HG12 | 2        | 0.23          |
| (1,2210) | 1:105:A:LEU:HG   | 1:110:A:VAL:HG13 | 3        | 0.23          |
| (1,2210) | 1:105:A:LEU:HG   | 1:110:A:VAL:HG12 | 8        | 0.23          |
| (1,2210) | 1:105:A:LEU:HG   | 1:110:A:VAL:HG11 | 9        | 0.23          |
| (1,2210) | 1:105:A:LEU:HG   | 1:110:A:VAL:HG13 | 13       | 0.23          |
| (1,2075) | 1:61:A:ALA:HB2   | 1:62:A:GLY:H     | 3        | 0.23          |
| (1,2037) | 1:57:A:VAL:HG23  | 1:57:A:VAL:HG11  | 4        | 0.23          |
| (1,2037) | 1:57:A:VAL:HG23  | 1:57:A:VAL:HG11  | 9        | 0.23          |
| (1,2035) | 1:52:A:ILE:HG13  | 1:97:A:LEU:HD23  | 6        | 0.23          |
| (1,2035) | 1:52:A:ILE:HG13  | 1:97:A:LEU:HD23  | 10       | 0.23          |
| (1,2035) | 1:52:A:ILE:HG13  | 1:97:A:LEU:HD21  | 11       | 0.23          |
| (1,2025) | 1:97:A:LEU:HD22  | 1:35:A:PHE:HD2   | 5        | 0.23          |
| (1,1947) | 1:93:A:THR:HB    | 1:88:A:VAL:HG12  | 13       | 0.23          |
| (1,1947) | 1:93:A:THR:HB    | 1:88:A:VAL:HG13  | 15       | 0.23          |
| (1,1904) | 1:74:A:ALA:HB3   | 1:28:A:ILE:HA    | 11       | 0.23          |
| (1,1890) | 1:100:A:ASN:HD22 | 1:98:A:ASP:HB3   | 8        | 0.23          |
| (1,1890) | 1:100:A:ASN:HD22 | 1:98:A:ASP:HB3   | 13       | 0.23          |
| (1,1886) | 1:102:A:CYS:HB3  | 1:49:A:LYS:HA    | 11       | 0.23          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1881) | 1:113:A:ALA:HB2 | 1:88:A:VAL:HA    | 10       | 0.23          |
| (1,1831) | 1:21:A:LEU:HG   | 1:21:A:LEU:HB3   | 1        | 0.23          |
| (1,1831) | 1:21:A:LEU:HG   | 1:21:A:LEU:HB3   | 11       | 0.23          |
| (1,1817) | 1:77:A:LEU:HG   | 1:77:A:LEU:HD23  | 7        | 0.23          |
| (1,1812) | 1:117:A:LEU:HA  | 1:117:A:LEU:HD11 | 17       | 0.23          |
| (1,1811) | 1:86:A:TYR:H    | 1:117:A:LEU:HD11 | 4        | 0.23          |
| (1,1799) | 1:71:A:LEU:HA   | 1:74:A:ALA:HB3   | 13       | 0.23          |
| (1,1773) | 1:24:A:SER:HA   | 1:27:A:VAL:HG23  | 1        | 0.23          |
| (1,1773) | 1:24:A:SER:HA   | 1:27:A:VAL:HG23  | 4        | 0.23          |
| (1,1773) | 1:24:A:SER:HA   | 1:27:A:VAL:HG23  | 8        | 0.23          |
| (1,1773) | 1:24:A:SER:HA   | 1:27:A:VAL:HG22  | 12       | 0.23          |
| (1,1773) | 1:24:A:SER:HA   | 1:27:A:VAL:HG23  | 14       | 0.23          |
| (1,1773) | 1:24:A:SER:HA   | 1:27:A:VAL:HG21  | 15       | 0.23          |
| (1,1752) | 1:41:A:ALA:HB3  | 1:28:A:ILE:HG22  | 11       | 0.23          |
| (1,1746) | 1:71:A:LEU:HD21 | 1:74:A:ALA:H     | 3        | 0.23          |
| (1,1741) | 1:55:A:ASP:HB2  | 1:56:A:LEU:HD23  | 10       | 0.23          |
| (1,1741) | 1:55:A:ASP:HB2  | 1:56:A:LEU:HD21  | 12       | 0.23          |
| (1,1736) | 1:77:A:LEU:HB3  | 1:77:A:LEU:HD13  | 3        | 0.23          |
| (1,1736) | 1:77:A:LEU:HB3  | 1:77:A:LEU:HD11  | 6        | 0.23          |
| (1,1736) | 1:77:A:LEU:HB3  | 1:77:A:LEU:HD11  | 13       | 0.23          |
| (1,1736) | 1:77:A:LEU:HB3  | 1:77:A:LEU:HD11  | 16       | 0.23          |
| (1,1735) | 1:66:A:LEU:HD23 | 1:67:A:SER:H     | 15       | 0.23          |
| (1,1733) | 1:30:A:PHE:HD1  | 1:66:A:LEU:HD21  | 1        | 0.23          |
| (1,1733) | 1:30:A:PHE:HD2  | 1:66:A:LEU:HD23  | 2        | 0.23          |
| (1,1733) | 1:30:A:PHE:HD2  | 1:66:A:LEU:HD21  | 4        | 0.23          |
| (1,1733) | 1:30:A:PHE:HD2  | 1:66:A:LEU:HD21  | 6        | 0.23          |
| (1,1733) | 1:30:A:PHE:HD1  | 1:66:A:LEU:HD21  | 7        | 0.23          |
| (1,1733) | 1:30:A:PHE:HD2  | 1:66:A:LEU:HD22  | 8        | 0.23          |
| (1,1733) | 1:30:A:PHE:HD1  | 1:66:A:LEU:HD23  | 16       | 0.23          |
| (1,1730) | 1:27:A:VAL:HA   | 1:66:A:LEU:HD23  | 2        | 0.23          |
| (1,1730) | 1:27:A:VAL:HA   | 1:66:A:LEU:HD21  | 13       | 0.23          |
| (1,1730) | 1:27:A:VAL:HA   | 1:66:A:LEU:HD23  | 16       | 0.23          |
| (1,1723) | 1:68:A:LYS:HD3  | 1:57:A:VAL:HG11  | 8        | 0.23          |
| (1,1723) | 1:68:A:LYS:HD3  | 1:57:A:VAL:HG11  | 10       | 0.23          |
| (1,1713) | 1:20:A:LYS:H    | 1:20:A:LYS:HD3   | 3        | 0.23          |
| (1,1698) | 1:44:A:GLU:HG2  | 1:45:A:ALA:HB1   | 5        | 0.23          |
| (1,1686) | 1:85:A:LEU:HD12 | 1:85:A:LEU:HD22  | 17       | 0.23          |
| (1,1681) | 1:40:A:SER:HA   | 1:41:A:ALA:HB1   | 13       | 0.23          |
| (1,1668) | 1:52:A:ILE:HG13 | 1:48:A:LEU:HD12  | 14       | 0.23          |
| (1,1629) | 1:116:A:GLN:HG3 | 1:113:A:ALA:HB3  | 5        | 0.23          |
| (1,1618) | 1:109:A:HIS:HB2 | 1:110:A:VAL:HG13 | 6        | 0.23          |
| (1,1616) | 1:109:A:HIS:HB2 | 1:108:A:GLN:H    | 1        | 0.23          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1592) | 1:126:A:ALA:HB1  | 1:125:A:GLN:HG3 | 2        | 0.23          |
| (1,1592) | 1:126:A:ALA:HB1  | 1:125:A:GLN:HG3 | 7        | 0.23          |
| (1,1592) | 1:126:A:ALA:HB3  | 1:125:A:GLN:HG3 | 13       | 0.23          |
| (1,1592) | 1:126:A:ALA:HB1  | 1:125:A:GLN:HG3 | 15       | 0.23          |
| (1,1588) | 1:74:A:ALA:HB1   | 1:74:A:ALA:HA   | 9        | 0.23          |
| (1,1588) | 1:74:A:ALA:HB1   | 1:74:A:ALA:HA   | 13       | 0.23          |
| (1,1552) | 1:124:A:VAL:HG12 | 1:124:A:VAL:HB  | 1        | 0.23          |
| (1,1552) | 1:124:A:VAL:HG12 | 1:124:A:VAL:HB  | 6        | 0.23          |
| (1,1552) | 1:124:A:VAL:HG13 | 1:124:A:VAL:HB  | 13       | 0.23          |
| (1,1552) | 1:124:A:VAL:HG11 | 1:124:A:VAL:HB  | 15       | 0.23          |
| (1,1552) | 1:124:A:VAL:HG11 | 1:124:A:VAL:HB  | 17       | 0.23          |
| (1,1521) | 1:30:A:PHE:HB3   | 1:29:A:ALA:HB1  | 4        | 0.23          |
| (1,1513) | 1:52:A:ILE:HG22  | 1:53:A:PHE:HB3  | 13       | 0.23          |
| (1,1508) | 1:29:A:ALA:H     | 1:28:A:ILE:HG22 | 1        | 0.23          |
| (1,1508) | 1:29:A:ALA:H     | 1:28:A:ILE:HG23 | 15       | 0.23          |
| (1,1485) | 1:71:A:LEU:HD13  | 1:72:A:ARG:HA   | 11       | 0.23          |
| (1,1478) | 1:64:A:MET:HE3   | 1:66:A:LEU:H    | 14       | 0.23          |
| (1,1428) | 1:93:A:THR:HG22  | 1:101:A:PRO:HB3 | 8        | 0.23          |
| (1,1428) | 1:93:A:THR:HG21  | 1:101:A:PRO:HB3 | 14       | 0.23          |
| (1,1399) | 1:95:A:VAL:HG22  | 1:95:A:VAL:H    | 11       | 0.23          |
| (1,1397) | 1:31:A:LEU:HD22  | 1:60:A:VAL:HG11 | 15       | 0.23          |
| (1,1395) | 1:31:A:LEU:HD23  | 1:39:A:PHE:HD2  | 3        | 0.23          |
| (1,1395) | 1:31:A:LEU:HD22  | 1:39:A:PHE:HD2  | 6        | 0.23          |
| (1,1395) | 1:31:A:LEU:HD23  | 1:39:A:PHE:HD1  | 8        | 0.23          |
| (1,1395) | 1:31:A:LEU:HD23  | 1:39:A:PHE:HD2  | 11       | 0.23          |
| (1,1395) | 1:31:A:LEU:HD22  | 1:39:A:PHE:HD1  | 13       | 0.23          |
| (1,1395) | 1:31:A:LEU:HD22  | 1:39:A:PHE:HD1  | 14       | 0.23          |
| (1,1395) | 1:31:A:LEU:HD23  | 1:39:A:PHE:HD1  | 15       | 0.23          |
| (1,1382) | 1:57:A:VAL:HG22  | 1:53:A:PHE:HE2  | 15       | 0.23          |
| (1,1371) | 1:28:A:ILE:HD11  | 1:75:A:LEU:H    | 12       | 0.23          |
| (1,1365) | 1:32:A:ALA:HB2   | 1:28:A:ILE:HG23 | 16       | 0.23          |
| (1,1350) | 1:129:A:ALA:HB2  | 1:129:A:ALA:H   | 9        | 0.23          |
| (1,1337) | 1:78:A:TYR:HD1   | 1:28:A:ILE:HD12 | 16       | 0.23          |
| (1,1232) | 1:60:A:VAL:HG13  | 1:59:A:ARG:HD3  | 6        | 0.23          |
| (1,1232) | 1:60:A:VAL:HG12  | 1:59:A:ARG:HD3  | 10       | 0.23          |
| (1,1232) | 1:60:A:VAL:HG11  | 1:59:A:ARG:HD3  | 12       | 0.23          |
| (1,1232) | 1:60:A:VAL:HG13  | 1:59:A:ARG:HD3  | 14       | 0.23          |
| (1,1232) | 1:60:A:VAL:HG11  | 1:59:A:ARG:HD3  | 17       | 0.23          |
| (1,1210) | 1:86:A:TYR:HB3   | 1:86:A:TYR:H    | 1        | 0.23          |
| (1,1210) | 1:86:A:TYR:HB3   | 1:86:A:TYR:H    | 2        | 0.23          |
| (1,1210) | 1:86:A:TYR:HB3   | 1:86:A:TYR:H    | 6        | 0.23          |
| (1,1210) | 1:86:A:TYR:HB3   | 1:86:A:TYR:H    | 7        | 0.23          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1210) | 1:86:A:TYR:HB3   | 1:86:A:TYR:H    | 15       | 0.23          |
| (1,1194) | 1:39:A:PHE:HB3   | 1:35:A:PHE:HB3  | 1        | 0.23          |
| (1,1194) | 1:39:A:PHE:HB3   | 1:35:A:PHE:HB3  | 3        | 0.23          |
| (1,1194) | 1:39:A:PHE:HB3   | 1:35:A:PHE:HB3  | 9        | 0.23          |
| (1,1194) | 1:39:A:PHE:HB3   | 1:35:A:PHE:HB3  | 11       | 0.23          |
| (1,1194) | 1:39:A:PHE:HB3   | 1:35:A:PHE:HB3  | 12       | 0.23          |
| (1,1194) | 1:39:A:PHE:HB3   | 1:35:A:PHE:HB3  | 16       | 0.23          |
| (1,1136) | 1:31:A:LEU:HD12  | 1:35:A:PHE:HD2  | 7        | 0.23          |
| (1,1080) | 1:105:A:LEU:HD11 | 1:92:A:ALA:H    | 1        | 0.23          |
| (1,1080) | 1:105:A:LEU:HD12 | 1:92:A:ALA:H    | 3        | 0.23          |
| (1,1080) | 1:105:A:LEU:HD11 | 1:92:A:ALA:H    | 7        | 0.23          |
| (1,1080) | 1:105:A:LEU:HD13 | 1:92:A:ALA:H    | 9        | 0.23          |
| (1,1080) | 1:105:A:LEU:HD13 | 1:92:A:ALA:H    | 13       | 0.23          |
| (1,1062) | 1:27:A:VAL:HG21  | 1:27:A:VAL:HG11 | 5        | 0.23          |
| (1,1062) | 1:27:A:VAL:HG22  | 1:27:A:VAL:HG13 | 12       | 0.23          |
| (1,1060) | 1:74:A:ALA:HB3   | 1:27:A:VAL:HG13 | 12       | 0.23          |
| (1,993)  | 1:79:A:THR:HG22  | 1:75:A:LEU:HA   | 4        | 0.23          |
| (1,895)  | 1:129:A:ALA:HB2  | 1:129:A:ALA:HA  | 13       | 0.23          |
| (1,853)  | 1:65:A:ASN:HB2   | 1:65:A:ASN:HD21 | 15       | 0.23          |
| (1,852)  | 1:65:A:ASN:HB3   | 1:65:A:ASN:HD21 | 7        | 0.23          |
| (1,829)  | 1:41:A:ALA:HB2   | 1:41:A:ALA:H    | 11       | 0.23          |
| (1,827)  | 1:45:A:ALA:HB1   | 1:45:A:ALA:H    | 7        | 0.23          |
| (1,827)  | 1:45:A:ALA:HB3   | 1:45:A:ALA:H    | 12       | 0.23          |
| (1,691)  | 1:75:A:LEU:HD22  | 1:54:A:GLN:H    | 13       | 0.23          |
| (1,618)  | 1:95:A:VAL:H     | 1:48:A:LEU:HD12 | 10       | 0.23          |
| (1,618)  | 1:95:A:VAL:H     | 1:48:A:LEU:HD11 | 13       | 0.23          |
| (1,564)  | 1:59:A:ARG:HE    | 1:97:A:LEU:HD11 | 1        | 0.23          |
| (1,557)  | 1:66:A:LEU:HB2   | 1:70:A:GLN:HE22 | 7        | 0.23          |
| (1,552)  | 1:65:A:ASN:H     | 1:65:A:ASN:HD21 | 1        | 0.23          |
| (1,552)  | 1:65:A:ASN:H     | 1:65:A:ASN:HD21 | 11       | 0.23          |
| (1,552)  | 1:65:A:ASN:H     | 1:65:A:ASN:HD21 | 12       | 0.23          |
| (1,552)  | 1:65:A:ASN:H     | 1:65:A:ASN:HD21 | 15       | 0.23          |
| (1,524)  | 1:20:A:LYS:HB3   | 1:22:A:ASN:HD22 | 13       | 0.23          |
| (1,451)  | 1:32:A:ALA:HB2   | 1:35:A:PHE:H    | 15       | 0.23          |
| (1,441)  | 1:42:A:GLU:HB3   | 1:41:A:ALA:H    | 3        | 0.23          |
| (1,441)  | 1:42:A:GLU:HB3   | 1:41:A:ALA:H    | 6        | 0.23          |
| (1,441)  | 1:42:A:GLU:HB3   | 1:41:A:ALA:H    | 10       | 0.23          |
| (1,441)  | 1:42:A:GLU:HB3   | 1:41:A:ALA:H    | 12       | 0.23          |
| (1,241)  | 1:95:A:VAL:HG13  | 1:96:A:ASP:H    | 2        | 0.23          |
| (1,234)  | 1:95:A:VAL:HG21  | 1:99:A:GLY:H    | 17       | 0.23          |
| (1,172)  | 1:27:A:VAL:HG12  | 1:21:A:LEU:H    | 2        | 0.23          |
| (1,172)  | 1:27:A:VAL:HG12  | 1:21:A:LEU:H    | 4        | 0.23          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,154)  | 1:130:A:GLU:H   | 1:129:A:ALA:HB3  | 4        | 0.23          |
| (1,154)  | 1:130:A:GLU:H   | 1:129:A:ALA:HB1  | 16       | 0.23          |
| (1,117)  | 1:27:A:VAL:HG13 | 1:26:A:GLU:H     | 16       | 0.23          |
| (1,100)  | 1:35:A:PHE:HE1  | 1:35:A:PHE:H     | 2        | 0.23          |
| (1,100)  | 1:35:A:PHE:HE1  | 1:35:A:PHE:H     | 12       | 0.23          |
| (1,100)  | 1:35:A:PHE:HE2  | 1:35:A:PHE:H     | 14       | 0.23          |
| (1,100)  | 1:35:A:PHE:HE2  | 1:35:A:PHE:H     | 17       | 0.23          |
| (1,56)   | 1:84:A:TYR:H    | 1:84:A:TYR:HD1   | 1        | 0.23          |
| (1,56)   | 1:84:A:TYR:H    | 1:84:A:TYR:HD1   | 3        | 0.23          |
| (1,56)   | 1:84:A:TYR:H    | 1:84:A:TYR:HD2   | 12       | 0.23          |
| (1,12)   | 1:100:A:ASN:H   | 1:100:A:ASN:HD21 | 5        | 0.23          |
| (1,12)   | 1:100:A:ASN:H   | 1:100:A:ASN:HD21 | 17       | 0.23          |
| (3,122)  | 1:27:A:VAL:HG23 | 1:28:A:ILE:HD11  | 13       | 0.22          |
| (3,111)  | 1:111:A:GLU:HG2 | 1:112:A:HIS:HA   | 14       | 0.22          |
| (3,92)   | 1:88:A:VAL:HG21 | 1:87:A:GLY:HA2   | 7        | 0.22          |
| (3,83)   | 1:114:A:ARG:HB2 | 1:113:A:ALA:HB3  | 8        | 0.22          |
| (3,59)   | 1:117:A:LEU:HA  | 1:85:A:LEU:HD22  | 13       | 0.22          |
| (3,16)   | 1:90:A:PRO:HA   | 1:110:A:VAL:HG12 | 1        | 0.22          |
| (3,16)   | 1:90:A:PRO:HA   | 1:110:A:VAL:HG11 | 13       | 0.22          |
| (1,4342) | 1:38:A:CYS:H    | 1:95:A:VAL:HG13  | 13       | 0.22          |
| (1,4299) | 1:65:A:ASN:HD22 | 1:65:A:ASN:HD21  | 13       | 0.22          |
| (1,4176) | 1:97:A:LEU:HD13 | 1:97:A:LEU:H     | 9        | 0.22          |
| (1,4172) | 1:105:A:LEU:H   | 1:92:A:ALA:H     | 3        | 0.22          |
| (1,4153) | 1:18:A:GLN:HB3  | 1:18:A:GLN:H     | 2        | 0.22          |
| (1,4153) | 1:18:A:GLN:HB3  | 1:18:A:GLN:H     | 11       | 0.22          |
| (1,4144) | 1:21:A:LEU:H    | 1:65:A:ASN:HB3   | 14       | 0.22          |
| (1,4127) | 1:34:A:ARG:HE   | 1:30:A:PHE:HD2   | 17       | 0.22          |
| (1,4109) | 1:97:A:LEU:HD11 | 1:98:A:ASP:H     | 15       | 0.22          |
| (1,4036) | 1:31:A:LEU:H    | 1:31:A:LEU:HD11  | 15       | 0.22          |
| (1,4017) | 1:32:A:ALA:HB3  | 1:35:A:PHE:H     | 14       | 0.22          |
| (1,3961) | 1:57:A:VAL:H    | 1:56:A:LEU:HB3   | 6        | 0.22          |
| (1,3941) | 1:63:A:GLU:H    | 1:61:A:ALA:HB3   | 7        | 0.22          |
| (1,3941) | 1:63:A:GLU:H    | 1:61:A:ALA:HB3   | 8        | 0.22          |
| (1,3941) | 1:63:A:GLU:H    | 1:61:A:ALA:HB3   | 10       | 0.22          |
| (1,3901) | 1:79:A:THR:H    | 1:77:A:LEU:HB2   | 1        | 0.22          |
| (1,3901) | 1:79:A:THR:H    | 1:77:A:LEU:HB2   | 2        | 0.22          |
| (1,3874) | 1:85:A:LEU:HB3  | 1:86:A:TYR:H     | 1        | 0.22          |
| (1,3874) | 1:85:A:LEU:HB3  | 1:86:A:TYR:H     | 5        | 0.22          |
| (1,3874) | 1:85:A:LEU:HB3  | 1:86:A:TYR:H     | 8        | 0.22          |
| (1,3845) | 1:95:A:VAL:HG11 | 1:96:A:ASP:H     | 16       | 0.22          |
| (1,3816) | 1:105:A:LEU:H   | 1:105:A:LEU:HD21 | 15       | 0.22          |
| (1,3781) | 1:119:A:GLU:HA  | 1:119:A:GLU:H    | 6        | 0.22          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3776) | 1:121:A:LYS:HA  | 1:122:A:ALA:H    | 11       | 0.22          |
| (1,3775) | 1:124:A:VAL:HA  | 1:125:A:GLN:H    | 5        | 0.22          |
| (1,3775) | 1:124:A:VAL:HA  | 1:125:A:GLN:H    | 7        | 0.22          |
| (1,3775) | 1:124:A:VAL:HA  | 1:125:A:GLN:H    | 12       | 0.22          |
| (1,3775) | 1:124:A:VAL:HA  | 1:125:A:GLN:H    | 15       | 0.22          |
| (1,3775) | 1:124:A:VAL:HA  | 1:125:A:GLN:H    | 17       | 0.22          |
| (1,3773) | 1:123:A:ARG:HA  | 1:124:A:VAL:H    | 10       | 0.22          |
| (1,3769) | 1:130:A:GLU:H   | 1:129:A:ALA:HB3  | 1        | 0.22          |
| (1,3749) | 1:123:A:ARG:H   | 1:121:A:LYS:H    | 1        | 0.22          |
| (1,3716) | 1:35:A:PHE:HE2  | 1:35:A:PHE:H     | 4        | 0.22          |
| (1,3698) | 1:30:A:PHE:HD2  | 1:30:A:PHE:H     | 4        | 0.22          |
| (1,3698) | 1:30:A:PHE:HD2  | 1:30:A:PHE:H     | 6        | 0.22          |
| (1,3698) | 1:30:A:PHE:HD2  | 1:30:A:PHE:H     | 8        | 0.22          |
| (1,3698) | 1:30:A:PHE:HD2  | 1:30:A:PHE:H     | 9        | 0.22          |
| (1,3698) | 1:30:A:PHE:HD1  | 1:30:A:PHE:H     | 13       | 0.22          |
| (1,3668) | 1:84:A:TYR:H    | 1:84:A:TYR:HD2   | 10       | 0.22          |
| (1,3668) | 1:84:A:TYR:H    | 1:84:A:TYR:HD2   | 14       | 0.22          |
| (1,3662) | 1:83:A:ARG:H    | 1:82:A:TRP:HD1   | 5        | 0.22          |
| (1,3662) | 1:83:A:ARG:H    | 1:82:A:TRP:HD1   | 17       | 0.22          |
| (1,3592) | 1:109:A:HIS:HB2 | 1:110:A:VAL:HG11 | 5        | 0.22          |
| (1,3592) | 1:109:A:HIS:HB2 | 1:110:A:VAL:HG13 | 12       | 0.22          |
| (1,3591) | 1:93:A:THR:HB   | 1:88:A:VAL:HG13  | 1        | 0.22          |
| (1,3588) | 1:105:A:LEU:HB3 | 1:110:A:VAL:HG23 | 6        | 0.22          |
| (1,3583) | 1:112:A:HIS:H   | 1:109:A:HIS:HA   | 2        | 0.22          |
| (1,3583) | 1:112:A:HIS:H   | 1:109:A:HIS:HA   | 5        | 0.22          |
| (1,3580) | 1:111:A:GLU:HB2 | 1:109:A:HIS:HA   | 3        | 0.22          |
| (1,3580) | 1:111:A:GLU:HB2 | 1:109:A:HIS:HA   | 5        | 0.22          |
| (1,3580) | 1:111:A:GLU:HB2 | 1:109:A:HIS:HA   | 6        | 0.22          |
| (1,3580) | 1:111:A:GLU:HB2 | 1:109:A:HIS:HA   | 10       | 0.22          |
| (1,3580) | 1:111:A:GLU:HB2 | 1:109:A:HIS:HA   | 13       | 0.22          |
| (1,3580) | 1:111:A:GLU:HB2 | 1:109:A:HIS:HA   | 17       | 0.22          |
| (1,3562) | 1:104:A:GLU:HB3 | 1:91:A:GLY:HA3   | 4        | 0.22          |
| (1,3562) | 1:104:A:GLU:HB3 | 1:91:A:GLY:HA3   | 6        | 0.22          |
| (1,3562) | 1:104:A:GLU:HB3 | 1:91:A:GLY:HA3   | 12       | 0.22          |
| (1,3537) | 1:51:A:GLY:HA2  | 1:54:A:GLN:HB2   | 16       | 0.22          |
| (1,3536) | 1:66:A:LEU:HB3  | 1:62:A:GLY:HA3   | 2        | 0.22          |
| (1,3535) | 1:74:A:ALA:HB3  | 1:28:A:ILE:HA    | 3        | 0.22          |
| (1,3535) | 1:74:A:ALA:HB1  | 1:28:A:ILE:HA    | 7        | 0.22          |
| (1,3535) | 1:74:A:ALA:HB2  | 1:28:A:ILE:HA    | 9        | 0.22          |
| (1,3535) | 1:74:A:ALA:HB1  | 1:28:A:ILE:HA    | 17       | 0.22          |
| (1,3534) | 1:122:A:ALA:HB3 | 1:121:A:LYS:HE3  | 13       | 0.22          |
| (1,3516) | 1:21:A:LEU:HG   | 1:65:A:ASN:HB3   | 10       | 0.22          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3516) | 1:21:A:LEU:HG   | 1:65:A:ASN:HB3   | 17       | 0.22          |
| (1,3515) | 1:102:A:CYS:HB3 | 1:49:A:LYS:HA    | 5        | 0.22          |
| (1,3515) | 1:102:A:CYS:HB3 | 1:49:A:LYS:HA    | 9        | 0.22          |
| (1,3508) | 1:113:A:ALA:HB1 | 1:88:A:VAL:HA    | 9        | 0.22          |
| (1,3506) | 1:60:A:VAL:HG11 | 1:35:A:PHE:HZ    | 4        | 0.22          |
| (1,3503) | 1:27:A:VAL:HG23 | 1:31:A:LEU:H     | 3        | 0.22          |
| (1,3498) | 1:70:A:GLN:HE21 | 1:27:A:VAL:HG13  | 3        | 0.22          |
| (1,3492) | 1:105:A:LEU:HB3 | 1:105:A:LEU:HD11 | 1        | 0.22          |
| (1,3492) | 1:105:A:LEU:HB3 | 1:105:A:LEU:HD11 | 5        | 0.22          |
| (1,3492) | 1:105:A:LEU:HB3 | 1:105:A:LEU:HD11 | 7        | 0.22          |
| (1,3492) | 1:105:A:LEU:HB3 | 1:105:A:LEU:HD12 | 11       | 0.22          |
| (1,3492) | 1:105:A:LEU:HB3 | 1:105:A:LEU:HD13 | 14       | 0.22          |
| (1,3492) | 1:105:A:LEU:HB3 | 1:105:A:LEU:HD13 | 16       | 0.22          |
| (1,3479) | 1:45:A:ALA:HB1  | 1:44:A:GLU:HB3   | 7        | 0.22          |
| (1,3476) | 1:107:A:GLU:HG2 | 1:108:A:GLN:H    | 17       | 0.22          |
| (1,3465) | 1:88:A:VAL:HG23 | 1:85:A:LEU:HB3   | 1        | 0.22          |
| (1,3465) | 1:88:A:VAL:HG23 | 1:85:A:LEU:HB3   | 12       | 0.22          |
| (1,3457) | 1:20:A:LYS:HE3  | 1:19:A:PRO:HA    | 14       | 0.22          |
| (1,3437) | 1:21:A:LEU:HB2  | 1:21:A:LEU:HD13  | 17       | 0.22          |
| (1,3436) | 1:64:A:MET:HE2  | 1:21:A:LEU:HD13  | 7        | 0.22          |
| (1,3430) | 1:45:A:ALA:HB3  | 1:84:A:TYR:HA    | 13       | 0.22          |
| (1,3430) | 1:45:A:ALA:HB3  | 1:84:A:TYR:HA    | 16       | 0.22          |
| (1,3422) | 1:77:A:LEU:HG   | 1:77:A:LEU:HD23  | 9        | 0.22          |
| (1,3422) | 1:77:A:LEU:HG   | 1:77:A:LEU:HD23  | 11       | 0.22          |
| (1,3422) | 1:77:A:LEU:HG   | 1:77:A:LEU:HD23  | 12       | 0.22          |
| (1,3417) | 1:117:A:LEU:HG  | 1:117:A:LEU:HD11 | 1        | 0.22          |
| (1,3417) | 1:117:A:LEU:HG  | 1:117:A:LEU:HD13 | 2        | 0.22          |
| (1,3417) | 1:117:A:LEU:HG  | 1:117:A:LEU:HD12 | 6        | 0.22          |
| (1,3417) | 1:117:A:LEU:HG  | 1:117:A:LEU:HD12 | 10       | 0.22          |
| (1,3415) | 1:117:A:LEU:HA  | 1:117:A:LEU:HD13 | 7        | 0.22          |
| (1,3415) | 1:117:A:LEU:HA  | 1:117:A:LEU:HD13 | 15       | 0.22          |
| (1,3412) | 1:82:A:TRP:HZ3  | 1:117:A:LEU:HD13 | 4        | 0.22          |
| (1,3412) | 1:82:A:TRP:HZ3  | 1:117:A:LEU:HD13 | 16       | 0.22          |
| (1,3401) | 1:86:A:TYR:HE1  | 1:86:A:TYR:HA    | 9        | 0.22          |
| (1,3401) | 1:86:A:TYR:HE1  | 1:86:A:TYR:HA    | 10       | 0.22          |
| (1,3396) | 1:71:A:LEU:HA   | 1:74:A:ALA:HB3   | 9        | 0.22          |
| (1,3395) | 1:33:A:GLU:HB3  | 1:33:A:GLU:HA    | 4        | 0.22          |
| (1,3395) | 1:33:A:GLU:HB3  | 1:33:A:GLU:HA    | 11       | 0.22          |
| (1,3358) | 1:28:A:ILE:HB   | 1:29:A:ALA:HA    | 14       | 0.22          |
| (1,3341) | 1:41:A:ALA:HB2  | 1:28:A:ILE:HG22  | 1        | 0.22          |
| (1,3341) | 1:41:A:ALA:HB3  | 1:28:A:ILE:HG21  | 2        | 0.22          |
| (1,3341) | 1:41:A:ALA:HB2  | 1:28:A:ILE:HG23  | 8        | 0.22          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3341) | 1:41:A:ALA:HB2   | 1:28:A:ILE:HG23 | 13       | 0.22          |
| (1,3341) | 1:41:A:ALA:HB2   | 1:28:A:ILE:HG23 | 16       | 0.22          |
| (1,3326) | 1:77:A:LEU:HG    | 1:77:A:LEU:HD11 | 8        | 0.22          |
| (1,3325) | 1:77:A:LEU:HB3   | 1:77:A:LEU:HD12 | 9        | 0.22          |
| (1,3325) | 1:77:A:LEU:HB3   | 1:77:A:LEU:HD12 | 10       | 0.22          |
| (1,3325) | 1:77:A:LEU:HB3   | 1:77:A:LEU:HD12 | 17       | 0.22          |
| (1,3322) | 1:30:A:PHE:HD1   | 1:66:A:LEU:HD23 | 14       | 0.22          |
| (1,3311) | 1:68:A:LYS:HD3   | 1:57:A:VAL:HG13 | 1        | 0.22          |
| (1,3311) | 1:68:A:LYS:HD3   | 1:57:A:VAL:HG12 | 7        | 0.22          |
| (1,3311) | 1:68:A:LYS:HD3   | 1:57:A:VAL:HG13 | 15       | 0.22          |
| (1,3270) | 1:42:A:GLU:HG2   | 1:41:A:ALA:HB2  | 12       | 0.22          |
| (1,3266) | 1:85:A:LEU:HD11  | 1:85:A:LEU:HD22 | 15       | 0.22          |
| (1,3260) | 1:121:A:LYS:HG2  | 1:121:A:LYS:HB2 | 3        | 0.22          |
| (1,3260) | 1:121:A:LYS:HG2  | 1:121:A:LYS:HB2 | 12       | 0.22          |
| (1,3260) | 1:121:A:LYS:HG2  | 1:121:A:LYS:HB2 | 15       | 0.22          |
| (1,3258) | 1:48:A:LEU:HD12  | 1:50:A:ILE:HA   | 6        | 0.22          |
| (1,3258) | 1:48:A:LEU:HD12  | 1:50:A:ILE:HA   | 7        | 0.22          |
| (1,3250) | 1:41:A:ALA:HA    | 1:41:A:ALA:HB2  | 9        | 0.22          |
| (1,3250) | 1:41:A:ALA:HA    | 1:41:A:ALA:HB3  | 11       | 0.22          |
| (1,3250) | 1:41:A:ALA:HA    | 1:41:A:ALA:HB2  | 14       | 0.22          |
| (1,3223) | 1:84:A:TYR:HE2   | 1:79:A:THR:HA   | 2        | 0.22          |
| (1,3223) | 1:84:A:TYR:HE2   | 1:79:A:THR:HA   | 7        | 0.22          |
| (1,3209) | 1:124:A:VAL:HG13 | 1:124:A:VAL:HB  | 3        | 0.22          |
| (1,3200) | 1:116:A:GLN:HG3  | 1:113:A:ALA:HB3 | 17       | 0.22          |
| (1,3196) | 1:64:A:MET:HB2   | 1:64:A:MET:HA   | 7        | 0.22          |
| (1,3195) | 1:113:A:ALA:HA   | 1:113:A:ALA:H   | 2        | 0.22          |
| (1,3195) | 1:113:A:ALA:HA   | 1:113:A:ALA:H   | 4        | 0.22          |
| (1,3195) | 1:113:A:ALA:HA   | 1:113:A:ALA:H   | 11       | 0.22          |
| (1,3195) | 1:113:A:ALA:HA   | 1:113:A:ALA:H   | 12       | 0.22          |
| (1,3183) | 1:124:A:VAL:HG22 | 1:121:A:LYS:HA  | 6        | 0.22          |
| (1,3183) | 1:124:A:VAL:HG22 | 1:121:A:LYS:HA  | 7        | 0.22          |
| (1,3183) | 1:124:A:VAL:HG21 | 1:121:A:LYS:HA  | 8        | 0.22          |
| (1,3183) | 1:124:A:VAL:HG22 | 1:121:A:LYS:HA  | 15       | 0.22          |
| (1,3181) | 1:108:A:GLN:HG3  | 1:108:A:GLN:HA  | 1        | 0.22          |
| (1,3181) | 1:108:A:GLN:HG3  | 1:108:A:GLN:HA  | 2        | 0.22          |
| (1,3181) | 1:108:A:GLN:HG3  | 1:108:A:GLN:HA  | 5        | 0.22          |
| (1,3181) | 1:108:A:GLN:HG3  | 1:108:A:GLN:HA  | 6        | 0.22          |
| (1,3181) | 1:108:A:GLN:HG3  | 1:108:A:GLN:HA  | 9        | 0.22          |
| (1,3181) | 1:108:A:GLN:HG3  | 1:108:A:GLN:HA  | 12       | 0.22          |
| (1,3181) | 1:108:A:GLN:HG3  | 1:108:A:GLN:HA  | 13       | 0.22          |
| (1,3181) | 1:108:A:GLN:HG3  | 1:108:A:GLN:HA  | 15       | 0.22          |
| (1,3181) | 1:108:A:GLN:HG3  | 1:108:A:GLN:HA  | 16       | 0.22          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3166) | 1:75:A:LEU:HD21 | 1:53:A:PHE:HD2  | 12       | 0.22          |
| (1,3166) | 1:75:A:LEU:HD21 | 1:53:A:PHE:HD1  | 15       | 0.22          |
| (1,3165) | 1:126:A:ALA:HB3 | 1:125:A:GLN:HG3 | 8        | 0.22          |
| (1,3165) | 1:126:A:ALA:HB3 | 1:125:A:GLN:HG3 | 9        | 0.22          |
| (1,3139) | 1:69:A:THR:HB   | 1:69:A:THR:H    | 2        | 0.22          |
| (1,3139) | 1:69:A:THR:HB   | 1:69:A:THR:H    | 5        | 0.22          |
| (1,3132) | 1:68:A:LYS:HB2  | 1:53:A:PHE:HE2  | 1        | 0.22          |
| (1,3132) | 1:68:A:LYS:HB2  | 1:53:A:PHE:HE2  | 8        | 0.22          |
| (1,3080) | 1:125:A:GLN:HB2 | 1:125:A:GLN:HA  | 4        | 0.22          |
| (1,3080) | 1:125:A:GLN:HB2 | 1:125:A:GLN:HA  | 6        | 0.22          |
| (1,3080) | 1:125:A:GLN:HB2 | 1:125:A:GLN:HA  | 11       | 0.22          |
| (1,3080) | 1:125:A:GLN:HB2 | 1:125:A:GLN:HA  | 13       | 0.22          |
| (1,3068) | 1:52:A:ILE:HG21 | 1:53:A:PHE:HB2  | 6        | 0.22          |
| (1,3067) | 1:52:A:ILE:HG21 | 1:53:A:PHE:HB3  | 6        | 0.22          |
| (1,3066) | 1:30:A:PHE:HB3  | 1:29:A:ALA:HB2  | 7        | 0.22          |
| (1,3066) | 1:30:A:PHE:HB3  | 1:29:A:ALA:HB3  | 9        | 0.22          |
| (1,3066) | 1:30:A:PHE:HB3  | 1:29:A:ALA:HB1  | 16       | 0.22          |
| (1,3055) | 1:52:A:ILE:HG23 | 1:50:A:ILE:H    | 10       | 0.22          |
| (1,3035) | 1:25:A:LYS:H    | 1:25:A:LYS:HG2  | 1        | 0.22          |
| (1,3035) | 1:25:A:LYS:H    | 1:25:A:LYS:HG2  | 2        | 0.22          |
| (1,3028) | 1:71:A:LEU:HD12 | 1:72:A:ARG:HA   | 3        | 0.22          |
| (1,3028) | 1:71:A:LEU:HD12 | 1:72:A:ARG:HA   | 5        | 0.22          |
| (1,2992) | 1:20:A:LYS:HB3  | 1:20:A:LYS:H    | 5        | 0.22          |
| (1,2969) | 1:93:A:THR:HG22 | 1:101:A:PRO:HB3 | 12       | 0.22          |
| (1,2960) | 1:77:A:LEU:HD13 | 1:25:A:LYS:HA   | 15       | 0.22          |
| (1,2946) | 1:88:A:VAL:HG11 | 1:84:A:TYR:HE2  | 8        | 0.22          |
| (1,2937) | 1:95:A:VAL:HG23 | 1:95:A:VAL:HG13 | 10       | 0.22          |
| (1,2937) | 1:95:A:VAL:HG23 | 1:95:A:VAL:HG12 | 16       | 0.22          |
| (1,2932) | 1:95:A:VAL:HG21 | 1:95:A:VAL:H    | 1        | 0.22          |
| (1,2931) | 1:88:A:VAL:HG23 | 1:85:A:LEU:H    | 1        | 0.22          |
| (1,2927) | 1:31:A:LEU:HD21 | 1:39:A:PHE:HD2  | 7        | 0.22          |
| (1,2888) | 1:29:A:ALA:HA   | 1:32:A:ALA:HB3  | 5        | 0.22          |
| (1,2888) | 1:29:A:ALA:HA   | 1:32:A:ALA:HB1  | 11       | 0.22          |
| (1,2881) | 1:74:A:ALA:HB2  | 1:31:A:LEU:HD11 | 12       | 0.22          |
| (1,2877) | 1:61:A:ALA:HB3  | 1:61:A:ALA:HA   | 3        | 0.22          |
| (1,2855) | 1:78:A:TYR:HD1  | 1:28:A:ILE:HD11 | 12       | 0.22          |
| (1,2832) | 1:97:A:LEU:HD22 | 1:97:A:LEU:H    | 8        | 0.22          |
| (1,2829) | 1:97:A:LEU:HD21 | 1:97:A:LEU:HB2  | 1        | 0.22          |
| (1,2824) | 1:97:A:LEU:HD21 | 1:56:A:LEU:HA   | 1        | 0.22          |
| (1,2769) | 1:43:A:GLY:HA2  | 1:42:A:GLU:HB2  | 13       | 0.22          |
| (1,2754) | 1:60:A:VAL:HG12 | 1:59:A:ARG:HD3  | 1        | 0.22          |
| (1,2745) | 1:34:A:ARG:HD3  | 1:34:A:ARG:HG3  | 7        | 0.22          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2745) | 1:34:A:ARG:HD3   | 1:34:A:ARG:HG3  | 12       | 0.22          |
| (1,2745) | 1:34:A:ARG:HD3   | 1:34:A:ARG:HG3  | 17       | 0.22          |
| (1,2729) | 1:17:A:ASN:HB3   | 1:17:A:ASN:HB2  | 3        | 0.22          |
| (1,2729) | 1:17:A:ASN:HB3   | 1:17:A:ASN:HB2  | 6        | 0.22          |
| (1,2713) | 1:53:A:PHE:HB3   | 1:75:A:LEU:HD13 | 1        | 0.22          |
| (1,2713) | 1:53:A:PHE:HB3   | 1:75:A:LEU:HD13 | 2        | 0.22          |
| (1,2711) | 1:35:A:PHE:HB2   | 1:35:A:PHE:HE1  | 6        | 0.22          |
| (1,2711) | 1:35:A:PHE:HB2   | 1:35:A:PHE:HE1  | 8        | 0.22          |
| (1,2672) | 1:31:A:LEU:HD11  | 1:35:A:PHE:HD1  | 8        | 0.22          |
| (1,2662) | 1:97:A:LEU:HD12  | 1:57:A:VAL:H    | 3        | 0.22          |
| (1,2662) | 1:97:A:LEU:HD11  | 1:57:A:VAL:H    | 7        | 0.22          |
| (1,2662) | 1:97:A:LEU:HD11  | 1:57:A:VAL:H    | 9        | 0.22          |
| (1,2639) | 1:71:A:LEU:HD13  | 1:71:A:LEU:HB2  | 5        | 0.22          |
| (1,2629) | 1:53:A:PHE:HZ    | 1:71:A:LEU:HB2  | 5        | 0.22          |
| (1,2622) | 1:71:A:LEU:HD11  | 1:57:A:VAL:H    | 5        | 0.22          |
| (1,2618) | 1:34:A:ARG:HG3   | 1:34:A:ARG:H    | 7        | 0.22          |
| (1,2618) | 1:34:A:ARG:HG3   | 1:34:A:ARG:H    | 12       | 0.22          |
| (1,2605) | 1:31:A:LEU:HD21  | 1:30:A:PHE:HD2  | 6        | 0.22          |
| (1,2605) | 1:31:A:LEU:HD21  | 1:30:A:PHE:HD2  | 10       | 0.22          |
| (1,2605) | 1:31:A:LEU:HD21  | 1:30:A:PHE:HD1  | 14       | 0.22          |
| (1,2598) | 1:27:A:VAL:HG21  | 1:27:A:VAL:HG12 | 15       | 0.22          |
| (1,2583) | 1:60:A:VAL:HG11  | 1:34:A:ARG:HG2  | 14       | 0.22          |
| (1,2583) | 1:60:A:VAL:HG12  | 1:34:A:ARG:HG2  | 17       | 0.22          |
| (1,2576) | 1:124:A:VAL:HG23 | 1:120:A:ALA:HA  | 3        | 0.22          |
| (1,2576) | 1:124:A:VAL:HG23 | 1:120:A:ALA:HA  | 14       | 0.22          |
| (1,2560) | 1:86:A:TYR:HE2   | 1:86:A:TYR:HD2  | 12       | 0.22          |
| (1,2560) | 1:86:A:TYR:HE2   | 1:86:A:TYR:HD2  | 17       | 0.22          |
| (1,2559) | 1:86:A:TYR:HE1   | 1:86:A:TYR:HB2  | 4        | 0.22          |
| (1,2559) | 1:86:A:TYR:HE2   | 1:86:A:TYR:HB2  | 16       | 0.22          |
| (1,2529) | 1:79:A:THR:HG23  | 1:75:A:LEU:HA   | 9        | 0.22          |
| (1,2527) | 1:123:A:ARG:H    | 1:123:A:ARG:HA  | 2        | 0.22          |
| (1,2527) | 1:123:A:ARG:H    | 1:123:A:ARG:HA  | 3        | 0.22          |
| (1,2527) | 1:123:A:ARG:H    | 1:123:A:ARG:HA  | 13       | 0.22          |
| (1,2527) | 1:123:A:ARG:H    | 1:123:A:ARG:HA  | 14       | 0.22          |
| (1,2515) | 1:122:A:ALA:HA   | 1:122:A:ALA:H   | 1        | 0.22          |
| (1,2515) | 1:122:A:ALA:HA   | 1:122:A:ALA:H   | 2        | 0.22          |
| (1,2515) | 1:122:A:ALA:HA   | 1:122:A:ALA:H   | 15       | 0.22          |
| (1,2505) | 1:126:A:ALA:HA   | 1:126:A:ALA:H   | 7        | 0.22          |
| (1,2505) | 1:126:A:ALA:HA   | 1:126:A:ALA:H   | 8        | 0.22          |
| (1,2505) | 1:126:A:ALA:HA   | 1:126:A:ALA:H   | 10       | 0.22          |
| (1,2444) | 1:53:A:PHE:HE2   | 1:53:A:PHE:HB2  | 4        | 0.22          |
| (1,2444) | 1:53:A:PHE:HE2   | 1:53:A:PHE:HB2  | 10       | 0.22          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2444) | 1:53:A:PHE:HE2   | 1:53:A:PHE:HB2   | 13       | 0.22          |
| (1,2434) | 1:86:A:TYR:HB2   | 1:117:A:LEU:HB3  | 6        | 0.22          |
| (1,2434) | 1:86:A:TYR:HB2   | 1:117:A:LEU:HB3  | 7        | 0.22          |
| (1,2434) | 1:86:A:TYR:HB2   | 1:117:A:LEU:HB3  | 14       | 0.22          |
| (1,2434) | 1:86:A:TYR:HB2   | 1:117:A:LEU:HB3  | 15       | 0.22          |
| (1,2424) | 1:64:A:MET:HE1   | 1:30:A:PHE:HD2   | 12       | 0.22          |
| (1,2409) | 1:49:A:LYS:H     | 1:52:A:ILE:HD11  | 3        | 0.22          |
| (1,2409) | 1:49:A:LYS:H     | 1:52:A:ILE:HD11  | 7        | 0.22          |
| (1,2404) | 1:28:A:ILE:HD11  | 1:74:A:ALA:HA    | 10       | 0.22          |
| (1,2346) | 1:105:A:LEU:HD12 | 1:107:A:GLU:HA   | 15       | 0.22          |
| (1,2341) | 1:66:A:LEU:HD23  | 1:70:A:GLN:H     | 6        | 0.22          |
| (1,2341) | 1:66:A:LEU:HD23  | 1:70:A:GLN:H     | 13       | 0.22          |
| (1,2336) | 1:64:A:MET:HE3   | 1:31:A:LEU:HA    | 10       | 0.22          |
| (1,2334) | 1:60:A:VAL:HG12  | 1:63:A:GLU:HG3   | 11       | 0.22          |
| (1,2307) | 1:117:A:LEU:HD12 | 1:86:A:TYR:HB2   | 17       | 0.22          |
| (1,2268) | 1:110:A:VAL:HG11 | 1:89:A:LYS:H     | 13       | 0.22          |
| (1,2221) | 1:31:A:LEU:HA    | 1:60:A:VAL:HB    | 7        | 0.22          |
| (1,2221) | 1:31:A:LEU:HA    | 1:60:A:VAL:HB    | 17       | 0.22          |
| (1,2210) | 1:105:A:LEU:HG   | 1:110:A:VAL:HG11 | 7        | 0.22          |
| (1,2210) | 1:105:A:LEU:HG   | 1:110:A:VAL:HG12 | 11       | 0.22          |
| (1,2210) | 1:105:A:LEU:HG   | 1:110:A:VAL:HG11 | 14       | 0.22          |
| (1,2210) | 1:105:A:LEU:HG   | 1:110:A:VAL:HG12 | 15       | 0.22          |
| (1,2190) | 1:61:A:ALA:HB1   | 1:62:A:GLY:HA2   | 14       | 0.22          |
| (1,2164) | 1:120:A:ALA:HA   | 1:121:A:LYS:H    | 3        | 0.22          |
| (1,2164) | 1:120:A:ALA:HA   | 1:121:A:LYS:H    | 7        | 0.22          |
| (1,2164) | 1:120:A:ALA:HA   | 1:121:A:LYS:H    | 17       | 0.22          |
| (1,2035) | 1:52:A:ILE:HG13  | 1:97:A:LEU:HD21  | 4        | 0.22          |
| (1,2035) | 1:52:A:ILE:HG13  | 1:97:A:LEU:HD21  | 8        | 0.22          |
| (1,1951) | 1:108:A:GLN:HA   | 1:111:A:GLU:HB3  | 12       | 0.22          |
| (1,1951) | 1:108:A:GLN:HA   | 1:111:A:GLU:HB3  | 14       | 0.22          |
| (1,1890) | 1:100:A:ASN:HD22 | 1:98:A:ASP:HB3   | 10       | 0.22          |
| (1,1890) | 1:100:A:ASN:HD22 | 1:98:A:ASP:HB3   | 12       | 0.22          |
| (1,1889) | 1:65:A:ASN:H     | 1:65:A:ASN:HB3   | 5        | 0.22          |
| (1,1889) | 1:65:A:ASN:H     | 1:65:A:ASN:HB3   | 11       | 0.22          |
| (1,1886) | 1:102:A:CYS:HB3  | 1:49:A:LYS:HA    | 1        | 0.22          |
| (1,1831) | 1:21:A:LEU:HG    | 1:21:A:LEU:HB3   | 3        | 0.22          |
| (1,1831) | 1:21:A:LEU:HG    | 1:21:A:LEU:HB3   | 15       | 0.22          |
| (1,1831) | 1:21:A:LEU:HG    | 1:21:A:LEU:HB3   | 16       | 0.22          |
| (1,1824) | 1:27:A:VAL:HA    | 1:21:A:LEU:HD13  | 7        | 0.22          |
| (1,1817) | 1:77:A:LEU:HG    | 1:77:A:LEU:HD21  | 16       | 0.22          |
| (1,1817) | 1:77:A:LEU:HG    | 1:77:A:LEU:HD21  | 17       | 0.22          |
| (1,1811) | 1:86:A:TYR:H     | 1:117:A:LEU:HD13 | 1        | 0.22          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1799) | 1:71:A:LEU:HA    | 1:74:A:ALA:HB3   | 14       | 0.22          |
| (1,1751) | 1:32:A:ALA:HB2   | 1:41:A:ALA:H     | 2        | 0.22          |
| (1,1736) | 1:77:A:LEU:HB3   | 1:77:A:LEU:HD13  | 4        | 0.22          |
| (1,1736) | 1:77:A:LEU:HB3   | 1:77:A:LEU:HD13  | 5        | 0.22          |
| (1,1736) | 1:77:A:LEU:HB3   | 1:77:A:LEU:HD13  | 15       | 0.22          |
| (1,1733) | 1:30:A:PHE:HD2   | 1:66:A:LEU:HD21  | 10       | 0.22          |
| (1,1733) | 1:30:A:PHE:HD2   | 1:66:A:LEU:HD21  | 15       | 0.22          |
| (1,1730) | 1:27:A:VAL:HA    | 1:66:A:LEU:HD22  | 8        | 0.22          |
| (1,1726) | 1:66:A:LEU:HD12  | 1:66:A:LEU:HA    | 3        | 0.22          |
| (1,1723) | 1:68:A:LYS:HD3   | 1:57:A:VAL:HG11  | 12       | 0.22          |
| (1,1698) | 1:44:A:GLU:HG2   | 1:45:A:ALA:HB3   | 2        | 0.22          |
| (1,1686) | 1:85:A:LEU:HD11  | 1:85:A:LEU:HD22  | 7        | 0.22          |
| (1,1629) | 1:116:A:GLN:HG3  | 1:113:A:ALA:HB3  | 2        | 0.22          |
| (1,1629) | 1:116:A:GLN:HG3  | 1:113:A:ALA:HB2  | 14       | 0.22          |
| (1,1628) | 1:87:A:GLY:HA3   | 1:113:A:ALA:HB2  | 9        | 0.22          |
| (1,1618) | 1:109:A:HIS:HB2  | 1:110:A:VAL:HG11 | 5        | 0.22          |
| (1,1618) | 1:109:A:HIS:HB2  | 1:110:A:VAL:HG13 | 12       | 0.22          |
| (1,1616) | 1:109:A:HIS:HB2  | 1:108:A:GLN:H    | 3        | 0.22          |
| (1,1613) | 1:124:A:VAL:HG23 | 1:121:A:LYS:HA   | 17       | 0.22          |
| (1,1592) | 1:126:A:ALA:HB3  | 1:125:A:GLN:HG3  | 3        | 0.22          |
| (1,1592) | 1:126:A:ALA:HB2  | 1:125:A:GLN:HG3  | 6        | 0.22          |
| (1,1592) | 1:126:A:ALA:HB3  | 1:125:A:GLN:HG3  | 16       | 0.22          |
| (1,1588) | 1:74:A:ALA:HB3   | 1:74:A:ALA:HA    | 4        | 0.22          |
| (1,1588) | 1:74:A:ALA:HB3   | 1:74:A:ALA:HA    | 16       | 0.22          |
| (1,1552) | 1:124:A:VAL:HG11 | 1:124:A:VAL:HB   | 2        | 0.22          |
| (1,1552) | 1:124:A:VAL:HG13 | 1:124:A:VAL:HB   | 5        | 0.22          |
| (1,1552) | 1:124:A:VAL:HG13 | 1:124:A:VAL:HB   | 9        | 0.22          |
| (1,1513) | 1:52:A:ILE:HG23  | 1:53:A:PHE:HB3   | 7        | 0.22          |
| (1,1508) | 1:29:A:ALA:H     | 1:28:A:ILE:HG23  | 13       | 0.22          |
| (1,1508) | 1:29:A:ALA:H     | 1:28:A:ILE:HG22  | 14       | 0.22          |
| (1,1456) | 1:57:A:VAL:HA    | 1:60:A:VAL:HB    | 14       | 0.22          |
| (1,1428) | 1:93:A:THR:HG23  | 1:101:A:PRO:HB3  | 6        | 0.22          |
| (1,1428) | 1:93:A:THR:HG22  | 1:101:A:PRO:HB3  | 13       | 0.22          |
| (1,1428) | 1:93:A:THR:HG21  | 1:101:A:PRO:HB3  | 16       | 0.22          |
| (1,1419) | 1:77:A:LEU:HD13  | 1:25:A:LYS:HA    | 4        | 0.22          |
| (1,1419) | 1:77:A:LEU:HD11  | 1:25:A:LYS:HA    | 16       | 0.22          |
| (1,1410) | 1:110:A:VAL:HG22 | 1:108:A:GLN:H    | 15       | 0.22          |
| (1,1409) | 1:57:A:VAL:HG23  | 1:57:A:VAL:HG11  | 4        | 0.22          |
| (1,1409) | 1:57:A:VAL:HG23  | 1:57:A:VAL:HG11  | 9        | 0.22          |
| (1,1397) | 1:31:A:LEU:HD21  | 1:60:A:VAL:HG12  | 17       | 0.22          |
| (1,1395) | 1:31:A:LEU:HD22  | 1:39:A:PHE:HD1   | 10       | 0.22          |
| (1,1395) | 1:31:A:LEU:HD21  | 1:39:A:PHE:HD1   | 12       | 0.22          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1395) | 1:31:A:LEU:HD22  | 1:39:A:PHE:HD2  | 17       | 0.22          |
| (1,1371) | 1:28:A:ILE:HD11  | 1:75:A:LEU:H    | 10       | 0.22          |
| (1,1365) | 1:32:A:ALA:HB1   | 1:28:A:ILE:HG23 | 5        | 0.22          |
| (1,1363) | 1:29:A:ALA:HA    | 1:32:A:ALA:HB3  | 3        | 0.22          |
| (1,1363) | 1:29:A:ALA:HA    | 1:32:A:ALA:HB1  | 8        | 0.22          |
| (1,1363) | 1:29:A:ALA:HA    | 1:32:A:ALA:HB2  | 10       | 0.22          |
| (1,1357) | 1:74:A:ALA:HB2   | 1:31:A:LEU:HD11 | 6        | 0.22          |
| (1,1331) | 1:78:A:TYR:HE1   | 1:84:A:TYR:HD2  | 7        | 0.22          |
| (1,1321) | 1:124:A:VAL:HG11 | 1:125:A:GLN:H   | 11       | 0.22          |
| (1,1285) | 1:48:A:LEU:HD23  | 1:48:A:LEU:HB3  | 17       | 0.22          |
| (1,1232) | 1:60:A:VAL:HG13  | 1:59:A:ARG:HD3  | 2        | 0.22          |
| (1,1232) | 1:60:A:VAL:HG11  | 1:59:A:ARG:HD3  | 4        | 0.22          |
| (1,1232) | 1:60:A:VAL:HG11  | 1:59:A:ARG:HD3  | 8        | 0.22          |
| (1,1232) | 1:60:A:VAL:HG11  | 1:59:A:ARG:HD3  | 9        | 0.22          |
| (1,1232) | 1:60:A:VAL:HG11  | 1:59:A:ARG:HD3  | 13       | 0.22          |
| (1,1231) | 1:97:A:LEU:HD11  | 1:59:A:ARG:HD3  | 6        | 0.22          |
| (1,1194) | 1:39:A:PHE:HB3   | 1:35:A:PHE:HB3  | 2        | 0.22          |
| (1,1194) | 1:39:A:PHE:HB3   | 1:35:A:PHE:HB3  | 4        | 0.22          |
| (1,1194) | 1:39:A:PHE:HB3   | 1:35:A:PHE:HB3  | 5        | 0.22          |
| (1,1194) | 1:39:A:PHE:HB3   | 1:35:A:PHE:HB3  | 10       | 0.22          |
| (1,1194) | 1:39:A:PHE:HB3   | 1:35:A:PHE:HB3  | 13       | 0.22          |
| (1,1194) | 1:39:A:PHE:HB3   | 1:35:A:PHE:HB3  | 15       | 0.22          |
| (1,1194) | 1:39:A:PHE:HB3   | 1:35:A:PHE:HB3  | 17       | 0.22          |
| (1,1136) | 1:31:A:LEU:HD13  | 1:35:A:PHE:HD1  | 2        | 0.22          |
| (1,1136) | 1:31:A:LEU:HD12  | 1:35:A:PHE:HD1  | 6        | 0.22          |
| (1,1136) | 1:31:A:LEU:HD13  | 1:35:A:PHE:HD2  | 15       | 0.22          |
| (1,1126) | 1:86:A:TYR:HE2   | 1:86:A:TYR:HB3  | 4        | 0.22          |
| (1,1080) | 1:105:A:LEU:HD11 | 1:92:A:ALA:H    | 2        | 0.22          |
| (1,1080) | 1:105:A:LEU:HD12 | 1:92:A:ALA:H    | 4        | 0.22          |
| (1,1080) | 1:105:A:LEU:HD13 | 1:92:A:ALA:H    | 16       | 0.22          |
| (1,1078) | 1:48:A:LEU:HD23  | 1:84:A:TYR:HE1  | 4        | 0.22          |
| (1,1060) | 1:74:A:ALA:HB1   | 1:27:A:VAL:HG13 | 8        | 0.22          |
| (1,993)  | 1:79:A:THR:HG22  | 1:75:A:LEU:HA   | 15       | 0.22          |
| (1,895)  | 1:129:A:ALA:HB1  | 1:129:A:ALA:HA  | 10       | 0.22          |
| (1,853)  | 1:65:A:ASN:HB2   | 1:65:A:ASN:HD21 | 1        | 0.22          |
| (1,853)  | 1:65:A:ASN:HB2   | 1:65:A:ASN:HD21 | 5        | 0.22          |
| (1,853)  | 1:65:A:ASN:HB2   | 1:65:A:ASN:HD21 | 14       | 0.22          |
| (1,829)  | 1:41:A:ALA:HB1   | 1:41:A:ALA:H    | 14       | 0.22          |
| (1,700)  | 1:95:A:VAL:HG22  | 1:38:A:CYS:H    | 4        | 0.22          |
| (1,630)  | 1:61:A:ALA:HB1   | 1:67:A:SER:H    | 3        | 0.22          |
| (1,630)  | 1:61:A:ALA:HB2   | 1:67:A:SER:H    | 10       | 0.22          |
| (1,527)  | 1:65:A:ASN:HB3   | 1:65:A:ASN:HD21 | 7        | 0.22          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,527)  | 1:65:A:ASN:HB3   | 1:65:A:ASN:HD21 | 9        | 0.22          |
| (1,512)  | 1:13:A:ASP:HB2   | 1:13:A:ASP:H    | 15       | 0.22          |
| (1,478)  | 1:27:A:VAL:HG23  | 1:29:A:ALA:H    | 8        | 0.22          |
| (1,451)  | 1:32:A:ALA:HB2   | 1:35:A:PHE:H    | 4        | 0.22          |
| (1,451)  | 1:32:A:ALA:HB3   | 1:35:A:PHE:H    | 12       | 0.22          |
| (1,451)  | 1:32:A:ALA:HB2   | 1:35:A:PHE:H    | 17       | 0.22          |
| (1,441)  | 1:42:A:GLU:HB3   | 1:41:A:ALA:H    | 5        | 0.22          |
| (1,441)  | 1:42:A:GLU:HB3   | 1:41:A:ALA:H    | 8        | 0.22          |
| (1,441)  | 1:42:A:GLU:HB3   | 1:41:A:ALA:H    | 14       | 0.22          |
| (1,397)  | 1:57:A:VAL:H     | 1:56:A:LEU:HB3  | 10       | 0.22          |
| (1,263)  | 1:110:A:VAL:HG21 | 1:91:A:GLY:H    | 7        | 0.22          |
| (1,116)  | 1:21:A:LEU:HD13  | 1:30:A:PHE:H    | 7        | 0.22          |
| (1,100)  | 1:35:A:PHE:HE2   | 1:35:A:PHE:H    | 7        | 0.22          |
| (1,100)  | 1:35:A:PHE:HE2   | 1:35:A:PHE:H    | 10       | 0.22          |
| (3,143)  | 1:25:A:LYS:H     | 1:77:A:LEU:HD21 | 8        | 0.21          |
| (3,143)  | 1:25:A:LYS:H     | 1:77:A:LEU:HD21 | 9        | 0.21          |
| (3,129)  | 1:71:A:LEU:HD12  | 1:60:A:VAL:HB   | 1        | 0.21          |
| (3,129)  | 1:71:A:LEU:HD12  | 1:60:A:VAL:HB   | 6        | 0.21          |
| (3,129)  | 1:71:A:LEU:HD11  | 1:60:A:VAL:HB   | 7        | 0.21          |
| (3,129)  | 1:71:A:LEU:HD13  | 1:60:A:VAL:HB   | 9        | 0.21          |
| (3,129)  | 1:71:A:LEU:HD12  | 1:60:A:VAL:HB   | 14       | 0.21          |
| (3,123)  | 1:50:A:ILE:HD13  | 1:79:A:THR:HA   | 10       | 0.21          |
| (3,117)  | 1:48:A:LEU:HD23  | 1:39:A:PHE:HD1  | 3        | 0.21          |
| (3,111)  | 1:111:A:GLU:HG2  | 1:112:A:HIS:HA  | 9        | 0.21          |
| (3,111)  | 1:111:A:GLU:HG2  | 1:112:A:HIS:HA  | 15       | 0.21          |
| (3,109)  | 1:92:A:ALA:H     | 1:110:A:VAL:HB  | 1        | 0.21          |
| (3,106)  | 1:68:A:LYS:HD2   | 1:68:A:LYS:HA   | 13       | 0.21          |
| (3,102)  | 1:65:A:ASN:HB2   | 1:64:A:MET:HG2  | 11       | 0.21          |
| (3,94)   | 1:56:A:LEU:HB2   | 1:75:A:LEU:HD12 | 5        | 0.21          |
| (3,94)   | 1:56:A:LEU:HB2   | 1:75:A:LEU:HD13 | 6        | 0.21          |
| (3,92)   | 1:88:A:VAL:HG23  | 1:87:A:GLY:HA2  | 11       | 0.21          |
| (3,83)   | 1:114:A:ARG:HB2  | 1:113:A:ALA:HB1 | 16       | 0.21          |
| (3,59)   | 1:117:A:LEU:HA   | 1:85:A:LEU:HD22 | 10       | 0.21          |
| (3,15)   | 1:85:A:LEU:HB3   | 1:82:A:TRP:HA   | 2        | 0.21          |
| (1,4344) | 1:120:A:ALA:H    | 1:119:A:GLU:HG2 | 12       | 0.21          |
| (1,4342) | 1:38:A:CYS:H     | 1:95:A:VAL:HG12 | 12       | 0.21          |
| (1,4316) | 1:95:A:VAL:H     | 1:94:A:ARG:HB3  | 15       | 0.21          |
| (1,4310) | 1:64:A:MET:HA    | 1:65:A:ASN:H    | 16       | 0.21          |
| (1,4299) | 1:65:A:ASN:HD22  | 1:65:A:ASN:HD21 | 4        | 0.21          |
| (1,4299) | 1:65:A:ASN:HD22  | 1:65:A:ASN:HD21 | 8        | 0.21          |
| (1,4299) | 1:65:A:ASN:HD22  | 1:65:A:ASN:HD21 | 9        | 0.21          |
| (1,4202) | 1:127:A:GLN:H    | 1:127:A:GLN:HB3 | 3        | 0.21          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,4202) | 1:127:A:GLN:H   | 1:127:A:GLN:HB3  | 6        | 0.21          |
| (1,4202) | 1:127:A:GLN:H   | 1:127:A:GLN:HB3  | 7        | 0.21          |
| (1,4176) | 1:97:A:LEU:HD11 | 1:97:A:LEU:H     | 13       | 0.21          |
| (1,4153) | 1:18:A:GLN:HB3  | 1:18:A:GLN:H     | 5        | 0.21          |
| (1,4153) | 1:18:A:GLN:HB3  | 1:18:A:GLN:H     | 15       | 0.21          |
| (1,4150) | 1:17:A:ASN:HB3  | 1:18:A:GLN:H     | 9        | 0.21          |
| (1,4150) | 1:17:A:ASN:HB3  | 1:18:A:GLN:H     | 13       | 0.21          |
| (1,4141) | 1:98:A:ASP:HB2  | 1:100:A:ASN:HD21 | 14       | 0.21          |
| (1,4141) | 1:98:A:ASP:HB2  | 1:100:A:ASN:HD21 | 16       | 0.21          |
| (1,4127) | 1:34:A:ARG:HE   | 1:30:A:PHE:HD1   | 10       | 0.21          |
| (1,4109) | 1:97:A:LEU:HD11 | 1:98:A:ASP:H     | 4        | 0.21          |
| (1,4069) | 1:13:A:ASP:HB2  | 1:13:A:ASP:H     | 2        | 0.21          |
| (1,4069) | 1:13:A:ASP:HB2  | 1:13:A:ASP:H     | 7        | 0.21          |
| (1,4069) | 1:13:A:ASP:HB2  | 1:13:A:ASP:H     | 8        | 0.21          |
| (1,4037) | 1:27:A:VAL:HG21 | 1:29:A:ALA:H     | 2        | 0.21          |
| (1,4036) | 1:31:A:LEU:H    | 1:31:A:LEU:HD13  | 3        | 0.21          |
| (1,4036) | 1:31:A:LEU:H    | 1:31:A:LEU:HD13  | 14       | 0.21          |
| (1,4017) | 1:32:A:ALA:HB2  | 1:35:A:PHE:H     | 11       | 0.21          |
| (1,3961) | 1:57:A:VAL:H    | 1:56:A:LEU:HB3   | 2        | 0.21          |
| (1,3961) | 1:57:A:VAL:H    | 1:56:A:LEU:HB3   | 14       | 0.21          |
| (1,3961) | 1:57:A:VAL:H    | 1:56:A:LEU:HB3   | 15       | 0.21          |
| (1,3961) | 1:57:A:VAL:H    | 1:56:A:LEU:HB3   | 16       | 0.21          |
| (1,3935) | 1:63:A:GLU:HB3  | 1:65:A:ASN:H     | 1        | 0.21          |
| (1,3874) | 1:85:A:LEU:HB3  | 1:86:A:TYR:H     | 4        | 0.21          |
| (1,3775) | 1:124:A:VAL:HA  | 1:125:A:GLN:H    | 6        | 0.21          |
| (1,3775) | 1:124:A:VAL:HA  | 1:125:A:GLN:H    | 10       | 0.21          |
| (1,3775) | 1:124:A:VAL:HA  | 1:125:A:GLN:H    | 11       | 0.21          |
| (1,3775) | 1:124:A:VAL:HA  | 1:125:A:GLN:H    | 16       | 0.21          |
| (1,3771) | 1:126:A:ALA:HB1 | 1:126:A:ALA:H    | 2        | 0.21          |
| (1,3768) | 1:130:A:GLU:H   | 1:130:A:GLU:HA   | 2        | 0.21          |
| (1,3749) | 1:123:A:ARG:H   | 1:121:A:LYS:H    | 2        | 0.21          |
| (1,3749) | 1:123:A:ARG:H   | 1:121:A:LYS:H    | 4        | 0.21          |
| (1,3749) | 1:123:A:ARG:H   | 1:121:A:LYS:H    | 5        | 0.21          |
| (1,3749) | 1:123:A:ARG:H   | 1:121:A:LYS:H    | 8        | 0.21          |
| (1,3749) | 1:123:A:ARG:H   | 1:121:A:LYS:H    | 10       | 0.21          |
| (1,3744) | 1:35:A:PHE:HD2  | 1:39:A:PHE:H     | 4        | 0.21          |
| (1,3744) | 1:35:A:PHE:HD2  | 1:39:A:PHE:H     | 9        | 0.21          |
| (1,3717) | 1:35:A:PHE:H    | 1:39:A:PHE:HE2   | 1        | 0.21          |
| (1,3717) | 1:35:A:PHE:H    | 1:39:A:PHE:HE2   | 2        | 0.21          |
| (1,3717) | 1:35:A:PHE:H    | 1:39:A:PHE:HE1   | 16       | 0.21          |
| (1,3716) | 1:35:A:PHE:HE2  | 1:35:A:PHE:H     | 9        | 0.21          |
| (1,3698) | 1:30:A:PHE:HD1  | 1:30:A:PHE:H     | 7        | 0.21          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3678) | 1:95:A:VAL:H    | 1:96:A:ASP:H     | 1        | 0.21          |
| (1,3668) | 1:84:A:TYR:H    | 1:84:A:TYR:HD2   | 8        | 0.21          |
| (1,3668) | 1:84:A:TYR:H    | 1:84:A:TYR:HD2   | 9        | 0.21          |
| (1,3662) | 1:83:A:ARG:H    | 1:82:A:TRP:HD1   | 4        | 0.21          |
| (1,3662) | 1:83:A:ARG:H    | 1:82:A:TRP:HD1   | 8        | 0.21          |
| (1,3662) | 1:83:A:ARG:H    | 1:82:A:TRP:HD1   | 15       | 0.21          |
| (1,3662) | 1:83:A:ARG:H    | 1:82:A:TRP:HD1   | 16       | 0.21          |
| (1,3627) | 1:100:A:ASN:H   | 1:100:A:ASN:HD21 | 6        | 0.21          |
| (1,3591) | 1:93:A:THR:HB   | 1:88:A:VAL:HG12  | 3        | 0.21          |
| (1,3591) | 1:93:A:THR:HB   | 1:88:A:VAL:HG12  | 5        | 0.21          |
| (1,3588) | 1:105:A:LEU:HB3 | 1:110:A:VAL:HG21 | 12       | 0.21          |
| (1,3583) | 1:112:A:HIS:H   | 1:109:A:HIS:HA   | 15       | 0.21          |
| (1,3580) | 1:111:A:GLU:HB2 | 1:109:A:HIS:HA   | 2        | 0.21          |
| (1,3580) | 1:111:A:GLU:HB2 | 1:109:A:HIS:HA   | 15       | 0.21          |
| (1,3562) | 1:104:A:GLU:HB3 | 1:91:A:GLY:HA3   | 1        | 0.21          |
| (1,3562) | 1:104:A:GLU:HB3 | 1:91:A:GLY:HA3   | 2        | 0.21          |
| (1,3562) | 1:104:A:GLU:HB3 | 1:91:A:GLY:HA3   | 3        | 0.21          |
| (1,3562) | 1:104:A:GLU:HB3 | 1:91:A:GLY:HA3   | 5        | 0.21          |
| (1,3562) | 1:104:A:GLU:HB3 | 1:91:A:GLY:HA3   | 8        | 0.21          |
| (1,3562) | 1:104:A:GLU:HB3 | 1:91:A:GLY:HA3   | 10       | 0.21          |
| (1,3562) | 1:104:A:GLU:HB3 | 1:91:A:GLY:HA3   | 11       | 0.21          |
| (1,3562) | 1:104:A:GLU:HB3 | 1:91:A:GLY:HA3   | 14       | 0.21          |
| (1,3562) | 1:104:A:GLU:HB3 | 1:91:A:GLY:HA3   | 16       | 0.21          |
| (1,3535) | 1:74:A:ALA:HB1  | 1:28:A:ILE:HA    | 12       | 0.21          |
| (1,3535) | 1:74:A:ALA:HB2  | 1:28:A:ILE:HA    | 13       | 0.21          |
| (1,3535) | 1:74:A:ALA:HB2  | 1:28:A:ILE:HA    | 14       | 0.21          |
| (1,3534) | 1:122:A:ALA:HB3 | 1:121:A:LYS:HE3  | 1        | 0.21          |
| (1,3515) | 1:102:A:CYS:HB3 | 1:49:A:LYS:HA    | 6        | 0.21          |
| (1,3515) | 1:102:A:CYS:HB3 | 1:49:A:LYS:HA    | 14       | 0.21          |
| (1,3506) | 1:60:A:VAL:HG12 | 1:35:A:PHE:HZ    | 3        | 0.21          |
| (1,3506) | 1:60:A:VAL:HG11 | 1:35:A:PHE:HZ    | 8        | 0.21          |
| (1,3506) | 1:60:A:VAL:HG13 | 1:35:A:PHE:HZ    | 15       | 0.21          |
| (1,3503) | 1:27:A:VAL:HG23 | 1:31:A:LEU:H     | 7        | 0.21          |
| (1,3503) | 1:27:A:VAL:HG22 | 1:31:A:LEU:H     | 8        | 0.21          |
| (1,3501) | 1:27:A:VAL:HG23 | 1:28:A:ILE:HA    | 10       | 0.21          |
| (1,3492) | 1:105:A:LEU:HB3 | 1:105:A:LEU:HD13 | 9        | 0.21          |
| (1,3479) | 1:45:A:ALA:HB2  | 1:44:A:GLU:HB3   | 8        | 0.21          |
| (1,3479) | 1:45:A:ALA:HB1  | 1:44:A:GLU:HB3   | 11       | 0.21          |
| (1,3476) | 1:107:A:GLU:HG2 | 1:108:A:GLN:H    | 8        | 0.21          |
| (1,3465) | 1:88:A:VAL:HG23 | 1:85:A:LEU:HB3   | 5        | 0.21          |
| (1,3465) | 1:88:A:VAL:HG22 | 1:85:A:LEU:HB3   | 10       | 0.21          |
| (1,3441) | 1:21:A:LEU:HG   | 1:21:A:LEU:HB3   | 2        | 0.21          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3441) | 1:21:A:LEU:HG    | 1:21:A:LEU:HB3   | 6        | 0.21          |
| (1,3441) | 1:21:A:LEU:HG    | 1:21:A:LEU:HB3   | 8        | 0.21          |
| (1,3441) | 1:21:A:LEU:HG    | 1:21:A:LEU:HB3   | 13       | 0.21          |
| (1,3436) | 1:64:A:MET:HE1   | 1:21:A:LEU:HD12  | 4        | 0.21          |
| (1,3422) | 1:77:A:LEU:HG    | 1:77:A:LEU:HD23  | 7        | 0.21          |
| (1,3422) | 1:77:A:LEU:HG    | 1:77:A:LEU:HD23  | 8        | 0.21          |
| (1,3422) | 1:77:A:LEU:HG    | 1:77:A:LEU:HD23  | 10       | 0.21          |
| (1,3417) | 1:117:A:LEU:HG   | 1:117:A:LEU:HD12 | 4        | 0.21          |
| (1,3417) | 1:117:A:LEU:HG   | 1:117:A:LEU:HD13 | 14       | 0.21          |
| (1,3415) | 1:117:A:LEU:HA   | 1:117:A:LEU:HD12 | 3        | 0.21          |
| (1,3401) | 1:86:A:TYR:HE2   | 1:86:A:TYR:HA    | 5        | 0.21          |
| (1,3401) | 1:86:A:TYR:HE1   | 1:86:A:TYR:HA    | 6        | 0.21          |
| (1,3401) | 1:86:A:TYR:HE2   | 1:86:A:TYR:HA    | 16       | 0.21          |
| (1,3396) | 1:71:A:LEU:HA    | 1:74:A:ALA:HB1   | 2        | 0.21          |
| (1,3395) | 1:33:A:GLU:HB3   | 1:33:A:GLU:HA    | 13       | 0.21          |
| (1,3395) | 1:33:A:GLU:HB3   | 1:33:A:GLU:HA    | 17       | 0.21          |
| (1,3370) | 1:24:A:SER:HA    | 1:27:A:VAL:HG13  | 6        | 0.21          |
| (1,3370) | 1:24:A:SER:HA    | 1:27:A:VAL:HG13  | 9        | 0.21          |
| (1,3341) | 1:41:A:ALA:HB2   | 1:28:A:ILE:HG23  | 10       | 0.21          |
| (1,3336) | 1:71:A:LEU:HD23  | 1:74:A:ALA:H     | 9        | 0.21          |
| (1,3336) | 1:71:A:LEU:HD21  | 1:74:A:ALA:H     | 15       | 0.21          |
| (1,3325) | 1:77:A:LEU:HB3   | 1:77:A:LEU:HD13  | 1        | 0.21          |
| (1,3325) | 1:77:A:LEU:HB3   | 1:77:A:LEU:HD13  | 2        | 0.21          |
| (1,3325) | 1:77:A:LEU:HB3   | 1:77:A:LEU:HD12  | 7        | 0.21          |
| (1,3325) | 1:77:A:LEU:HB3   | 1:77:A:LEU:HD13  | 11       | 0.21          |
| (1,3325) | 1:77:A:LEU:HB3   | 1:77:A:LEU:HD12  | 12       | 0.21          |
| (1,3325) | 1:77:A:LEU:HB3   | 1:77:A:LEU:HD12  | 14       | 0.21          |
| (1,3311) | 1:68:A:LYS:HD3   | 1:57:A:VAL:HG12  | 14       | 0.21          |
| (1,3266) | 1:85:A:LEU:HD13  | 1:85:A:LEU:HD23  | 4        | 0.21          |
| (1,3266) | 1:85:A:LEU:HD12  | 1:85:A:LEU:HD22  | 17       | 0.21          |
| (1,3260) | 1:121:A:LYS:HG2  | 1:121:A:LYS:HB2  | 7        | 0.21          |
| (1,3260) | 1:121:A:LYS:HG2  | 1:121:A:LYS:HB2  | 14       | 0.21          |
| (1,3260) | 1:121:A:LYS:HG2  | 1:121:A:LYS:HB2  | 16       | 0.21          |
| (1,3260) | 1:121:A:LYS:HG2  | 1:121:A:LYS:HB2  | 17       | 0.21          |
| (1,3255) | 1:40:A:SER:HA    | 1:41:A:ALA:HB3   | 7        | 0.21          |
| (1,3232) | 1:92:A:ALA:H     | 1:105:A:LEU:HB2  | 11       | 0.21          |
| (1,3232) | 1:92:A:ALA:H     | 1:105:A:LEU:HB2  | 14       | 0.21          |
| (1,3228) | 1:31:A:LEU:HB2   | 1:39:A:PHE:HE2   | 9        | 0.21          |
| (1,3223) | 1:84:A:TYR:HE1   | 1:79:A:THR:HA    | 14       | 0.21          |
| (1,3209) | 1:124:A:VAL:HG13 | 1:124:A:VAL:HB   | 7        | 0.21          |
| (1,3209) | 1:124:A:VAL:HG11 | 1:124:A:VAL:HB   | 11       | 0.21          |
| (1,3195) | 1:113:A:ALA:HA   | 1:113:A:ALA:H    | 3        | 0.21          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3195) | 1:113:A:ALA:HA   | 1:113:A:ALA:H   | 6        | 0.21          |
| (1,3195) | 1:113:A:ALA:HA   | 1:113:A:ALA:H   | 9        | 0.21          |
| (1,3195) | 1:113:A:ALA:HA   | 1:113:A:ALA:H   | 14       | 0.21          |
| (1,3195) | 1:113:A:ALA:HA   | 1:113:A:ALA:H   | 15       | 0.21          |
| (1,3183) | 1:124:A:VAL:HG22 | 1:121:A:LYS:HA  | 2        | 0.21          |
| (1,3181) | 1:108:A:GLN:HG3  | 1:108:A:GLN:HA  | 3        | 0.21          |
| (1,3181) | 1:108:A:GLN:HG3  | 1:108:A:GLN:HA  | 4        | 0.21          |
| (1,3181) | 1:108:A:GLN:HG3  | 1:108:A:GLN:HA  | 17       | 0.21          |
| (1,3179) | 1:111:A:GLU:HA   | 1:111:A:GLU:H   | 11       | 0.21          |
| (1,3179) | 1:111:A:GLU:HA   | 1:111:A:GLU:H   | 12       | 0.21          |
| (1,3179) | 1:111:A:GLU:HA   | 1:111:A:GLU:H   | 14       | 0.21          |
| (1,3179) | 1:111:A:GLU:HA   | 1:111:A:GLU:H   | 15       | 0.21          |
| (1,3172) | 1:25:A:LYS:HE3   | 1:25:A:LYS:HA   | 14       | 0.21          |
| (1,3166) | 1:75:A:LEU:HD23  | 1:53:A:PHE:HD1  | 5        | 0.21          |
| (1,3166) | 1:75:A:LEU:HD23  | 1:53:A:PHE:HD2  | 9        | 0.21          |
| (1,3166) | 1:75:A:LEU:HD21  | 1:53:A:PHE:HD2  | 11       | 0.21          |
| (1,3166) | 1:75:A:LEU:HD21  | 1:53:A:PHE:HD1  | 16       | 0.21          |
| (1,3166) | 1:75:A:LEU:HD22  | 1:53:A:PHE:HD2  | 17       | 0.21          |
| (1,3139) | 1:69:A:THR:HB    | 1:69:A:THR:H    | 1        | 0.21          |
| (1,3139) | 1:69:A:THR:HB    | 1:69:A:THR:H    | 3        | 0.21          |
| (1,3139) | 1:69:A:THR:HB    | 1:69:A:THR:H    | 4        | 0.21          |
| (1,3139) | 1:69:A:THR:HB    | 1:69:A:THR:H    | 6        | 0.21          |
| (1,3139) | 1:69:A:THR:HB    | 1:69:A:THR:H    | 7        | 0.21          |
| (1,3139) | 1:69:A:THR:HB    | 1:69:A:THR:H    | 8        | 0.21          |
| (1,3139) | 1:69:A:THR:HB    | 1:69:A:THR:H    | 9        | 0.21          |
| (1,3139) | 1:69:A:THR:HB    | 1:69:A:THR:H    | 11       | 0.21          |
| (1,3139) | 1:69:A:THR:HB    | 1:69:A:THR:H    | 12       | 0.21          |
| (1,3139) | 1:69:A:THR:HB    | 1:69:A:THR:H    | 13       | 0.21          |
| (1,3139) | 1:69:A:THR:HB    | 1:69:A:THR:H    | 14       | 0.21          |
| (1,3139) | 1:69:A:THR:HB    | 1:69:A:THR:H    | 15       | 0.21          |
| (1,3139) | 1:69:A:THR:HB    | 1:69:A:THR:H    | 16       | 0.21          |
| (1,3132) | 1:68:A:LYS:HB2   | 1:53:A:PHE:HE2  | 5        | 0.21          |
| (1,3113) | 1:57:A:VAL:HG11  | 1:61:A:ALA:H    | 17       | 0.21          |
| (1,3066) | 1:30:A:PHE:HB3   | 1:29:A:ALA:HB1  | 5        | 0.21          |
| (1,3066) | 1:30:A:PHE:HB3   | 1:29:A:ALA:HB1  | 6        | 0.21          |
| (1,3066) | 1:30:A:PHE:HB3   | 1:29:A:ALA:HB1  | 14       | 0.21          |
| (1,3055) | 1:52:A:ILE:HG23  | 1:50:A:ILE:H    | 12       | 0.21          |
| (1,3052) | 1:39:A:PHE:HZ    | 1:52:A:ILE:HG22 | 17       | 0.21          |
| (1,3036) | 1:78:A:TYR:HH    | 1:45:A:ALA:HB2  | 12       | 0.21          |
| (1,3028) | 1:71:A:LEU:HD13  | 1:72:A:ARG:HA   | 1        | 0.21          |
| (1,3023) | 1:64:A:MET:HE2   | 1:27:A:VAL:HA   | 7        | 0.21          |
| (1,2969) | 1:93:A:THR:HG21  | 1:101:A:PRO:HB3 | 5        | 0.21          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2969) | 1:93:A:THR:HG22 | 1:101:A:PRO:HB3  | 7        | 0.21          |
| (1,2969) | 1:93:A:THR:HG23 | 1:101:A:PRO:HB3  | 11       | 0.21          |
| (1,2945) | 1:110:A:VAL:HB  | 1:110:A:VAL:HG12 | 5        | 0.21          |
| (1,2927) | 1:31:A:LEU:HD21 | 1:39:A:PHE:HD2   | 1        | 0.21          |
| (1,2927) | 1:31:A:LEU:HD22 | 1:39:A:PHE:HD1   | 5        | 0.21          |
| (1,2891) | 1:32:A:ALA:HB3  | 1:28:A:ILE:HG23  | 10       | 0.21          |
| (1,2876) | 1:61:A:ALA:HB3  | 1:62:A:GLY:H     | 11       | 0.21          |
| (1,2855) | 1:78:A:TYR:HD2  | 1:28:A:ILE:HD12  | 6        | 0.21          |
| (1,2851) | 1:50:A:ILE:HG21 | 1:50:A:ILE:HA    | 2        | 0.21          |
| (1,2819) | 1:97:A:LEU:HD12 | 1:35:A:PHE:HE2   | 9        | 0.21          |
| (1,2769) | 1:43:A:GLY:HA2  | 1:42:A:GLU:HB2   | 1        | 0.21          |
| (1,2754) | 1:60:A:VAL:HG13 | 1:59:A:ARG:HD3   | 15       | 0.21          |
| (1,2745) | 1:34:A:ARG:HD3  | 1:34:A:ARG:HG3   | 11       | 0.21          |
| (1,2727) | 1:86:A:TYR:HB3  | 1:86:A:TYR:H     | 8        | 0.21          |
| (1,2727) | 1:86:A:TYR:HB3  | 1:86:A:TYR:H     | 9        | 0.21          |
| (1,2727) | 1:86:A:TYR:HB3  | 1:86:A:TYR:H     | 10       | 0.21          |
| (1,2727) | 1:86:A:TYR:HB3  | 1:86:A:TYR:H     | 13       | 0.21          |
| (1,2727) | 1:86:A:TYR:HB3  | 1:86:A:TYR:H     | 14       | 0.21          |
| (1,2727) | 1:86:A:TYR:HB3  | 1:86:A:TYR:H     | 16       | 0.21          |
| (1,2713) | 1:53:A:PHE:HB3  | 1:75:A:LEU:HD11  | 8        | 0.21          |
| (1,2694) | 1:73:A:SER:HB2  | 1:74:A:ALA:H     | 6        | 0.21          |
| (1,2694) | 1:73:A:SER:HB2  | 1:74:A:ALA:H     | 9        | 0.21          |
| (1,2672) | 1:31:A:LEU:HD12 | 1:35:A:PHE:HD2   | 3        | 0.21          |
| (1,2639) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2   | 1        | 0.21          |
| (1,2639) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HB2   | 15       | 0.21          |
| (1,2622) | 1:71:A:LEU:HD13 | 1:57:A:VAL:H     | 4        | 0.21          |
| (1,2622) | 1:71:A:LEU:HD11 | 1:57:A:VAL:H     | 7        | 0.21          |
| (1,2618) | 1:34:A:ARG:HG3  | 1:34:A:ARG:H     | 8        | 0.21          |
| (1,2605) | 1:31:A:LEU:HD21 | 1:30:A:PHE:HD2   | 5        | 0.21          |
| (1,2605) | 1:31:A:LEU:HD21 | 1:30:A:PHE:HD1   | 13       | 0.21          |
| (1,2598) | 1:27:A:VAL:HG21 | 1:27:A:VAL:HG11  | 5        | 0.21          |
| (1,2596) | 1:74:A:ALA:HB1  | 1:27:A:VAL:HG11  | 14       | 0.21          |
| (1,2515) | 1:122:A:ALA:HA  | 1:122:A:ALA:H    | 3        | 0.21          |
| (1,2515) | 1:122:A:ALA:HA  | 1:122:A:ALA:H    | 4        | 0.21          |
| (1,2515) | 1:122:A:ALA:HA  | 1:122:A:ALA:H    | 5        | 0.21          |
| (1,2515) | 1:122:A:ALA:HA  | 1:122:A:ALA:H    | 7        | 0.21          |
| (1,2515) | 1:122:A:ALA:HA  | 1:122:A:ALA:H    | 10       | 0.21          |
| (1,2515) | 1:122:A:ALA:HA  | 1:122:A:ALA:H    | 14       | 0.21          |
| (1,2515) | 1:122:A:ALA:HA  | 1:122:A:ALA:H    | 17       | 0.21          |
| (1,2489) | 1:28:A:ILE:HA   | 1:28:A:ILE:HG23  | 7        | 0.21          |
| (1,2444) | 1:53:A:PHE:HE1  | 1:53:A:PHE:HB2   | 1        | 0.21          |
| (1,2444) | 1:53:A:PHE:HE1  | 1:53:A:PHE:HB2   | 8        | 0.21          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2444) | 1:53:A:PHE:HE2   | 1:53:A:PHE:HB2   | 12       | 0.21          |
| (1,2444) | 1:53:A:PHE:HE2   | 1:53:A:PHE:HB2   | 17       | 0.21          |
| (1,2434) | 1:86:A:TYR:HB2   | 1:117:A:LEU:HB3  | 1        | 0.21          |
| (1,2434) | 1:86:A:TYR:HB2   | 1:117:A:LEU:HB3  | 2        | 0.21          |
| (1,2434) | 1:86:A:TYR:HB2   | 1:117:A:LEU:HB3  | 3        | 0.21          |
| (1,2434) | 1:86:A:TYR:HB2   | 1:117:A:LEU:HB3  | 9        | 0.21          |
| (1,2434) | 1:86:A:TYR:HB2   | 1:117:A:LEU:HB3  | 12       | 0.21          |
| (1,2416) | 1:45:A:ALA:HB1   | 1:45:A:ALA:H     | 1        | 0.21          |
| (1,2411) | 1:45:A:ALA:HB3   | 1:84:A:TYR:HB3   | 4        | 0.21          |
| (1,2404) | 1:28:A:ILE:HD12  | 1:74:A:ALA:HA    | 3        | 0.21          |
| (1,2404) | 1:28:A:ILE:HD13  | 1:74:A:ALA:HA    | 8        | 0.21          |
| (1,2404) | 1:28:A:ILE:HD13  | 1:74:A:ALA:HA    | 13       | 0.21          |
| (1,2341) | 1:66:A:LEU:HD22  | 1:70:A:GLN:H     | 3        | 0.21          |
| (1,2341) | 1:66:A:LEU:HD21  | 1:70:A:GLN:H     | 8        | 0.21          |
| (1,2341) | 1:66:A:LEU:HD22  | 1:70:A:GLN:H     | 16       | 0.21          |
| (1,2307) | 1:117:A:LEU:HD13 | 1:86:A:TYR:HB2   | 3        | 0.21          |
| (1,2288) | 1:70:A:GLN:HA    | 1:70:A:GLN:HG3   | 10       | 0.21          |
| (1,2283) | 1:33:A:GLU:HG2   | 1:33:A:GLU:HA    | 5        | 0.21          |
| (1,2210) | 1:105:A:LEU:HG   | 1:110:A:VAL:HG11 | 1        | 0.21          |
| (1,2169) | 1:22:A:ASN:HB3   | 1:22:A:ASN:H     | 13       | 0.21          |
| (1,2169) | 1:22:A:ASN:HB3   | 1:22:A:ASN:H     | 17       | 0.21          |
| (1,2164) | 1:120:A:ALA:HA   | 1:121:A:LYS:H    | 5        | 0.21          |
| (1,2164) | 1:120:A:ALA:HA   | 1:121:A:LYS:H    | 9        | 0.21          |
| (1,2164) | 1:120:A:ALA:HA   | 1:121:A:LYS:H    | 15       | 0.21          |
| (1,2116) | 1:45:A:ALA:HB1   | 1:84:A:TYR:HA    | 8        | 0.21          |
| (1,2094) | 1:95:A:VAL:HG21  | 1:97:A:LEU:HD21  | 10       | 0.21          |
| (1,2037) | 1:57:A:VAL:HG22  | 1:57:A:VAL:HG11  | 3        | 0.21          |
| (1,2037) | 1:57:A:VAL:HG22  | 1:57:A:VAL:HG11  | 13       | 0.21          |
| (1,2035) | 1:52:A:ILE:HG13  | 1:97:A:LEU:HD21  | 9        | 0.21          |
| (1,2035) | 1:52:A:ILE:HG13  | 1:97:A:LEU:HD23  | 12       | 0.21          |
| (1,2035) | 1:52:A:ILE:HG13  | 1:97:A:LEU:HD21  | 13       | 0.21          |
| (1,2035) | 1:52:A:ILE:HG13  | 1:97:A:LEU:HD23  | 17       | 0.21          |
| (1,2021) | 1:53:A:PHE:HE2   | 1:57:A:VAL:HG11  | 11       | 0.21          |
| (1,1951) | 1:108:A:GLN:HA   | 1:111:A:GLU:HB3  | 1        | 0.21          |
| (1,1951) | 1:108:A:GLN:HA   | 1:111:A:GLU:HB3  | 2        | 0.21          |
| (1,1951) | 1:108:A:GLN:HA   | 1:111:A:GLU:HB3  | 3        | 0.21          |
| (1,1951) | 1:108:A:GLN:HA   | 1:111:A:GLU:HB3  | 4        | 0.21          |
| (1,1951) | 1:108:A:GLN:HA   | 1:111:A:GLU:HB3  | 6        | 0.21          |
| (1,1951) | 1:108:A:GLN:HA   | 1:111:A:GLU:HB3  | 7        | 0.21          |
| (1,1951) | 1:108:A:GLN:HA   | 1:111:A:GLU:HB3  | 8        | 0.21          |
| (1,1951) | 1:108:A:GLN:HA   | 1:111:A:GLU:HB3  | 9        | 0.21          |
| (1,1951) | 1:108:A:GLN:HA   | 1:111:A:GLU:HB3  | 10       | 0.21          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1951) | 1:108:A:GLN:HA  | 1:111:A:GLU:HB3  | 11       | 0.21          |
| (1,1951) | 1:108:A:GLN:HA  | 1:111:A:GLU:HB3  | 13       | 0.21          |
| (1,1951) | 1:108:A:GLN:HA  | 1:111:A:GLU:HB3  | 16       | 0.21          |
| (1,1951) | 1:108:A:GLN:HA  | 1:111:A:GLU:HB3  | 17       | 0.21          |
| (1,1947) | 1:93:A:THR:HB   | 1:88:A:VAL:HG12  | 8        | 0.21          |
| (1,1947) | 1:93:A:THR:HB   | 1:88:A:VAL:HG12  | 12       | 0.21          |
| (1,1877) | 1:27:A:VAL:HG21 | 1:27:A:VAL:H     | 7        | 0.21          |
| (1,1865) | 1:45:A:ALA:HB1  | 1:44:A:GLU:HB3   | 16       | 0.21          |
| (1,1831) | 1:21:A:LEU:HG   | 1:21:A:LEU:HB3   | 5        | 0.21          |
| (1,1831) | 1:21:A:LEU:HG   | 1:21:A:LEU:HB3   | 12       | 0.21          |
| (1,1817) | 1:77:A:LEU:HG   | 1:77:A:LEU:HD21  | 5        | 0.21          |
| (1,1817) | 1:77:A:LEU:HG   | 1:77:A:LEU:HD21  | 15       | 0.21          |
| (1,1812) | 1:117:A:LEU:HA  | 1:117:A:LEU:HD12 | 9        | 0.21          |
| (1,1812) | 1:117:A:LEU:HA  | 1:117:A:LEU:HD13 | 11       | 0.21          |
| (1,1793) | 1:88:A:VAL:HG23 | 1:84:A:TYR:HA    | 4        | 0.21          |
| (1,1756) | 1:79:A:THR:HG22 | 1:84:A:TYR:HE1   | 6        | 0.21          |
| (1,1746) | 1:71:A:LEU:HD22 | 1:74:A:ALA:H     | 11       | 0.21          |
| (1,1733) | 1:30:A:PHE:HD2  | 1:66:A:LEU:HD23  | 3        | 0.21          |
| (1,1733) | 1:30:A:PHE:HD1  | 1:66:A:LEU:HD21  | 13       | 0.21          |
| (1,1733) | 1:30:A:PHE:HD1  | 1:66:A:LEU:HD22  | 17       | 0.21          |
| (1,1730) | 1:27:A:VAL:HA   | 1:66:A:LEU:HD23  | 5        | 0.21          |
| (1,1730) | 1:27:A:VAL:HA   | 1:66:A:LEU:HD22  | 12       | 0.21          |
| (1,1720) | 1:117:A:LEU:HG  | 1:117:A:LEU:HD11 | 7        | 0.21          |
| (1,1713) | 1:20:A:LYS:H    | 1:20:A:LYS:HD3   | 17       | 0.21          |
| (1,1690) | 1:42:A:GLU:HG2  | 1:41:A:ALA:HB1   | 6        | 0.21          |
| (1,1681) | 1:40:A:SER:HA   | 1:41:A:ALA:HB1   | 8        | 0.21          |
| (1,1681) | 1:40:A:SER:HA   | 1:41:A:ALA:HB1   | 17       | 0.21          |
| (1,1671) | 1:78:A:TYR:HA   | 1:28:A:ILE:HG12  | 2        | 0.21          |
| (1,1629) | 1:116:A:GLN:HG3 | 1:113:A:ALA:HB2  | 8        | 0.21          |
| (1,1628) | 1:87:A:GLY:HA3  | 1:113:A:ALA:HB1  | 2        | 0.21          |
| (1,1628) | 1:87:A:GLY:HA3  | 1:113:A:ALA:HB1  | 11       | 0.21          |
| (1,1628) | 1:87:A:GLY:HA3  | 1:113:A:ALA:HB3  | 14       | 0.21          |
| (1,1628) | 1:87:A:GLY:HA3  | 1:113:A:ALA:HB1  | 15       | 0.21          |
| (1,1628) | 1:87:A:GLY:HA3  | 1:113:A:ALA:HB1  | 16       | 0.21          |
| (1,1616) | 1:109:A:HIS:HB2 | 1:108:A:GLN:H    | 4        | 0.21          |
| (1,1616) | 1:109:A:HIS:HB2 | 1:108:A:GLN:H    | 6        | 0.21          |
| (1,1616) | 1:109:A:HIS:HB2 | 1:108:A:GLN:H    | 9        | 0.21          |
| (1,1616) | 1:109:A:HIS:HB2 | 1:108:A:GLN:H    | 10       | 0.21          |
| (1,1616) | 1:109:A:HIS:HB2 | 1:108:A:GLN:H    | 14       | 0.21          |
| (1,1616) | 1:109:A:HIS:HB2 | 1:108:A:GLN:H    | 16       | 0.21          |
| (1,1616) | 1:109:A:HIS:HB2 | 1:108:A:GLN:H    | 17       | 0.21          |
| (1,1592) | 1:126:A:ALA:HB1 | 1:125:A:GLN:HG3  | 4        | 0.21          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1592) | 1:126:A:ALA:HB2  | 1:125:A:GLN:HG3 | 5        | 0.21          |
| (1,1592) | 1:126:A:ALA:HB2  | 1:125:A:GLN:HG3 | 11       | 0.21          |
| (1,1592) | 1:126:A:ALA:HB1  | 1:125:A:GLN:HG3 | 12       | 0.21          |
| (1,1592) | 1:126:A:ALA:HB3  | 1:125:A:GLN:HG3 | 17       | 0.21          |
| (1,1588) | 1:74:A:ALA:HB1   | 1:74:A:ALA:HA   | 7        | 0.21          |
| (1,1567) | 1:68:A:LYS:HB2   | 1:68:A:LYS:HA   | 17       | 0.21          |
| (1,1552) | 1:124:A:VAL:HG13 | 1:124:A:VAL:HB  | 3        | 0.21          |
| (1,1552) | 1:124:A:VAL:HG13 | 1:124:A:VAL:HB  | 12       | 0.21          |
| (1,1552) | 1:124:A:VAL:HG11 | 1:124:A:VAL:HB  | 14       | 0.21          |
| (1,1513) | 1:52:A:ILE:HG23  | 1:53:A:PHE:HB3  | 17       | 0.21          |
| (1,1511) | 1:28:A:ILE:HA    | 1:28:A:ILE:HG23 | 7        | 0.21          |
| (1,1508) | 1:29:A:ALA:H     | 1:28:A:ILE:HG22 | 9        | 0.21          |
| (1,1508) | 1:29:A:ALA:H     | 1:28:A:ILE:HG22 | 11       | 0.21          |
| (1,1508) | 1:29:A:ALA:H     | 1:28:A:ILE:HG21 | 12       | 0.21          |
| (1,1508) | 1:29:A:ALA:H     | 1:28:A:ILE:HG23 | 16       | 0.21          |
| (1,1508) | 1:29:A:ALA:H     | 1:28:A:ILE:HG23 | 17       | 0.21          |
| (1,1481) | 1:64:A:MET:HE2   | 1:30:A:PHE:HA   | 11       | 0.21          |
| (1,1478) | 1:64:A:MET:HE2   | 1:66:A:LEU:H    | 4        | 0.21          |
| (1,1478) | 1:64:A:MET:HE1   | 1:66:A:LEU:H    | 16       | 0.21          |
| (1,1456) | 1:57:A:VAL:HA    | 1:60:A:VAL:HB   | 2        | 0.21          |
| (1,1456) | 1:57:A:VAL:HA    | 1:60:A:VAL:HB   | 4        | 0.21          |
| (1,1456) | 1:57:A:VAL:HA    | 1:60:A:VAL:HB   | 6        | 0.21          |
| (1,1456) | 1:57:A:VAL:HA    | 1:60:A:VAL:HB   | 16       | 0.21          |
| (1,1428) | 1:93:A:THR:HG21  | 1:101:A:PRO:HB3 | 4        | 0.21          |
| (1,1428) | 1:93:A:THR:HG23  | 1:101:A:PRO:HB3 | 17       | 0.21          |
| (1,1419) | 1:77:A:LEU:HD13  | 1:25:A:LYS:HA   | 3        | 0.21          |
| (1,1419) | 1:77:A:LEU:HD11  | 1:25:A:LYS:HA   | 6        | 0.21          |
| (1,1410) | 1:110:A:VAL:HG22 | 1:108:A:GLN:H   | 11       | 0.21          |
| (1,1409) | 1:57:A:VAL:HG22  | 1:57:A:VAL:HG11 | 3        | 0.21          |
| (1,1409) | 1:57:A:VAL:HG22  | 1:57:A:VAL:HG11 | 13       | 0.21          |
| (1,1403) | 1:95:A:VAL:HG22  | 1:95:A:VAL:HG12 | 17       | 0.21          |
| (1,1382) | 1:57:A:VAL:HG22  | 1:53:A:PHE:HE2  | 8        | 0.21          |
| (1,1371) | 1:28:A:ILE:HD11  | 1:75:A:LEU:H    | 7        | 0.21          |
| (1,1365) | 1:32:A:ALA:HB3   | 1:28:A:ILE:HG23 | 15       | 0.21          |
| (1,1363) | 1:29:A:ALA:HA    | 1:32:A:ALA:HB3  | 2        | 0.21          |
| (1,1363) | 1:29:A:ALA:HA    | 1:32:A:ALA:HB3  | 7        | 0.21          |
| (1,1363) | 1:29:A:ALA:HA    | 1:32:A:ALA:HB1  | 13       | 0.21          |
| (1,1342) | 1:48:A:LEU:HD13  | 1:84:A:TYR:HE2  | 17       | 0.21          |
| (1,1337) | 1:78:A:TYR:HD2   | 1:28:A:ILE:HD13 | 8        | 0.21          |
| (1,1337) | 1:78:A:TYR:HD1   | 1:28:A:ILE:HD13 | 14       | 0.21          |
| (1,1331) | 1:78:A:TYR:HE1   | 1:84:A:TYR:HD1  | 10       | 0.21          |
| (1,1315) | 1:95:A:VAL:HG23  | 1:97:A:LEU:HD22 | 11       | 0.21          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1303) | 1:97:A:LEU:HD13  | 1:35:A:PHE:HE2   | 15       | 0.21          |
| (1,1275) | 1:84:A:TYR:HE1   | 1:84:A:TYR:HB3   | 2        | 0.21          |
| (1,1253) | 1:47:A:PRO:HB3   | 1:87:A:GLY:HA2   | 5        | 0.21          |
| (1,1253) | 1:47:A:PRO:HB3   | 1:87:A:GLY:HA2   | 16       | 0.21          |
| (1,1247) | 1:42:A:GLU:HB3   | 1:43:A:GLY:HA2   | 17       | 0.21          |
| (1,1232) | 1:60:A:VAL:HG12  | 1:59:A:ARG:HD3   | 3        | 0.21          |
| (1,1206) | 1:117:A:LEU:HD11 | 1:86:A:TYR:HB2   | 4        | 0.21          |
| (1,1206) | 1:117:A:LEU:HD11 | 1:86:A:TYR:HB2   | 16       | 0.21          |
| (1,1194) | 1:39:A:PHE:HB3   | 1:35:A:PHE:HB3   | 6        | 0.21          |
| (1,1194) | 1:39:A:PHE:HB3   | 1:35:A:PHE:HB3   | 8        | 0.21          |
| (1,1194) | 1:39:A:PHE:HB3   | 1:35:A:PHE:HB3   | 14       | 0.21          |
| (1,1136) | 1:31:A:LEU:HD13  | 1:35:A:PHE:HD2   | 10       | 0.21          |
| (1,1080) | 1:105:A:LEU:HD13 | 1:92:A:ALA:H     | 8        | 0.21          |
| (1,1080) | 1:105:A:LEU:HD11 | 1:92:A:ALA:H     | 10       | 0.21          |
| (1,1080) | 1:105:A:LEU:HD12 | 1:92:A:ALA:H     | 11       | 0.21          |
| (1,1080) | 1:105:A:LEU:HD11 | 1:92:A:ALA:H     | 12       | 0.21          |
| (1,1080) | 1:105:A:LEU:HD13 | 1:92:A:ALA:H     | 15       | 0.21          |
| (1,1080) | 1:105:A:LEU:HD12 | 1:92:A:ALA:H     | 17       | 0.21          |
| (1,838)  | 1:64:A:MET:HE1   | 1:30:A:PHE:HD2   | 17       | 0.21          |
| (1,829)  | 1:41:A:ALA:HB2   | 1:41:A:ALA:H     | 16       | 0.21          |
| (1,635)  | 1:127:A:GLN:H    | 1:127:A:GLN:HB3  | 15       | 0.21          |
| (1,630)  | 1:61:A:ALA:HB1   | 1:67:A:SER:H     | 5        | 0.21          |
| (1,630)  | 1:61:A:ALA:HB2   | 1:67:A:SER:H     | 12       | 0.21          |
| (1,618)  | 1:95:A:VAL:H     | 1:48:A:LEU:HD12  | 5        | 0.21          |
| (1,580)  | 1:98:A:ASP:HB2   | 1:100:A:ASN:HD21 | 8        | 0.21          |
| (1,580)  | 1:98:A:ASP:HB2   | 1:100:A:ASN:HD21 | 10       | 0.21          |
| (1,512)  | 1:13:A:ASP:HB2   | 1:13:A:ASP:H     | 6        | 0.21          |
| (1,477)  | 1:31:A:LEU:H     | 1:31:A:LEU:HD11  | 5        | 0.21          |
| (1,397)  | 1:57:A:VAL:H     | 1:56:A:LEU:HB3   | 12       | 0.21          |
| (1,397)  | 1:57:A:VAL:H     | 1:56:A:LEU:HB3   | 17       | 0.21          |
| (1,263)  | 1:110:A:VAL:HG21 | 1:91:A:GLY:H     | 5        | 0.21          |
| (1,234)  | 1:95:A:VAL:HG22  | 1:99:A:GLY:H     | 3        | 0.21          |
| (1,117)  | 1:27:A:VAL:HG13  | 1:26:A:GLU:H     | 8        | 0.21          |
| (1,100)  | 1:35:A:PHE:HE2   | 1:35:A:PHE:H     | 1        | 0.21          |
| (1,56)   | 1:84:A:TYR:H     | 1:84:A:TYR:HD2   | 13       | 0.21          |
| (3,148)  | 1:22:A:ASN:H     | 1:22:A:ASN:HB2   | 12       | 0.2           |
| (3,135)  | 1:123:A:ARG:HB3  | 1:120:A:ALA:HA   | 8        | 0.2           |
| (3,126)  | 1:21:A:LEU:HD23  | 1:22:A:ASN:H     | 4        | 0.2           |
| (3,111)  | 1:111:A:GLU:HG2  | 1:112:A:HIS:HA   | 3        | 0.2           |
| (3,111)  | 1:111:A:GLU:HG2  | 1:112:A:HIS:HA   | 6        | 0.2           |
| (3,111)  | 1:111:A:GLU:HG2  | 1:112:A:HIS:HA   | 16       | 0.2           |
| (3,94)   | 1:56:A:LEU:HB2   | 1:75:A:LEU:HD13  | 14       | 0.2           |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (3,83)   | 1:114:A:ARG:HB2 | 1:113:A:ALA:HB1  | 5        | 0.2           |
| (3,54)   | 1:71:A:LEU:HB3  | 1:75:A:LEU:HD12  | 15       | 0.2           |
| (3,16)   | 1:90:A:PRO:HA   | 1:110:A:VAL:HG13 | 7        | 0.2           |
| (3,14)   | 1:82:A:TRP:HA   | 1:85:A:LEU:HB2   | 1        | 0.2           |
| (3,14)   | 1:82:A:TRP:HA   | 1:85:A:LEU:HB2   | 12       | 0.2           |
| (1,4323) | 1:62:A:GLY:H    | 1:68:A:LYS:HD2   | 14       | 0.2           |
| (1,4317) | 1:93:A:THR:HB   | 1:102:A:CYS:H    | 1        | 0.2           |
| (1,4316) | 1:95:A:VAL:H    | 1:94:A:ARG:HB3   | 5        | 0.2           |
| (1,4225) | 1:122:A:ALA:HB2 | 1:123:A:ARG:H    | 13       | 0.2           |
| (1,4212) | 1:115:A:LYS:HE3 | 1:115:A:LYS:H    | 6        | 0.2           |
| (1,4212) | 1:115:A:LYS:HE3 | 1:115:A:LYS:H    | 9        | 0.2           |
| (1,4176) | 1:97:A:LEU:HD11 | 1:97:A:LEU:H     | 3        | 0.2           |
| (1,4165) | 1:40:A:SER:HA   | 1:43:A:GLY:H     | 12       | 0.2           |
| (1,4164) | 1:32:A:ALA:HB2  | 1:41:A:ALA:H     | 2        | 0.2           |
| (1,4153) | 1:18:A:GLN:HB3  | 1:18:A:GLN:H     | 3        | 0.2           |
| (1,4150) | 1:17:A:ASN:HB3  | 1:18:A:GLN:H     | 1        | 0.2           |
| (1,4150) | 1:17:A:ASN:HB3  | 1:18:A:GLN:H     | 6        | 0.2           |
| (1,4127) | 1:34:A:ARG:HE   | 1:30:A:PHE:HD2   | 12       | 0.2           |
| (1,4109) | 1:97:A:LEU:HD13 | 1:98:A:ASP:H     | 9        | 0.2           |
| (1,4069) | 1:13:A:ASP:HB2  | 1:13:A:ASP:H     | 3        | 0.2           |
| (1,4069) | 1:13:A:ASP:HB2  | 1:13:A:ASP:H     | 9        | 0.2           |
| (1,4069) | 1:13:A:ASP:HB2  | 1:13:A:ASP:H     | 12       | 0.2           |
| (1,4069) | 1:13:A:ASP:HB2  | 1:13:A:ASP:H     | 14       | 0.2           |
| (1,4069) | 1:13:A:ASP:HB2  | 1:13:A:ASP:H     | 16       | 0.2           |
| (1,4037) | 1:27:A:VAL:HG21 | 1:29:A:ALA:H     | 3        | 0.2           |
| (1,4037) | 1:27:A:VAL:HG21 | 1:29:A:ALA:H     | 10       | 0.2           |
| (1,4036) | 1:31:A:LEU:H    | 1:31:A:LEU:HD13  | 4        | 0.2           |
| (1,4036) | 1:31:A:LEU:H    | 1:31:A:LEU:HD13  | 6        | 0.2           |
| (1,4017) | 1:32:A:ALA:HB3  | 1:35:A:PHE:H     | 10       | 0.2           |
| (1,4016) | 1:15:A:MET:HA   | 1:15:A:MET:H     | 2        | 0.2           |
| (1,4016) | 1:15:A:MET:HA   | 1:15:A:MET:H     | 7        | 0.2           |
| (1,4016) | 1:15:A:MET:HA   | 1:15:A:MET:H     | 11       | 0.2           |
| (1,3987) | 1:50:A:ILE:HG21 | 1:50:A:ILE:H     | 10       | 0.2           |
| (1,3933) | 1:65:A:ASN:HB2  | 1:65:A:ASN:H     | 14       | 0.2           |
| (1,3901) | 1:79:A:THR:H    | 1:77:A:LEU:HB2   | 3        | 0.2           |
| (1,3901) | 1:79:A:THR:H    | 1:77:A:LEU:HB2   | 8        | 0.2           |
| (1,3901) | 1:79:A:THR:H    | 1:77:A:LEU:HB2   | 10       | 0.2           |
| (1,3781) | 1:119:A:GLU:HA  | 1:119:A:GLU:H    | 1        | 0.2           |
| (1,3781) | 1:119:A:GLU:HA  | 1:119:A:GLU:H    | 4        | 0.2           |
| (1,3781) | 1:119:A:GLU:HA  | 1:119:A:GLU:H    | 9        | 0.2           |
| (1,3775) | 1:124:A:VAL:HA  | 1:125:A:GLN:H    | 3        | 0.2           |
| (1,3771) | 1:126:A:ALA:HB3 | 1:126:A:ALA:H    | 9        | 0.2           |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3771) | 1:126:A:ALA:HB3 | 1:126:A:ALA:H    | 14       | 0.2           |
| (1,3768) | 1:130:A:GLU:H   | 1:130:A:GLU:HA   | 5        | 0.2           |
| (1,3768) | 1:130:A:GLU:H   | 1:130:A:GLU:HA   | 8        | 0.2           |
| (1,3749) | 1:123:A:ARG:H   | 1:121:A:LYS:H    | 7        | 0.2           |
| (1,3749) | 1:123:A:ARG:H   | 1:121:A:LYS:H    | 9        | 0.2           |
| (1,3749) | 1:123:A:ARG:H   | 1:121:A:LYS:H    | 11       | 0.2           |
| (1,3749) | 1:123:A:ARG:H   | 1:121:A:LYS:H    | 15       | 0.2           |
| (1,3749) | 1:123:A:ARG:H   | 1:121:A:LYS:H    | 16       | 0.2           |
| (1,3744) | 1:35:A:PHE:HD1  | 1:39:A:PHE:H     | 12       | 0.2           |
| (1,3717) | 1:35:A:PHE:H    | 1:39:A:PHE:HE2   | 3        | 0.2           |
| (1,3717) | 1:35:A:PHE:H    | 1:39:A:PHE:HE2   | 4        | 0.2           |
| (1,3717) | 1:35:A:PHE:H    | 1:39:A:PHE:HE2   | 9        | 0.2           |
| (1,3717) | 1:35:A:PHE:H    | 1:39:A:PHE:HE1   | 13       | 0.2           |
| (1,3717) | 1:35:A:PHE:H    | 1:39:A:PHE:HE1   | 14       | 0.2           |
| (1,3698) | 1:30:A:PHE:HD2  | 1:30:A:PHE:H     | 15       | 0.2           |
| (1,3673) | 1:49:A:LYS:H    | 1:50:A:ILE:H     | 6        | 0.2           |
| (1,3673) | 1:49:A:LYS:H    | 1:50:A:ILE:H     | 12       | 0.2           |
| (1,3662) | 1:83:A:ARG:H    | 1:82:A:TRP:HD1   | 6        | 0.2           |
| (1,3662) | 1:83:A:ARG:H    | 1:82:A:TRP:HD1   | 7        | 0.2           |
| (1,3591) | 1:93:A:THR:HB   | 1:88:A:VAL:HG13  | 9        | 0.2           |
| (1,3591) | 1:93:A:THR:HB   | 1:88:A:VAL:HG12  | 14       | 0.2           |
| (1,3583) | 1:112:A:HIS:H   | 1:109:A:HIS:HA   | 13       | 0.2           |
| (1,3562) | 1:104:A:GLU:HB3 | 1:91:A:GLY:HA3   | 7        | 0.2           |
| (1,3562) | 1:104:A:GLU:HB3 | 1:91:A:GLY:HA3   | 9        | 0.2           |
| (1,3562) | 1:104:A:GLU:HB3 | 1:91:A:GLY:HA3   | 13       | 0.2           |
| (1,3536) | 1:66:A:LEU:HB3  | 1:62:A:GLY:HA3   | 1        | 0.2           |
| (1,3536) | 1:66:A:LEU:HB3  | 1:62:A:GLY:HA3   | 8        | 0.2           |
| (1,3535) | 1:74:A:ALA:HB2  | 1:28:A:ILE:HA    | 1        | 0.2           |
| (1,3535) | 1:74:A:ALA:HB2  | 1:28:A:ILE:HA    | 2        | 0.2           |
| (1,3535) | 1:74:A:ALA:HB1  | 1:28:A:ILE:HA    | 6        | 0.2           |
| (1,3535) | 1:74:A:ALA:HB2  | 1:28:A:ILE:HA    | 8        | 0.2           |
| (1,3519) | 1:65:A:ASN:H    | 1:65:A:ASN:HB3   | 15       | 0.2           |
| (1,3515) | 1:102:A:CYS:HB3 | 1:49:A:LYS:HA    | 4        | 0.2           |
| (1,3506) | 1:60:A:VAL:HG13 | 1:35:A:PHE:HZ    | 5        | 0.2           |
| (1,3506) | 1:60:A:VAL:HG13 | 1:35:A:PHE:HZ    | 6        | 0.2           |
| (1,3506) | 1:60:A:VAL:HG11 | 1:35:A:PHE:HZ    | 9        | 0.2           |
| (1,3494) | 1:56:A:LEU:HD21 | 1:55:A:ASP:HB3   | 8        | 0.2           |
| (1,3494) | 1:56:A:LEU:HD21 | 1:55:A:ASP:HB3   | 12       | 0.2           |
| (1,3494) | 1:56:A:LEU:HD23 | 1:55:A:ASP:HB3   | 17       | 0.2           |
| (1,3492) | 1:105:A:LEU:HB3 | 1:105:A:LEU:HD13 | 15       | 0.2           |
| (1,3489) | 1:21:A:LEU:HD22 | 1:20:A:LYS:HA    | 8        | 0.2           |
| (1,3479) | 1:45:A:ALA:HB1  | 1:44:A:GLU:HB3   | 1        | 0.2           |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3479) | 1:45:A:ALA:HB1  | 1:44:A:GLU:HB3   | 4        | 0.2           |
| (1,3479) | 1:45:A:ALA:HB1  | 1:44:A:GLU:HB3   | 5        | 0.2           |
| (1,3479) | 1:45:A:ALA:HB3  | 1:44:A:GLU:HB3   | 6        | 0.2           |
| (1,3477) | 1:15:A:MET:HG3  | 1:15:A:MET:HB2   | 12       | 0.2           |
| (1,3476) | 1:107:A:GLU:HG2 | 1:108:A:GLN:H    | 2        | 0.2           |
| (1,3476) | 1:107:A:GLU:HG2 | 1:108:A:GLN:H    | 7        | 0.2           |
| (1,3476) | 1:107:A:GLU:HG2 | 1:108:A:GLN:H    | 10       | 0.2           |
| (1,3476) | 1:107:A:GLU:HG2 | 1:108:A:GLN:H    | 12       | 0.2           |
| (1,3457) | 1:20:A:LYS:HE3  | 1:19:A:PRO:HA    | 3        | 0.2           |
| (1,3457) | 1:20:A:LYS:HE3  | 1:19:A:PRO:HA    | 13       | 0.2           |
| (1,3441) | 1:21:A:LEU:HG   | 1:21:A:LEU:HB3   | 1        | 0.2           |
| (1,3441) | 1:21:A:LEU:HG   | 1:21:A:LEU:HB3   | 11       | 0.2           |
| (1,3437) | 1:21:A:LEU:HB2  | 1:21:A:LEU:HD13  | 3        | 0.2           |
| (1,3437) | 1:21:A:LEU:HB2  | 1:21:A:LEU:HD12  | 11       | 0.2           |
| (1,3415) | 1:117:A:LEU:HA  | 1:117:A:LEU:HD11 | 17       | 0.2           |
| (1,3412) | 1:82:A:TRP:HZ3  | 1:117:A:LEU:HD13 | 13       | 0.2           |
| (1,3401) | 1:86:A:TYR:HE1  | 1:86:A:TYR:HA    | 13       | 0.2           |
| (1,3396) | 1:71:A:LEU:HA   | 1:74:A:ALA:HB3   | 13       | 0.2           |
| (1,3395) | 1:33:A:GLU:HB3  | 1:33:A:GLU:HA    | 1        | 0.2           |
| (1,3395) | 1:33:A:GLU:HB3  | 1:33:A:GLU:HA    | 3        | 0.2           |
| (1,3395) | 1:33:A:GLU:HB3  | 1:33:A:GLU:HA    | 9        | 0.2           |
| (1,3395) | 1:33:A:GLU:HB3  | 1:33:A:GLU:HA    | 10       | 0.2           |
| (1,3370) | 1:24:A:SER:HA   | 1:27:A:VAL:HG11  | 4        | 0.2           |
| (1,3370) | 1:24:A:SER:HA   | 1:27:A:VAL:HG11  | 11       | 0.2           |
| (1,3370) | 1:24:A:SER:HA   | 1:27:A:VAL:HG11  | 13       | 0.2           |
| (1,3370) | 1:24:A:SER:HA   | 1:27:A:VAL:HG13  | 16       | 0.2           |
| (1,3369) | 1:24:A:SER:HA   | 1:27:A:VAL:HG21  | 5        | 0.2           |
| (1,3344) | 1:113:A:ALA:HB1 | 1:89:A:LYS:H     | 7        | 0.2           |
| (1,3341) | 1:41:A:ALA:HB3  | 1:28:A:ILE:HG22  | 11       | 0.2           |
| (1,3336) | 1:71:A:LEU:HD23 | 1:74:A:ALA:H     | 4        | 0.2           |
| (1,3336) | 1:71:A:LEU:HD21 | 1:74:A:ALA:H     | 5        | 0.2           |
| (1,3325) | 1:77:A:LEU:HB3  | 1:77:A:LEU:HD13  | 3        | 0.2           |
| (1,3325) | 1:77:A:LEU:HB3  | 1:77:A:LEU:HD11  | 6        | 0.2           |
| (1,3325) | 1:77:A:LEU:HB3  | 1:77:A:LEU:HD11  | 13       | 0.2           |
| (1,3325) | 1:77:A:LEU:HB3  | 1:77:A:LEU:HD11  | 16       | 0.2           |
| (1,3322) | 1:30:A:PHE:HD2  | 1:66:A:LEU:HD22  | 9        | 0.2           |
| (1,3322) | 1:30:A:PHE:HD1  | 1:66:A:LEU:HD22  | 12       | 0.2           |
| (1,3320) | 1:27:A:VAL:HA   | 1:66:A:LEU:HD21  | 4        | 0.2           |
| (1,3320) | 1:27:A:VAL:HA   | 1:66:A:LEU:HD21  | 7        | 0.2           |
| (1,3320) | 1:27:A:VAL:HA   | 1:66:A:LEU:HD22  | 9        | 0.2           |
| (1,3320) | 1:27:A:VAL:HA   | 1:66:A:LEU:HD21  | 11       | 0.2           |
| (1,3320) | 1:27:A:VAL:HA   | 1:66:A:LEU:HD23  | 14       | 0.2           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3320) | 1:27:A:VAL:HA   | 1:66:A:LEU:HD22 | 17       | 0.2           |
| (1,3266) | 1:85:A:LEU:HD11 | 1:85:A:LEU:HD22 | 7        | 0.2           |
| (1,3260) | 1:121:A:LYS:HG2 | 1:121:A:LYS:HB2 | 1        | 0.2           |
| (1,3260) | 1:121:A:LYS:HG2 | 1:121:A:LYS:HB2 | 5        | 0.2           |
| (1,3260) | 1:121:A:LYS:HG2 | 1:121:A:LYS:HB2 | 6        | 0.2           |
| (1,3250) | 1:41:A:ALA:HA   | 1:41:A:ALA:HB3  | 2        | 0.2           |
| (1,3250) | 1:41:A:ALA:HA   | 1:41:A:ALA:HB2  | 13       | 0.2           |
| (1,3232) | 1:92:A:ALA:H    | 1:105:A:LEU:HB2 | 1        | 0.2           |
| (1,3232) | 1:92:A:ALA:H    | 1:105:A:LEU:HB2 | 6        | 0.2           |
| (1,3232) | 1:92:A:ALA:H    | 1:105:A:LEU:HB2 | 7        | 0.2           |
| (1,3232) | 1:92:A:ALA:H    | 1:105:A:LEU:HB2 | 15       | 0.2           |
| (1,3230) | 1:68:A:LYS:HB2  | 1:68:A:LYS:HA   | 14       | 0.2           |
| (1,3200) | 1:116:A:GLN:HG3 | 1:113:A:ALA:HB1 | 9        | 0.2           |
| (1,3195) | 1:113:A:ALA:HA  | 1:113:A:ALA:H   | 1        | 0.2           |
| (1,3181) | 1:108:A:GLN:HG3 | 1:108:A:GLN:HA  | 11       | 0.2           |
| (1,3179) | 1:111:A:GLU:HA  | 1:111:A:GLU:H   | 1        | 0.2           |
| (1,3179) | 1:111:A:GLU:HA  | 1:111:A:GLU:H   | 2        | 0.2           |
| (1,3179) | 1:111:A:GLU:HA  | 1:111:A:GLU:H   | 3        | 0.2           |
| (1,3179) | 1:111:A:GLU:HA  | 1:111:A:GLU:H   | 4        | 0.2           |
| (1,3179) | 1:111:A:GLU:HA  | 1:111:A:GLU:H   | 5        | 0.2           |
| (1,3179) | 1:111:A:GLU:HA  | 1:111:A:GLU:H   | 6        | 0.2           |
| (1,3179) | 1:111:A:GLU:HA  | 1:111:A:GLU:H   | 8        | 0.2           |
| (1,3179) | 1:111:A:GLU:HA  | 1:111:A:GLU:H   | 9        | 0.2           |
| (1,3179) | 1:111:A:GLU:HA  | 1:111:A:GLU:H   | 13       | 0.2           |
| (1,3179) | 1:111:A:GLU:HA  | 1:111:A:GLU:H   | 16       | 0.2           |
| (1,3179) | 1:111:A:GLU:HA  | 1:111:A:GLU:H   | 17       | 0.2           |
| (1,3166) | 1:75:A:LEU:HD23 | 1:53:A:PHE:HD2  | 6        | 0.2           |
| (1,3166) | 1:75:A:LEU:HD23 | 1:53:A:PHE:HD1  | 14       | 0.2           |
| (1,3165) | 1:126:A:ALA:HB1 | 1:125:A:GLN:HG3 | 7        | 0.2           |
| (1,3165) | 1:126:A:ALA:HB3 | 1:125:A:GLN:HG3 | 13       | 0.2           |
| (1,3165) | 1:126:A:ALA:HB1 | 1:125:A:GLN:HG3 | 15       | 0.2           |
| (1,3160) | 1:74:A:ALA:HB1  | 1:74:A:ALA:HA   | 9        | 0.2           |
| (1,3160) | 1:74:A:ALA:HB1  | 1:74:A:ALA:HA   | 13       | 0.2           |
| (1,3139) | 1:69:A:THR:HB   | 1:69:A:THR:H    | 10       | 0.2           |
| (1,3139) | 1:69:A:THR:HB   | 1:69:A:THR:H    | 17       | 0.2           |
| (1,3132) | 1:68:A:LYS:HB2  | 1:53:A:PHE:HE1  | 7        | 0.2           |
| (1,3113) | 1:57:A:VAL:HG11 | 1:61:A:ALA:H    | 7        | 0.2           |
| (1,3113) | 1:57:A:VAL:HG13 | 1:61:A:ALA:H    | 8        | 0.2           |
| (1,3052) | 1:39:A:PHE:HZ   | 1:52:A:ILE:HG22 | 7        | 0.2           |
| (1,3021) | 1:64:A:MET:HE3  | 1:63:A:GLU:H    | 10       | 0.2           |
| (1,3021) | 1:64:A:MET:HE3  | 1:63:A:GLU:H    | 17       | 0.2           |
| (1,3019) | 1:64:A:MET:HE1  | 1:66:A:LEU:H    | 9        | 0.2           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2969) | 1:93:A:THR:HG22 | 1:101:A:PRO:HB3 | 8        | 0.2           |
| (1,2969) | 1:93:A:THR:HG23 | 1:101:A:PRO:HB3 | 10       | 0.2           |
| (1,2950) | 1:75:A:LEU:HD11 | 1:75:A:LEU:H    | 1        | 0.2           |
| (1,2950) | 1:75:A:LEU:HD11 | 1:75:A:LEU:H    | 14       | 0.2           |
| (1,2932) | 1:95:A:VAL:HG23 | 1:95:A:VAL:H    | 6        | 0.2           |
| (1,2930) | 1:31:A:LEU:HD22 | 1:60:A:VAL:HG11 | 15       | 0.2           |
| (1,2927) | 1:31:A:LEU:HD23 | 1:39:A:PHE:HD2  | 2        | 0.2           |
| (1,2927) | 1:31:A:LEU:HD22 | 1:39:A:PHE:HD2  | 4        | 0.2           |
| (1,2927) | 1:31:A:LEU:HD23 | 1:39:A:PHE:HD2  | 9        | 0.2           |
| (1,2927) | 1:31:A:LEU:HD22 | 1:39:A:PHE:HD1  | 16       | 0.2           |
| (1,2924) | 1:21:A:LEU:HD23 | 1:21:A:LEU:H    | 7        | 0.2           |
| (1,2899) | 1:28:A:ILE:HD11 | 1:75:A:LEU:H    | 1        | 0.2           |
| (1,2899) | 1:28:A:ILE:HD13 | 1:75:A:LEU:H    | 8        | 0.2           |
| (1,2881) | 1:74:A:ALA:HB3  | 1:31:A:LEU:HD11 | 14       | 0.2           |
| (1,2871) | 1:129:A:ALA:HB2 | 1:129:A:ALA:H   | 9        | 0.2           |
| (1,2855) | 1:78:A:TYR:HD1  | 1:28:A:ILE:HD12 | 16       | 0.2           |
| (1,2836) | 1:95:A:VAL:HG21 | 1:97:A:LEU:HD22 | 13       | 0.2           |
| (1,2769) | 1:43:A:GLY:HA2  | 1:42:A:GLU:HB2  | 11       | 0.2           |
| (1,2769) | 1:43:A:GLY:HA2  | 1:42:A:GLU:HB2  | 15       | 0.2           |
| (1,2754) | 1:60:A:VAL:HG13 | 1:59:A:ARG:HD3  | 16       | 0.2           |
| (1,2740) | 1:57:A:VAL:HG21 | 1:58:A:ASP:HB2  | 1        | 0.2           |
| (1,2727) | 1:86:A:TYR:HB3  | 1:86:A:TYR:H    | 3        | 0.2           |
| (1,2727) | 1:86:A:TYR:HB3  | 1:86:A:TYR:H    | 4        | 0.2           |
| (1,2727) | 1:86:A:TYR:HB3  | 1:86:A:TYR:H    | 5        | 0.2           |
| (1,2727) | 1:86:A:TYR:HB3  | 1:86:A:TYR:H    | 6        | 0.2           |
| (1,2727) | 1:86:A:TYR:HB3  | 1:86:A:TYR:H    | 11       | 0.2           |
| (1,2727) | 1:86:A:TYR:HB3  | 1:86:A:TYR:H    | 12       | 0.2           |
| (1,2727) | 1:86:A:TYR:HB3  | 1:86:A:TYR:H    | 15       | 0.2           |
| (1,2727) | 1:86:A:TYR:HB3  | 1:86:A:TYR:H    | 17       | 0.2           |
| (1,2711) | 1:35:A:PHE:HB2  | 1:35:A:PHE:HE2  | 1        | 0.2           |
| (1,2711) | 1:35:A:PHE:HB2  | 1:35:A:PHE:HE1  | 11       | 0.2           |
| (1,2662) | 1:97:A:LEU:HD13 | 1:57:A:VAL:H    | 11       | 0.2           |
| (1,2629) | 1:53:A:PHE:HZ   | 1:71:A:LEU:HB2  | 1        | 0.2           |
| (1,2629) | 1:53:A:PHE:HZ   | 1:71:A:LEU:HB2  | 2        | 0.2           |
| (1,2629) | 1:53:A:PHE:HZ   | 1:71:A:LEU:HB2  | 3        | 0.2           |
| (1,2629) | 1:53:A:PHE:HZ   | 1:71:A:LEU:HB2  | 15       | 0.2           |
| (1,2622) | 1:71:A:LEU:HD12 | 1:57:A:VAL:H    | 1        | 0.2           |
| (1,2622) | 1:71:A:LEU:HD13 | 1:57:A:VAL:H    | 12       | 0.2           |
| (1,2605) | 1:31:A:LEU:HD22 | 1:30:A:PHE:HD2  | 3        | 0.2           |
| (1,2598) | 1:27:A:VAL:HG22 | 1:27:A:VAL:HG13 | 12       | 0.2           |
| (1,2529) | 1:79:A:THR:HG22 | 1:75:A:LEU:HA   | 4        | 0.2           |
| (1,2515) | 1:122:A:ALA:HA  | 1:122:A:ALA:H   | 6        | 0.2           |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2515) | 1:122:A:ALA:HA   | 1:122:A:ALA:H   | 9        | 0.2           |
| (1,2505) | 1:126:A:ALA:HA   | 1:126:A:ALA:H   | 3        | 0.2           |
| (1,2505) | 1:126:A:ALA:HA   | 1:126:A:ALA:H   | 6        | 0.2           |
| (1,2489) | 1:28:A:ILE:HA    | 1:28:A:ILE:HG22 | 4        | 0.2           |
| (1,2489) | 1:28:A:ILE:HA    | 1:28:A:ILE:HG22 | 16       | 0.2           |
| (1,2444) | 1:53:A:PHE:HE2   | 1:53:A:PHE:HB2  | 11       | 0.2           |
| (1,2444) | 1:53:A:PHE:HE1   | 1:53:A:PHE:HB2  | 15       | 0.2           |
| (1,2434) | 1:86:A:TYR:HB2   | 1:117:A:LEU:HB3 | 11       | 0.2           |
| (1,2416) | 1:45:A:ALA:HB3   | 1:45:A:ALA:H    | 6        | 0.2           |
| (1,2416) | 1:45:A:ALA:HB1   | 1:45:A:ALA:H    | 7        | 0.2           |
| (1,2416) | 1:45:A:ALA:HB3   | 1:45:A:ALA:H    | 12       | 0.2           |
| (1,2409) | 1:49:A:LYS:H     | 1:52:A:ILE:HD11 | 1        | 0.2           |
| (1,2409) | 1:49:A:LYS:H     | 1:52:A:ILE:HD11 | 12       | 0.2           |
| (1,2367) | 1:52:A:ILE:H     | 1:52:A:ILE:HD12 | 6        | 0.2           |
| (1,2358) | 1:107:A:GLU:HA   | 1:111:A:GLU:H   | 5        | 0.2           |
| (1,2358) | 1:107:A:GLU:HA   | 1:111:A:GLU:H   | 15       | 0.2           |
| (1,2346) | 1:105:A:LEU:HD13 | 1:107:A:GLU:HA  | 2        | 0.2           |
| (1,2341) | 1:66:A:LEU:HD22  | 1:70:A:GLN:H    | 14       | 0.2           |
| (1,2341) | 1:66:A:LEU:HD23  | 1:70:A:GLN:H    | 15       | 0.2           |
| (1,2336) | 1:64:A:MET:HE3   | 1:31:A:LEU:HA   | 16       | 0.2           |
| (1,2334) | 1:60:A:VAL:HG13  | 1:63:A:GLU:HG3  | 5        | 0.2           |
| (1,2307) | 1:117:A:LEU:HD11 | 1:86:A:TYR:HB2  | 7        | 0.2           |
| (1,2299) | 1:55:A:ASP:HB3   | 1:96:A:ASP:HA   | 8        | 0.2           |
| (1,2283) | 1:33:A:GLU:HG2   | 1:33:A:GLU:HA   | 11       | 0.2           |
| (1,2221) | 1:31:A:LEU:HA    | 1:60:A:VAL:HB   | 10       | 0.2           |
| (1,2221) | 1:31:A:LEU:HA    | 1:60:A:VAL:HB   | 12       | 0.2           |
| (1,2169) | 1:22:A:ASN:HB3   | 1:22:A:ASN:H    | 8        | 0.2           |
| (1,2164) | 1:120:A:ALA:HA   | 1:121:A:LYS:H   | 10       | 0.2           |
| (1,2164) | 1:120:A:ALA:HA   | 1:121:A:LYS:H   | 11       | 0.2           |
| (1,2164) | 1:120:A:ALA:HA   | 1:121:A:LYS:H   | 12       | 0.2           |
| (1,2164) | 1:120:A:ALA:HA   | 1:121:A:LYS:H   | 16       | 0.2           |
| (1,2116) | 1:45:A:ALA:HB3   | 1:84:A:TYR:HA   | 4        | 0.2           |
| (1,2112) | 1:45:A:ALA:HB2   | 1:84:A:TYR:H    | 2        | 0.2           |
| (1,2045) | 1:77:A:LEU:H     | 1:78:A:TYR:H    | 1        | 0.2           |
| (1,2045) | 1:77:A:LEU:H     | 1:78:A:TYR:H    | 2        | 0.2           |
| (1,2045) | 1:77:A:LEU:H     | 1:78:A:TYR:H    | 7        | 0.2           |
| (1,2037) | 1:57:A:VAL:HG22  | 1:57:A:VAL:HG11 | 1        | 0.2           |
| (1,2035) | 1:52:A:ILE:HG13  | 1:97:A:LEU:HD23 | 15       | 0.2           |
| (1,2005) | 1:95:A:VAL:HG22  | 1:48:A:LEU:HD11 | 7        | 0.2           |
| (1,1963) | 1:120:A:ALA:HB2  | 1:82:A:TRP:HE1  | 2        | 0.2           |
| (1,1951) | 1:108:A:GLN:HA   | 1:111:A:GLU:HB3 | 5        | 0.2           |
| (1,1947) | 1:93:A:THR:HB    | 1:88:A:VAL:HG12 | 7        | 0.2           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1890) | 1:100:A:ASN:HD22 | 1:98:A:ASP:HB3   | 6        | 0.2           |
| (1,1890) | 1:100:A:ASN:HD22 | 1:98:A:ASP:HB3   | 16       | 0.2           |
| (1,1886) | 1:102:A:CYS:HB3  | 1:49:A:LYS:HA    | 2        | 0.2           |
| (1,1886) | 1:102:A:CYS:HB3  | 1:49:A:LYS:HA    | 3        | 0.2           |
| (1,1883) | 1:64:A:MET:HE3   | 1:21:A:LEU:H     | 1        | 0.2           |
| (1,1876) | 1:27:A:VAL:HG23  | 1:31:A:LEU:HD12  | 9        | 0.2           |
| (1,1831) | 1:21:A:LEU:HG    | 1:21:A:LEU:HB3   | 10       | 0.2           |
| (1,1831) | 1:21:A:LEU:HG    | 1:21:A:LEU:HB3   | 14       | 0.2           |
| (1,1831) | 1:21:A:LEU:HG    | 1:21:A:LEU:HB3   | 17       | 0.2           |
| (1,1817) | 1:77:A:LEU:HG    | 1:77:A:LEU:HD22  | 3        | 0.2           |
| (1,1817) | 1:77:A:LEU:HG    | 1:77:A:LEU:HD22  | 4        | 0.2           |
| (1,1817) | 1:77:A:LEU:HG    | 1:77:A:LEU:HD22  | 6        | 0.2           |
| (1,1812) | 1:117:A:LEU:HA   | 1:117:A:LEU:HD12 | 12       | 0.2           |
| (1,1811) | 1:86:A:TYR:H     | 1:117:A:LEU:HD12 | 5        | 0.2           |
| (1,1799) | 1:71:A:LEU:HA    | 1:74:A:ALA:HB2   | 6        | 0.2           |
| (1,1799) | 1:71:A:LEU:HA    | 1:74:A:ALA:HB2   | 11       | 0.2           |
| (1,1773) | 1:24:A:SER:HA    | 1:27:A:VAL:HG21  | 7        | 0.2           |
| (1,1773) | 1:24:A:SER:HA    | 1:27:A:VAL:HG21  | 9        | 0.2           |
| (1,1753) | 1:113:A:ALA:HB3  | 1:89:A:LYS:H     | 2        | 0.2           |
| (1,1753) | 1:113:A:ALA:HB1  | 1:89:A:LYS:H     | 12       | 0.2           |
| (1,1730) | 1:27:A:VAL:HA    | 1:66:A:LEU:HD21  | 15       | 0.2           |
| (1,1726) | 1:66:A:LEU:HD12  | 1:66:A:LEU:HA    | 5        | 0.2           |
| (1,1726) | 1:66:A:LEU:HD11  | 1:66:A:LEU:HA    | 6        | 0.2           |
| (1,1726) | 1:66:A:LEU:HD11  | 1:66:A:LEU:HA    | 9        | 0.2           |
| (1,1713) | 1:20:A:LYS:H     | 1:20:A:LYS:HD3   | 11       | 0.2           |
| (1,1713) | 1:20:A:LYS:H     | 1:20:A:LYS:HD3   | 13       | 0.2           |
| (1,1698) | 1:44:A:GLU:HG2   | 1:45:A:ALA:HB3   | 6        | 0.2           |
| (1,1698) | 1:44:A:GLU:HG2   | 1:45:A:ALA:HB3   | 8        | 0.2           |
| (1,1671) | 1:78:A:TYR:HA    | 1:28:A:ILE:HG12  | 11       | 0.2           |
| (1,1660) | 1:27:A:VAL:HA    | 1:27:A:VAL:HG11  | 9        | 0.2           |
| (1,1628) | 1:87:A:GLY:HA3   | 1:113:A:ALA:HB3  | 3        | 0.2           |
| (1,1628) | 1:87:A:GLY:HA3   | 1:113:A:ALA:HB1  | 5        | 0.2           |
| (1,1628) | 1:87:A:GLY:HA3   | 1:113:A:ALA:HB1  | 6        | 0.2           |
| (1,1628) | 1:87:A:GLY:HA3   | 1:113:A:ALA:HB2  | 7        | 0.2           |
| (1,1616) | 1:109:A:HIS:HB2  | 1:108:A:GLN:H    | 2        | 0.2           |
| (1,1616) | 1:109:A:HIS:HB2  | 1:108:A:GLN:H    | 7        | 0.2           |
| (1,1616) | 1:109:A:HIS:HB2  | 1:108:A:GLN:H    | 8        | 0.2           |
| (1,1616) | 1:109:A:HIS:HB2  | 1:108:A:GLN:H    | 12       | 0.2           |
| (1,1592) | 1:126:A:ALA:HB3  | 1:125:A:GLN:HG3  | 10       | 0.2           |
| (1,1588) | 1:74:A:ALA:HB3   | 1:74:A:ALA:HA    | 3        | 0.2           |
| (1,1588) | 1:74:A:ALA:HB1   | 1:74:A:ALA:HA    | 5        | 0.2           |
| (1,1588) | 1:74:A:ALA:HB1   | 1:74:A:ALA:HA    | 17       | 0.2           |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1568) | 1:68:A:LYS:HB2   | 1:57:A:VAL:HG11 | 11       | 0.2           |
| (1,1567) | 1:68:A:LYS:HB2   | 1:68:A:LYS:HA   | 11       | 0.2           |
| (1,1556) | 1:59:A:ARG:HB2   | 1:58:A:ASP:HB2  | 11       | 0.2           |
| (1,1553) | 1:57:A:VAL:HG12  | 1:61:A:ALA:H    | 6        | 0.2           |
| (1,1552) | 1:124:A:VAL:HG13 | 1:124:A:VAL:HB  | 7        | 0.2           |
| (1,1513) | 1:52:A:ILE:HG22  | 1:53:A:PHE:HB3  | 16       | 0.2           |
| (1,1511) | 1:28:A:ILE:HA    | 1:28:A:ILE:HG22 | 4        | 0.2           |
| (1,1511) | 1:28:A:ILE:HA    | 1:28:A:ILE:HG22 | 16       | 0.2           |
| (1,1508) | 1:29:A:ALA:H     | 1:28:A:ILE:HG21 | 2        | 0.2           |
| (1,1508) | 1:29:A:ALA:H     | 1:28:A:ILE:HG23 | 5        | 0.2           |
| (1,1508) | 1:29:A:ALA:H     | 1:28:A:ILE:HG23 | 10       | 0.2           |
| (1,1481) | 1:64:A:MET:HE3   | 1:30:A:PHE:HA   | 16       | 0.2           |
| (1,1456) | 1:57:A:VAL:HA    | 1:60:A:VAL:HB   | 7        | 0.2           |
| (1,1456) | 1:57:A:VAL:HA    | 1:60:A:VAL:HB   | 9        | 0.2           |
| (1,1456) | 1:57:A:VAL:HA    | 1:60:A:VAL:HB   | 12       | 0.2           |
| (1,1428) | 1:93:A:THR:HG22  | 1:101:A:PRO:HB3 | 2        | 0.2           |
| (1,1428) | 1:93:A:THR:HG23  | 1:101:A:PRO:HB3 | 3        | 0.2           |
| (1,1419) | 1:77:A:LEU:HD13  | 1:25:A:LYS:HA   | 5        | 0.2           |
| (1,1419) | 1:77:A:LEU:HD12  | 1:25:A:LYS:HA   | 17       | 0.2           |
| (1,1409) | 1:57:A:VAL:HG22  | 1:57:A:VAL:HG11 | 1        | 0.2           |
| (1,1399) | 1:95:A:VAL:HG22  | 1:95:A:VAL:H    | 17       | 0.2           |
| (1,1382) | 1:57:A:VAL:HG22  | 1:53:A:PHE:HE1  | 12       | 0.2           |
| (1,1382) | 1:57:A:VAL:HG23  | 1:53:A:PHE:HE1  | 13       | 0.2           |
| (1,1371) | 1:28:A:ILE:HD13  | 1:75:A:LEU:H    | 17       | 0.2           |
| (1,1363) | 1:29:A:ALA:HA    | 1:32:A:ALA:HB1  | 16       | 0.2           |
| (1,1357) | 1:74:A:ALA:HB3   | 1:31:A:LEU:HD12 | 5        | 0.2           |
| (1,1353) | 1:61:A:ALA:HB2   | 1:62:A:GLY:H    | 5        | 0.2           |
| (1,1337) | 1:78:A:TYR:HD2   | 1:28:A:ILE:HD12 | 4        | 0.2           |
| (1,1337) | 1:78:A:TYR:HD2   | 1:28:A:ILE:HD13 | 5        | 0.2           |
| (1,1337) | 1:78:A:TYR:HD2   | 1:28:A:ILE:HD13 | 13       | 0.2           |
| (1,1337) | 1:78:A:TYR:HD1   | 1:28:A:ILE:HD11 | 15       | 0.2           |
| (1,1331) | 1:78:A:TYR:HE2   | 1:84:A:TYR:HD1  | 6        | 0.2           |
| (1,1331) | 1:78:A:TYR:HE2   | 1:84:A:TYR:HD1  | 13       | 0.2           |
| (1,1321) | 1:124:A:VAL:HG13 | 1:125:A:GLN:H   | 3        | 0.2           |
| (1,1321) | 1:124:A:VAL:HG13 | 1:125:A:GLN:H   | 7        | 0.2           |
| (1,1321) | 1:124:A:VAL:HG13 | 1:125:A:GLN:H   | 9        | 0.2           |
| (1,1321) | 1:124:A:VAL:HG11 | 1:125:A:GLN:H   | 14       | 0.2           |
| (1,1321) | 1:124:A:VAL:HG11 | 1:125:A:GLN:H   | 17       | 0.2           |
| (1,1303) | 1:97:A:LEU:HD13  | 1:35:A:PHE:HE2  | 4        | 0.2           |
| (1,1253) | 1:47:A:PRO:HB3   | 1:87:A:GLY:HA2  | 4        | 0.2           |
| (1,1253) | 1:47:A:PRO:HB3   | 1:87:A:GLY:HA2  | 17       | 0.2           |
| (1,1243) | 1:43:A:GLY:HA2   | 1:44:A:GLU:H    | 17       | 0.2           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1232) | 1:60:A:VAL:HG13  | 1:59:A:ARG:HD3   | 5        | 0.2           |
| (1,1232) | 1:60:A:VAL:HG12  | 1:59:A:ARG:HD3   | 11       | 0.2           |
| (1,1231) | 1:97:A:LEU:HD12  | 1:59:A:ARG:HD3   | 8        | 0.2           |
| (1,1206) | 1:117:A:LEU:HD13 | 1:86:A:TYR:HB2   | 2        | 0.2           |
| (1,1206) | 1:117:A:LEU:HD12 | 1:86:A:TYR:HB2   | 5        | 0.2           |
| (1,1206) | 1:117:A:LEU:HD13 | 1:86:A:TYR:HB2   | 9        | 0.2           |
| (1,1206) | 1:117:A:LEU:HD11 | 1:86:A:TYR:HB2   | 10       | 0.2           |
| (1,1206) | 1:117:A:LEU:HD11 | 1:86:A:TYR:HB2   | 11       | 0.2           |
| (1,1206) | 1:117:A:LEU:HD11 | 1:86:A:TYR:HB2   | 13       | 0.2           |
| (1,1206) | 1:117:A:LEU:HD12 | 1:86:A:TYR:HB2   | 14       | 0.2           |
| (1,1167) | 1:34:A:ARG:HB3   | 1:30:A:PHE:HD1   | 8        | 0.2           |
| (1,1136) | 1:31:A:LEU:HD13  | 1:35:A:PHE:HD2   | 5        | 0.2           |
| (1,1136) | 1:31:A:LEU:HD12  | 1:35:A:PHE:HD1   | 13       | 0.2           |
| (1,1136) | 1:31:A:LEU:HD12  | 1:35:A:PHE:HD2   | 14       | 0.2           |
| (1,1081) | 1:71:A:LEU:HD12  | 1:57:A:VAL:H     | 11       | 0.2           |
| (1,1080) | 1:105:A:LEU:HD11 | 1:92:A:ALA:H     | 6        | 0.2           |
| (1,993)  | 1:79:A:THR:HG22  | 1:75:A:LEU:HA    | 2        | 0.2           |
| (1,852)  | 1:65:A:ASN:HB3   | 1:65:A:ASN:HD21  | 11       | 0.2           |
| (1,829)  | 1:41:A:ALA:HB1   | 1:41:A:ALA:H     | 15       | 0.2           |
| (1,827)  | 1:45:A:ALA:HB1   | 1:45:A:ALA:H     | 4        | 0.2           |
| (1,827)  | 1:45:A:ALA:HB2   | 1:45:A:ALA:H     | 8        | 0.2           |
| (1,827)  | 1:45:A:ALA:HB2   | 1:45:A:ALA:H     | 14       | 0.2           |
| (1,822)  | 1:49:A:LYS:H     | 1:52:A:ILE:HD11  | 11       | 0.2           |
| (1,753)  | 1:92:A:ALA:HB2   | 1:91:A:GLY:H     | 4        | 0.2           |
| (1,753)  | 1:92:A:ALA:HB2   | 1:91:A:GLY:H     | 12       | 0.2           |
| (1,580)  | 1:98:A:ASP:HB2   | 1:100:A:ASN:HD21 | 2        | 0.2           |
| (1,580)  | 1:98:A:ASP:HB2   | 1:100:A:ASN:HD21 | 12       | 0.2           |
| (1,580)  | 1:98:A:ASP:HB2   | 1:100:A:ASN:HD21 | 13       | 0.2           |
| (1,564)  | 1:59:A:ARG:HE    | 1:97:A:LEU:HD11  | 15       | 0.2           |
| (1,549)  | 1:97:A:LEU:HD11  | 1:98:A:ASP:H     | 3        | 0.2           |
| (1,549)  | 1:97:A:LEU:HD12  | 1:98:A:ASP:H     | 11       | 0.2           |
| (1,512)  | 1:13:A:ASP:HB2   | 1:13:A:ASP:H     | 10       | 0.2           |
| (1,512)  | 1:13:A:ASP:HB2   | 1:13:A:ASP:H     | 11       | 0.2           |
| (1,512)  | 1:13:A:ASP:HB2   | 1:13:A:ASP:H     | 13       | 0.2           |
| (1,478)  | 1:27:A:VAL:HG23  | 1:29:A:ALA:H     | 11       | 0.2           |
| (1,477)  | 1:31:A:LEU:H     | 1:31:A:LEU:HD13  | 7        | 0.2           |
| (1,451)  | 1:32:A:ALA:HB2   | 1:35:A:PHE:H     | 8        | 0.2           |
| (1,441)  | 1:42:A:GLU:HB3   | 1:41:A:ALA:H     | 7        | 0.2           |
| (1,397)  | 1:57:A:VAL:H     | 1:56:A:LEU:HB3   | 6        | 0.2           |
| (1,397)  | 1:57:A:VAL:H     | 1:56:A:LEU:HB3   | 8        | 0.2           |
| (1,308)  | 1:79:A:THR:HG21  | 1:80:A:SER:H     | 17       | 0.2           |
| (1,241)  | 1:95:A:VAL:HG13  | 1:96:A:ASP:H     | 5        | 0.2           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,234)  | 1:95:A:VAL:HG23 | 1:99:A:GLY:H    | 8        | 0.2           |
| (1,234)  | 1:95:A:VAL:HG21 | 1:99:A:GLY:H    | 9        | 0.2           |
| (1,172)  | 1:27:A:VAL:HG12 | 1:21:A:LEU:H    | 7        | 0.2           |
| (1,154)  | 1:130:A:GLU:H   | 1:129:A:ALA:HB2 | 13       | 0.2           |
| (1,152)  | 1:128:A:ARG:HB3 | 1:129:A:ALA:H   | 10       | 0.2           |
| (1,100)  | 1:35:A:PHE:HE2  | 1:35:A:PHE:H    | 5        | 0.2           |
| (1,100)  | 1:35:A:PHE:HE1  | 1:35:A:PHE:H    | 16       | 0.2           |
| (3,130)  | 1:52:A:ILE:HG22 | 1:50:A:ILE:HA   | 5        | 0.19          |
| (3,111)  | 1:111:A:GLU:HG2 | 1:112:A:HIS:HA  | 4        | 0.19          |
| (3,111)  | 1:111:A:GLU:HG2 | 1:112:A:HIS:HA  | 12       | 0.19          |
| (3,94)   | 1:56:A:LEU:HB2  | 1:75:A:LEU:HD11 | 13       | 0.19          |
| (3,92)   | 1:88:A:VAL:HG23 | 1:87:A:GLY:HA2  | 9        | 0.19          |
| (3,83)   | 1:114:A:ARG:HB2 | 1:113:A:ALA:HB2 | 9        | 0.19          |
| (3,64)   | 1:55:A:ASP:HB2  | 1:52:A:ILE:HG22 | 7        | 0.19          |
| (3,64)   | 1:55:A:ASP:HB2  | 1:52:A:ILE:HG22 | 13       | 0.19          |
| (3,59)   | 1:117:A:LEU:HA  | 1:85:A:LEU:HD21 | 14       | 0.19          |
| (3,58)   | 1:102:A:CYS:HB2 | 1:95:A:VAL:H    | 8        | 0.19          |
| (3,54)   | 1:71:A:LEU:HB3  | 1:75:A:LEU:HD13 | 10       | 0.19          |
| (3,54)   | 1:71:A:LEU:HB3  | 1:75:A:LEU:HD13 | 12       | 0.19          |
| (3,29)   | 1:48:A:LEU:HD22 | 1:39:A:PHE:HD1  | 7        | 0.19          |
| (3,22)   | 1:48:A:LEU:HD11 | 1:97:A:LEU:H    | 12       | 0.19          |
| (1,4345) | 1:117:A:LEU:HA  | 1:121:A:LYS:H   | 8        | 0.19          |
| (1,4344) | 1:120:A:ALA:H   | 1:119:A:GLU:HG2 | 6        | 0.19          |
| (1,4323) | 1:62:A:GLY:H    | 1:68:A:LYS:HD2  | 16       | 0.19          |
| (1,4317) | 1:93:A:THR:HB   | 1:102:A:CYS:H   | 17       | 0.19          |
| (1,4301) | 1:97:A:LEU:HB2  | 1:97:A:LEU:H    | 17       | 0.19          |
| (1,4299) | 1:65:A:ASN:HD22 | 1:65:A:ASN:HD21 | 7        | 0.19          |
| (1,4225) | 1:122:A:ALA:HB3 | 1:123:A:ARG:H   | 2        | 0.19          |
| (1,4225) | 1:122:A:ALA:HB1 | 1:123:A:ARG:H   | 8        | 0.19          |
| (1,4225) | 1:122:A:ALA:HB2 | 1:123:A:ARG:H   | 11       | 0.19          |
| (1,4225) | 1:122:A:ALA:HB3 | 1:123:A:ARG:H   | 15       | 0.19          |
| (1,4225) | 1:122:A:ALA:HB3 | 1:123:A:ARG:H   | 17       | 0.19          |
| (1,4202) | 1:127:A:GLN:H   | 1:127:A:GLN:HB3 | 4        | 0.19          |
| (1,4202) | 1:127:A:GLN:H   | 1:127:A:GLN:HB3 | 5        | 0.19          |
| (1,4202) | 1:127:A:GLN:H   | 1:127:A:GLN:HB3 | 12       | 0.19          |
| (1,4180) | 1:95:A:VAL:H    | 1:48:A:LEU:HD11 | 6        | 0.19          |
| (1,4180) | 1:95:A:VAL:H    | 1:48:A:LEU:HD11 | 9        | 0.19          |
| (1,4165) | 1:40:A:SER:HA   | 1:43:A:GLY:H    | 17       | 0.19          |
| (1,4154) | 1:17:A:ASN:HA   | 1:18:A:GLN:H    | 12       | 0.19          |
| (1,4153) | 1:18:A:GLN:HB3  | 1:18:A:GLN:H    | 14       | 0.19          |
| (1,4150) | 1:17:A:ASN:HB3  | 1:18:A:GLN:H    | 5        | 0.19          |
| (1,4150) | 1:17:A:ASN:HB3  | 1:18:A:GLN:H    | 16       | 0.19          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,4133) | 1:82:A:TRP:HE1  | 1:82:A:TRP:HD1  | 5        | 0.19          |
| (1,4133) | 1:82:A:TRP:HE1  | 1:82:A:TRP:HD1  | 17       | 0.19          |
| (1,4113) | 1:22:A:ASN:H    | 1:22:A:ASN:HD22 | 16       | 0.19          |
| (1,4069) | 1:13:A:ASP:HB2  | 1:13:A:ASP:H    | 5        | 0.19          |
| (1,4068) | 1:13:A:ASP:HB3  | 1:13:A:ASP:H    | 17       | 0.19          |
| (1,4036) | 1:31:A:LEU:H    | 1:31:A:LEU:HD11 | 9        | 0.19          |
| (1,4019) | 1:33:A:GLU:HB3  | 1:34:A:ARG:H    | 3        | 0.19          |
| (1,4019) | 1:33:A:GLU:HB3  | 1:34:A:ARG:H    | 16       | 0.19          |
| (1,4019) | 1:33:A:GLU:HB3  | 1:34:A:ARG:H    | 17       | 0.19          |
| (1,4017) | 1:32:A:ALA:HB2  | 1:35:A:PHE:H    | 5        | 0.19          |
| (1,4017) | 1:32:A:ALA:HB2  | 1:35:A:PHE:H    | 16       | 0.19          |
| (1,4016) | 1:15:A:MET:HA   | 1:15:A:MET:H    | 13       | 0.19          |
| (1,3987) | 1:50:A:ILE:HG22 | 1:50:A:ILE:H    | 1        | 0.19          |
| (1,3987) | 1:50:A:ILE:HG22 | 1:50:A:ILE:H    | 5        | 0.19          |
| (1,3987) | 1:50:A:ILE:HG23 | 1:50:A:ILE:H    | 13       | 0.19          |
| (1,3961) | 1:57:A:VAL:H    | 1:56:A:LEU:HB3  | 13       | 0.19          |
| (1,3941) | 1:63:A:GLU:H    | 1:61:A:ALA:HB3  | 6        | 0.19          |
| (1,3941) | 1:63:A:GLU:H    | 1:61:A:ALA:HB2  | 13       | 0.19          |
| (1,3901) | 1:79:A:THR:H    | 1:77:A:LEU:HB2  | 5        | 0.19          |
| (1,3901) | 1:79:A:THR:H    | 1:77:A:LEU:HB2  | 6        | 0.19          |
| (1,3901) | 1:79:A:THR:H    | 1:77:A:LEU:HB2  | 7        | 0.19          |
| (1,3901) | 1:79:A:THR:H    | 1:77:A:LEU:HB2  | 9        | 0.19          |
| (1,3901) | 1:79:A:THR:H    | 1:77:A:LEU:HB2  | 12       | 0.19          |
| (1,3901) | 1:79:A:THR:H    | 1:77:A:LEU:HB2  | 13       | 0.19          |
| (1,3901) | 1:79:A:THR:H    | 1:77:A:LEU:HB2  | 15       | 0.19          |
| (1,3901) | 1:79:A:THR:H    | 1:77:A:LEU:HB2  | 16       | 0.19          |
| (1,3901) | 1:79:A:THR:H    | 1:77:A:LEU:HB2  | 17       | 0.19          |
| (1,3898) | 1:79:A:THR:HG21 | 1:80:A:SER:H    | 6        | 0.19          |
| (1,3898) | 1:79:A:THR:HG22 | 1:80:A:SER:H    | 12       | 0.19          |
| (1,3879) | 1:127:A:GLN:H   | 1:127:A:GLN:HG2 | 13       | 0.19          |
| (1,3845) | 1:95:A:VAL:HG12 | 1:96:A:ASP:H    | 15       | 0.19          |
| (1,3797) | 1:44:A:GLU:HA   | 1:44:A:GLU:H    | 14       | 0.19          |
| (1,3797) | 1:44:A:GLU:HA   | 1:44:A:GLU:H    | 17       | 0.19          |
| (1,3781) | 1:119:A:GLU:HA  | 1:119:A:GLU:H   | 5        | 0.19          |
| (1,3781) | 1:119:A:GLU:HA  | 1:119:A:GLU:H   | 10       | 0.19          |
| (1,3781) | 1:119:A:GLU:HA  | 1:119:A:GLU:H   | 14       | 0.19          |
| (1,3781) | 1:119:A:GLU:HA  | 1:119:A:GLU:H   | 16       | 0.19          |
| (1,3749) | 1:123:A:ARG:H   | 1:121:A:LYS:H   | 3        | 0.19          |
| (1,3749) | 1:123:A:ARG:H   | 1:121:A:LYS:H   | 6        | 0.19          |
| (1,3749) | 1:123:A:ARG:H   | 1:121:A:LYS:H   | 12       | 0.19          |
| (1,3749) | 1:123:A:ARG:H   | 1:121:A:LYS:H   | 13       | 0.19          |
| (1,3749) | 1:123:A:ARG:H   | 1:121:A:LYS:H   | 14       | 0.19          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3749) | 1:123:A:ARG:H   | 1:121:A:LYS:H   | 17       | 0.19          |
| (1,3744) | 1:35:A:PHE:HD2  | 1:39:A:PHE:H    | 17       | 0.19          |
| (1,3717) | 1:35:A:PHE:H    | 1:39:A:PHE:HE2  | 7        | 0.19          |
| (1,3717) | 1:35:A:PHE:H    | 1:39:A:PHE:HE1  | 10       | 0.19          |
| (1,3717) | 1:35:A:PHE:H    | 1:39:A:PHE:HE1  | 12       | 0.19          |
| (1,3717) | 1:35:A:PHE:H    | 1:39:A:PHE:HE1  | 15       | 0.19          |
| (1,3717) | 1:35:A:PHE:H    | 1:39:A:PHE:HE2  | 17       | 0.19          |
| (1,3698) | 1:30:A:PHE:HD2  | 1:30:A:PHE:H    | 3        | 0.19          |
| (1,3698) | 1:30:A:PHE:HD1  | 1:30:A:PHE:H    | 17       | 0.19          |
| (1,3662) | 1:83:A:ARG:H    | 1:82:A:TRP:HD1  | 3        | 0.19          |
| (1,3595) | 1:108:A:GLN:HA  | 1:111:A:GLU:HB3 | 2        | 0.19          |
| (1,3595) | 1:108:A:GLN:HA  | 1:111:A:GLU:HB3 | 4        | 0.19          |
| (1,3595) | 1:108:A:GLN:HA  | 1:111:A:GLU:HB3 | 6        | 0.19          |
| (1,3595) | 1:108:A:GLN:HA  | 1:111:A:GLU:HB3 | 9        | 0.19          |
| (1,3595) | 1:108:A:GLN:HA  | 1:111:A:GLU:HB3 | 12       | 0.19          |
| (1,3595) | 1:108:A:GLN:HA  | 1:111:A:GLU:HB3 | 13       | 0.19          |
| (1,3595) | 1:108:A:GLN:HA  | 1:111:A:GLU:HB3 | 14       | 0.19          |
| (1,3595) | 1:108:A:GLN:HA  | 1:111:A:GLU:HB3 | 16       | 0.19          |
| (1,3591) | 1:93:A:THR:HB   | 1:88:A:VAL:HG12 | 10       | 0.19          |
| (1,3591) | 1:93:A:THR:HB   | 1:88:A:VAL:HG12 | 13       | 0.19          |
| (1,3591) | 1:93:A:THR:HB   | 1:88:A:VAL:HG13 | 15       | 0.19          |
| (1,3539) | 1:63:A:GLU:HG3  | 1:63:A:GLU:H    | 1        | 0.19          |
| (1,3536) | 1:66:A:LEU:HB3  | 1:62:A:GLY:HA3  | 16       | 0.19          |
| (1,3535) | 1:74:A:ALA:HB3  | 1:28:A:ILE:HA   | 11       | 0.19          |
| (1,3516) | 1:21:A:LEU:HG   | 1:65:A:ASN:HB3  | 3        | 0.19          |
| (1,3508) | 1:113:A:ALA:HB1 | 1:88:A:VAL:HA   | 12       | 0.19          |
| (1,3508) | 1:113:A:ALA:HB3 | 1:88:A:VAL:HA   | 16       | 0.19          |
| (1,3506) | 1:60:A:VAL:HG13 | 1:35:A:PHE:HZ   | 2        | 0.19          |
| (1,3506) | 1:60:A:VAL:HG12 | 1:35:A:PHE:HZ   | 7        | 0.19          |
| (1,3506) | 1:60:A:VAL:HG11 | 1:35:A:PHE:HZ   | 13       | 0.19          |
| (1,3506) | 1:60:A:VAL:HG13 | 1:35:A:PHE:HZ   | 16       | 0.19          |
| (1,3501) | 1:27:A:VAL:HG23 | 1:28:A:ILE:HA   | 17       | 0.19          |
| (1,3494) | 1:56:A:LEU:HD23 | 1:55:A:ASP:HB3  | 10       | 0.19          |
| (1,3476) | 1:107:A:GLU:HG2 | 1:108:A:GLN:H   | 13       | 0.19          |
| (1,3465) | 1:88:A:VAL:HG23 | 1:85:A:LEU:HB3  | 4        | 0.19          |
| (1,3446) | 1:65:A:ASN:HD22 | 1:20:A:LYS:HG2  | 9        | 0.19          |
| (1,3441) | 1:21:A:LEU:HG   | 1:21:A:LEU:HB3  | 3        | 0.19          |
| (1,3441) | 1:21:A:LEU:HG   | 1:21:A:LEU:HB3  | 15       | 0.19          |
| (1,3441) | 1:21:A:LEU:HG   | 1:21:A:LEU:HB3  | 16       | 0.19          |
| (1,3430) | 1:45:A:ALA:HB3  | 1:84:A:TYR:HA   | 5        | 0.19          |
| (1,3430) | 1:45:A:ALA:HB3  | 1:84:A:TYR:HA   | 11       | 0.19          |
| (1,3422) | 1:77:A:LEU:HG   | 1:77:A:LEU:HD21 | 15       | 0.19          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3422) | 1:77:A:LEU:HG   | 1:77:A:LEU:HD21  | 16       | 0.19          |
| (1,3422) | 1:77:A:LEU:HG   | 1:77:A:LEU:HD21  | 17       | 0.19          |
| (1,3417) | 1:117:A:LEU:HG  | 1:117:A:LEU:HD12 | 8        | 0.19          |
| (1,3417) | 1:117:A:LEU:HG  | 1:117:A:LEU:HD12 | 13       | 0.19          |
| (1,3412) | 1:82:A:TRP:HZ3  | 1:117:A:LEU:HD13 | 10       | 0.19          |
| (1,3401) | 1:86:A:TYR:HE1  | 1:86:A:TYR:HA    | 4        | 0.19          |
| (1,3401) | 1:86:A:TYR:HE1  | 1:86:A:TYR:HA    | 8        | 0.19          |
| (1,3401) | 1:86:A:TYR:HE1  | 1:86:A:TYR:HA    | 14       | 0.19          |
| (1,3396) | 1:71:A:LEU:HA   | 1:74:A:ALA:HB3   | 14       | 0.19          |
| (1,3395) | 1:33:A:GLU:HB3  | 1:33:A:GLU:HA    | 7        | 0.19          |
| (1,3378) | 1:67:A:SER:HB3  | 1:66:A:LEU:HA    | 14       | 0.19          |
| (1,3378) | 1:67:A:SER:HB3  | 1:66:A:LEU:HA    | 17       | 0.19          |
| (1,3370) | 1:24:A:SER:HA   | 1:27:A:VAL:HG12  | 17       | 0.19          |
| (1,3369) | 1:24:A:SER:HA   | 1:27:A:VAL:HG23  | 1        | 0.19          |
| (1,3369) | 1:24:A:SER:HA   | 1:27:A:VAL:HG23  | 4        | 0.19          |
| (1,3369) | 1:24:A:SER:HA   | 1:27:A:VAL:HG23  | 8        | 0.19          |
| (1,3369) | 1:24:A:SER:HA   | 1:27:A:VAL:HG22  | 12       | 0.19          |
| (1,3369) | 1:24:A:SER:HA   | 1:27:A:VAL:HG23  | 14       | 0.19          |
| (1,3369) | 1:24:A:SER:HA   | 1:27:A:VAL:HG21  | 15       | 0.19          |
| (1,3336) | 1:71:A:LEU:HD23 | 1:74:A:ALA:H     | 1        | 0.19          |
| (1,3336) | 1:71:A:LEU:HD23 | 1:74:A:ALA:H     | 13       | 0.19          |
| (1,3325) | 1:77:A:LEU:HB3  | 1:77:A:LEU:HD13  | 4        | 0.19          |
| (1,3325) | 1:77:A:LEU:HB3  | 1:77:A:LEU:HD13  | 5        | 0.19          |
| (1,3325) | 1:77:A:LEU:HB3  | 1:77:A:LEU:HD13  | 15       | 0.19          |
| (1,3322) | 1:30:A:PHE:HD1  | 1:66:A:LEU:HD21  | 1        | 0.19          |
| (1,3322) | 1:30:A:PHE:HD2  | 1:66:A:LEU:HD23  | 2        | 0.19          |
| (1,3322) | 1:30:A:PHE:HD2  | 1:66:A:LEU:HD21  | 4        | 0.19          |
| (1,3322) | 1:30:A:PHE:HD2  | 1:66:A:LEU:HD21  | 6        | 0.19          |
| (1,3322) | 1:30:A:PHE:HD2  | 1:66:A:LEU:HD22  | 8        | 0.19          |
| (1,3322) | 1:30:A:PHE:HD1  | 1:66:A:LEU:HD23  | 16       | 0.19          |
| (1,3320) | 1:27:A:VAL:HA   | 1:66:A:LEU:HD21  | 1        | 0.19          |
| (1,3320) | 1:27:A:VAL:HA   | 1:66:A:LEU:HD23  | 3        | 0.19          |
| (1,3320) | 1:27:A:VAL:HA   | 1:66:A:LEU:HD21  | 6        | 0.19          |
| (1,3320) | 1:27:A:VAL:HA   | 1:66:A:LEU:HD21  | 10       | 0.19          |
| (1,3311) | 1:68:A:LYS:HD3  | 1:57:A:VAL:HG11  | 8        | 0.19          |
| (1,3311) | 1:68:A:LYS:HD3  | 1:57:A:VAL:HG11  | 10       | 0.19          |
| (1,3311) | 1:68:A:LYS:HD3  | 1:57:A:VAL:HG11  | 12       | 0.19          |
| (1,3306) | 1:128:A:ARG:HG2 | 1:128:A:ARG:HD2  | 7        | 0.19          |
| (1,3299) | 1:20:A:LYS:H    | 1:20:A:LYS:HD3   | 3        | 0.19          |
| (1,3264) | 1:121:A:LYS:HG2 | 1:121:A:LYS:H    | 11       | 0.19          |
| (1,3260) | 1:121:A:LYS:HG2 | 1:121:A:LYS:HB2  | 4        | 0.19          |
| (1,3260) | 1:121:A:LYS:HG2 | 1:121:A:LYS:HB2  | 10       | 0.19          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3260) | 1:121:A:LYS:HG2  | 1:121:A:LYS:HB2 | 13       | 0.19          |
| (1,3258) | 1:48:A:LEU:HD13  | 1:50:A:ILE:HA   | 11       | 0.19          |
| (1,3257) | 1:48:A:LEU:HD12  | 1:38:A:CYS:HA   | 1        | 0.19          |
| (1,3257) | 1:48:A:LEU:HD13  | 1:38:A:CYS:HA   | 9        | 0.19          |
| (1,3250) | 1:41:A:ALA:HA    | 1:41:A:ALA:HB3  | 3        | 0.19          |
| (1,3250) | 1:41:A:ALA:HA    | 1:41:A:ALA:HB2  | 8        | 0.19          |
| (1,3250) | 1:41:A:ALA:HA    | 1:41:A:ALA:HB3  | 12       | 0.19          |
| (1,3241) | 1:52:A:ILE:HG13  | 1:97:A:LEU:HD23 | 6        | 0.19          |
| (1,3241) | 1:52:A:ILE:HG13  | 1:97:A:LEU:HD23 | 10       | 0.19          |
| (1,3241) | 1:52:A:ILE:HG13  | 1:97:A:LEU:HD21 | 11       | 0.19          |
| (1,3232) | 1:92:A:ALA:H     | 1:105:A:LEU:HB2 | 5        | 0.19          |
| (1,3232) | 1:92:A:ALA:H     | 1:105:A:LEU:HB2 | 9        | 0.19          |
| (1,3230) | 1:68:A:LYS:HB2   | 1:68:A:LYS:HA   | 4        | 0.19          |
| (1,3230) | 1:68:A:LYS:HB2   | 1:68:A:LYS:HA   | 6        | 0.19          |
| (1,3230) | 1:68:A:LYS:HB2   | 1:68:A:LYS:HA   | 9        | 0.19          |
| (1,3200) | 1:116:A:GLN:HG3  | 1:113:A:ALA:HB3 | 5        | 0.19          |
| (1,3183) | 1:124:A:VAL:HG23 | 1:121:A:LYS:HA  | 17       | 0.19          |
| (1,3181) | 1:108:A:GLN:HG3  | 1:108:A:GLN:HA  | 10       | 0.19          |
| (1,3180) | 1:111:A:GLU:HG2  | 1:111:A:GLU:HA  | 5        | 0.19          |
| (1,3179) | 1:111:A:GLU:HA   | 1:111:A:GLU:H   | 7        | 0.19          |
| (1,3179) | 1:111:A:GLU:HA   | 1:111:A:GLU:H   | 10       | 0.19          |
| (1,3165) | 1:126:A:ALA:HB1  | 1:125:A:GLN:HG3 | 2        | 0.19          |
| (1,3165) | 1:126:A:ALA:HB3  | 1:125:A:GLN:HG3 | 3        | 0.19          |
| (1,3165) | 1:126:A:ALA:HB2  | 1:125:A:GLN:HG3 | 6        | 0.19          |
| (1,3165) | 1:126:A:ALA:HB3  | 1:125:A:GLN:HG3 | 16       | 0.19          |
| (1,3160) | 1:74:A:ALA:HB3   | 1:74:A:ALA:HA   | 4        | 0.19          |
| (1,3160) | 1:74:A:ALA:HB3   | 1:74:A:ALA:HA   | 16       | 0.19          |
| (1,3136) | 1:68:A:LYS:HB2   | 1:57:A:VAL:HG12 | 17       | 0.19          |
| (1,3068) | 1:52:A:ILE:HG23  | 1:53:A:PHE:HB2  | 1        | 0.19          |
| (1,3068) | 1:52:A:ILE:HG21  | 1:53:A:PHE:HB2  | 3        | 0.19          |
| (1,3068) | 1:52:A:ILE:HG22  | 1:53:A:PHE:HB2  | 5        | 0.19          |
| (1,3068) | 1:52:A:ILE:HG22  | 1:53:A:PHE:HB2  | 10       | 0.19          |
| (1,3066) | 1:30:A:PHE:HB3   | 1:29:A:ALA:HB1  | 1        | 0.19          |
| (1,3053) | 1:29:A:ALA:H     | 1:28:A:ILE:HG22 | 1        | 0.19          |
| (1,3053) | 1:29:A:ALA:H     | 1:28:A:ILE:HG23 | 13       | 0.19          |
| (1,3053) | 1:29:A:ALA:H     | 1:28:A:ILE:HG23 | 15       | 0.19          |
| (1,2992) | 1:20:A:LYS:HB3   | 1:20:A:LYS:H    | 4        | 0.19          |
| (1,2992) | 1:20:A:LYS:HB3   | 1:20:A:LYS:H    | 6        | 0.19          |
| (1,2969) | 1:93:A:THR:HG21  | 1:101:A:PRO:HB3 | 14       | 0.19          |
| (1,2960) | 1:77:A:LEU:HD13  | 1:25:A:LYS:HA   | 4        | 0.19          |
| (1,2960) | 1:77:A:LEU:HD11  | 1:25:A:LYS:HA   | 16       | 0.19          |
| (1,2950) | 1:75:A:LEU:HD12  | 1:75:A:LEU:H    | 15       | 0.19          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2932) | 1:95:A:VAL:HG22  | 1:95:A:VAL:H    | 11       | 0.19          |
| (1,2930) | 1:31:A:LEU:HD21  | 1:60:A:VAL:HG12 | 17       | 0.19          |
| (1,2927) | 1:31:A:LEU:HD23  | 1:39:A:PHE:HD2  | 3        | 0.19          |
| (1,2927) | 1:31:A:LEU:HD23  | 1:39:A:PHE:HD1  | 8        | 0.19          |
| (1,2927) | 1:31:A:LEU:HD23  | 1:39:A:PHE:HD2  | 11       | 0.19          |
| (1,2927) | 1:31:A:LEU:HD22  | 1:39:A:PHE:HD1  | 13       | 0.19          |
| (1,2927) | 1:31:A:LEU:HD23  | 1:39:A:PHE:HD1  | 15       | 0.19          |
| (1,2899) | 1:28:A:ILE:HD11  | 1:75:A:LEU:H    | 12       | 0.19          |
| (1,2891) | 1:32:A:ALA:HB1   | 1:28:A:ILE:HG23 | 5        | 0.19          |
| (1,2891) | 1:32:A:ALA:HB2   | 1:28:A:ILE:HG23 | 16       | 0.19          |
| (1,2888) | 1:29:A:ALA:HA    | 1:32:A:ALA:HB3  | 3        | 0.19          |
| (1,2888) | 1:29:A:ALA:HA    | 1:32:A:ALA:HB1  | 8        | 0.19          |
| (1,2888) | 1:29:A:ALA:HA    | 1:32:A:ALA:HB2  | 10       | 0.19          |
| (1,2877) | 1:61:A:ALA:HB3   | 1:61:A:ALA:HA   | 5        | 0.19          |
| (1,2851) | 1:50:A:ILE:HG22  | 1:50:A:ILE:HA   | 8        | 0.19          |
| (1,2840) | 1:124:A:VAL:HG11 | 1:125:A:GLN:H   | 11       | 0.19          |
| (1,2754) | 1:60:A:VAL:HG12  | 1:59:A:ARG:HD3  | 10       | 0.19          |
| (1,2754) | 1:60:A:VAL:HG13  | 1:59:A:ARG:HD3  | 14       | 0.19          |
| (1,2729) | 1:17:A:ASN:HB3   | 1:17:A:ASN:HB2  | 10       | 0.19          |
| (1,2729) | 1:17:A:ASN:HB3   | 1:17:A:ASN:HB2  | 12       | 0.19          |
| (1,2727) | 1:86:A:TYR:HB3   | 1:86:A:TYR:H    | 1        | 0.19          |
| (1,2727) | 1:86:A:TYR:HB3   | 1:86:A:TYR:H    | 2        | 0.19          |
| (1,2727) | 1:86:A:TYR:HB3   | 1:86:A:TYR:H    | 7        | 0.19          |
| (1,2719) | 1:117:A:LEU:HD11 | 1:86:A:TYR:HB2  | 8        | 0.19          |
| (1,2711) | 1:35:A:PHE:HB2   | 1:35:A:PHE:HE1  | 2        | 0.19          |
| (1,2711) | 1:35:A:PHE:HB2   | 1:35:A:PHE:HE2  | 5        | 0.19          |
| (1,2711) | 1:35:A:PHE:HB2   | 1:35:A:PHE:HE2  | 7        | 0.19          |
| (1,2711) | 1:35:A:PHE:HB2   | 1:35:A:PHE:HE2  | 9        | 0.19          |
| (1,2711) | 1:35:A:PHE:HB2   | 1:35:A:PHE:HE2  | 14       | 0.19          |
| (1,2711) | 1:35:A:PHE:HB2   | 1:35:A:PHE:HE2  | 15       | 0.19          |
| (1,2639) | 1:71:A:LEU:HD13  | 1:71:A:LEU:HB2  | 8        | 0.19          |
| (1,2639) | 1:71:A:LEU:HD11  | 1:71:A:LEU:HB2  | 11       | 0.19          |
| (1,2629) | 1:53:A:PHE:HZ    | 1:71:A:LEU:HB2  | 13       | 0.19          |
| (1,2622) | 1:71:A:LEU:HD11  | 1:57:A:VAL:H    | 3        | 0.19          |
| (1,2622) | 1:71:A:LEU:HD13  | 1:57:A:VAL:H    | 13       | 0.19          |
| (1,2621) | 1:105:A:LEU:HD11 | 1:92:A:ALA:H    | 7        | 0.19          |
| (1,2596) | 1:74:A:ALA:HB1   | 1:27:A:VAL:HG13 | 8        | 0.19          |
| (1,2596) | 1:74:A:ALA:HB3   | 1:27:A:VAL:HG13 | 12       | 0.19          |
| (1,2559) | 1:86:A:TYR:HE1   | 1:86:A:TYR:HB2  | 6        | 0.19          |
| (1,2559) | 1:86:A:TYR:HE1   | 1:86:A:TYR:HB2  | 10       | 0.19          |
| (1,2547) | 1:11:A:SER:HA    | 1:12:A:GLN:HG3  | 5        | 0.19          |
| (1,2547) | 1:11:A:SER:HA    | 1:12:A:GLN:HG3  | 7        | 0.19          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2547) | 1:11:A:SER:HA    | 1:12:A:GLN:HG3  | 11       | 0.19          |
| (1,2547) | 1:11:A:SER:HA    | 1:12:A:GLN:HG3  | 16       | 0.19          |
| (1,2530) | 1:33:A:GLU:HA    | 1:34:A:ARG:H    | 7        | 0.19          |
| (1,2529) | 1:79:A:THR:HG22  | 1:75:A:LEU:HA   | 15       | 0.19          |
| (1,2514) | 1:120:A:ALA:H    | 1:120:A:ALA:HA  | 6        | 0.19          |
| (1,2489) | 1:28:A:ILE:HA    | 1:28:A:ILE:HG23 | 12       | 0.19          |
| (1,2480) | 1:71:A:LEU:HB2   | 1:27:A:VAL:HG12 | 12       | 0.19          |
| (1,2476) | 1:50:A:ILE:HD12  | 1:50:A:ILE:HB   | 4        | 0.19          |
| (1,2444) | 1:53:A:PHE:HE1   | 1:53:A:PHE:HB2  | 16       | 0.19          |
| (1,2411) | 1:45:A:ALA:HB1   | 1:84:A:TYR:HB3  | 16       | 0.19          |
| (1,2408) | 1:52:A:ILE:HD11  | 1:96:A:ASP:HA   | 1        | 0.19          |
| (1,2346) | 1:105:A:LEU:HD13 | 1:107:A:GLU:HA  | 12       | 0.19          |
| (1,2341) | 1:66:A:LEU:HD23  | 1:70:A:GLN:H    | 1        | 0.19          |
| (1,2336) | 1:64:A:MET:HE2   | 1:31:A:LEU:HA   | 3        | 0.19          |
| (1,2336) | 1:64:A:MET:HE1   | 1:31:A:LEU:HA   | 8        | 0.19          |
| (1,2336) | 1:64:A:MET:HE2   | 1:31:A:LEU:HA   | 15       | 0.19          |
| (1,2336) | 1:64:A:MET:HE3   | 1:31:A:LEU:HA   | 17       | 0.19          |
| (1,2307) | 1:117:A:LEU:HD13 | 1:86:A:TYR:HB2  | 12       | 0.19          |
| (1,2307) | 1:117:A:LEU:HD11 | 1:86:A:TYR:HB2  | 15       | 0.19          |
| (1,2299) | 1:55:A:ASP:HB3   | 1:96:A:ASP:HA   | 7        | 0.19          |
| (1,2288) | 1:70:A:GLN:HA    | 1:70:A:GLN:HG3  | 3        | 0.19          |
| (1,2288) | 1:70:A:GLN:HA    | 1:70:A:GLN:HG3  | 4        | 0.19          |
| (1,2288) | 1:70:A:GLN:HA    | 1:70:A:GLN:HG3  | 5        | 0.19          |
| (1,2288) | 1:70:A:GLN:HA    | 1:70:A:GLN:HG3  | 13       | 0.19          |
| (1,2288) | 1:70:A:GLN:HA    | 1:70:A:GLN:HG3  | 17       | 0.19          |
| (1,2268) | 1:110:A:VAL:HG13 | 1:89:A:LYS:H    | 16       | 0.19          |
| (1,2221) | 1:31:A:LEU:HA    | 1:60:A:VAL:HB   | 2        | 0.19          |
| (1,2221) | 1:31:A:LEU:HA    | 1:60:A:VAL:HB   | 4        | 0.19          |
| (1,2194) | 1:50:A:ILE:HD12  | 1:80:A:SER:H    | 2        | 0.19          |
| (1,2169) | 1:22:A:ASN:HB3   | 1:22:A:ASN:H    | 1        | 0.19          |
| (1,2169) | 1:22:A:ASN:HB3   | 1:22:A:ASN:H    | 2        | 0.19          |
| (1,2169) | 1:22:A:ASN:HB3   | 1:22:A:ASN:H    | 9        | 0.19          |
| (1,2164) | 1:120:A:ALA:HA   | 1:121:A:LYS:H   | 1        | 0.19          |
| (1,2164) | 1:120:A:ALA:HA   | 1:121:A:LYS:H   | 2        | 0.19          |
| (1,2164) | 1:120:A:ALA:HA   | 1:121:A:LYS:H   | 4        | 0.19          |
| (1,2164) | 1:120:A:ALA:HA   | 1:121:A:LYS:H   | 6        | 0.19          |
| (1,2164) | 1:120:A:ALA:HA   | 1:121:A:LYS:H   | 14       | 0.19          |
| (1,2116) | 1:45:A:ALA:HB3   | 1:84:A:TYR:HA   | 13       | 0.19          |
| (1,2116) | 1:45:A:ALA:HB3   | 1:84:A:TYR:HA   | 16       | 0.19          |
| (1,2045) | 1:77:A:LEU:H     | 1:78:A:TYR:H    | 8        | 0.19          |
| (1,2037) | 1:57:A:VAL:HG21  | 1:57:A:VAL:HG12 | 5        | 0.19          |
| (1,2037) | 1:57:A:VAL:HG22  | 1:57:A:VAL:HG11 | 6        | 0.19          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2037) | 1:57:A:VAL:HG23  | 1:57:A:VAL:HG12  | 10       | 0.19          |
| (1,2037) | 1:57:A:VAL:HG21  | 1:57:A:VAL:HG11  | 15       | 0.19          |
| (1,2037) | 1:57:A:VAL:HG22  | 1:57:A:VAL:HG11  | 16       | 0.19          |
| (1,2035) | 1:52:A:ILE:HG13  | 1:97:A:LEU:HD23  | 5        | 0.19          |
| (1,2035) | 1:52:A:ILE:HG13  | 1:97:A:LEU:HD23  | 14       | 0.19          |
| (1,2025) | 1:97:A:LEU:HD22  | 1:35:A:PHE:HD2   | 7        | 0.19          |
| (1,2005) | 1:95:A:VAL:HG22  | 1:48:A:LEU:HD12  | 5        | 0.19          |
| (1,2005) | 1:95:A:VAL:HG21  | 1:48:A:LEU:HD11  | 12       | 0.19          |
| (1,1951) | 1:108:A:GLN:HA   | 1:111:A:GLU:HB3  | 15       | 0.19          |
| (1,1890) | 1:100:A:ASN:HD22 | 1:98:A:ASP:HB3   | 2        | 0.19          |
| (1,1890) | 1:100:A:ASN:HD22 | 1:98:A:ASP:HB3   | 14       | 0.19          |
| (1,1890) | 1:100:A:ASN:HD22 | 1:98:A:ASP:HB3   | 17       | 0.19          |
| (1,1883) | 1:64:A:MET:HE3   | 1:21:A:LEU:H     | 15       | 0.19          |
| (1,1877) | 1:27:A:VAL:HG23  | 1:27:A:VAL:H     | 1        | 0.19          |
| (1,1877) | 1:27:A:VAL:HG21  | 1:27:A:VAL:H     | 3        | 0.19          |
| (1,1877) | 1:27:A:VAL:HG23  | 1:27:A:VAL:H     | 8        | 0.19          |
| (1,1877) | 1:27:A:VAL:HG21  | 1:27:A:VAL:H     | 10       | 0.19          |
| (1,1876) | 1:27:A:VAL:HG23  | 1:31:A:LEU:HD11  | 6        | 0.19          |
| (1,1876) | 1:27:A:VAL:HG22  | 1:31:A:LEU:HD11  | 13       | 0.19          |
| (1,1845) | 1:95:A:VAL:HG22  | 1:96:A:ASP:HA    | 10       | 0.19          |
| (1,1845) | 1:95:A:VAL:HG23  | 1:96:A:ASP:HA    | 12       | 0.19          |
| (1,1826) | 1:64:A:MET:HE3   | 1:21:A:LEU:HD11  | 9        | 0.19          |
| (1,1824) | 1:27:A:VAL:HA    | 1:21:A:LEU:HD11  | 4        | 0.19          |
| (1,1817) | 1:77:A:LEU:HG    | 1:77:A:LEU:HD22  | 13       | 0.19          |
| (1,1811) | 1:86:A:TYR:H     | 1:117:A:LEU:HD11 | 6        | 0.19          |
| (1,1811) | 1:86:A:TYR:H     | 1:117:A:LEU:HD11 | 10       | 0.19          |
| (1,1801) | 1:117:A:LEU:HA   | 1:120:A:ALA:HB1  | 15       | 0.19          |
| (1,1799) | 1:71:A:LEU:HA    | 1:74:A:ALA:HB3   | 5        | 0.19          |
| (1,1799) | 1:71:A:LEU:HA    | 1:74:A:ALA:HB2   | 12       | 0.19          |
| (1,1799) | 1:71:A:LEU:HA    | 1:74:A:ALA:HB2   | 15       | 0.19          |
| (1,1773) | 1:24:A:SER:HA    | 1:27:A:VAL:HG23  | 11       | 0.19          |
| (1,1773) | 1:24:A:SER:HA    | 1:27:A:VAL:HG23  | 16       | 0.19          |
| (1,1756) | 1:79:A:THR:HG23  | 1:84:A:TYR:HE1   | 12       | 0.19          |
| (1,1733) | 1:30:A:PHE:HD2   | 1:66:A:LEU:HD23  | 5        | 0.19          |
| (1,1733) | 1:30:A:PHE:HD2   | 1:66:A:LEU:HD21  | 11       | 0.19          |
| (1,1726) | 1:66:A:LEU:HD11  | 1:66:A:LEU:HA    | 7        | 0.19          |
| (1,1725) | 1:71:A:LEU:HD13  | 1:71:A:LEU:HG    | 10       | 0.19          |
| (1,1725) | 1:71:A:LEU:HD11  | 1:71:A:LEU:HG    | 17       | 0.19          |
| (1,1720) | 1:117:A:LEU:HG   | 1:117:A:LEU:HD11 | 15       | 0.19          |
| (1,1718) | 1:18:A:GLN:HB3   | 1:19:A:PRO:HD2   | 12       | 0.19          |
| (1,1713) | 1:20:A:LYS:H     | 1:20:A:LYS:HD3   | 6        | 0.19          |
| (1,1713) | 1:20:A:LYS:H     | 1:20:A:LYS:HD3   | 14       | 0.19          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1713) | 1:20:A:LYS:H     | 1:20:A:LYS:HD3  | 15       | 0.19          |
| (1,1690) | 1:42:A:GLU:HG2   | 1:41:A:ALA:HB1  | 17       | 0.19          |
| (1,1683) | 1:48:A:LEU:HD11  | 1:38:A:CYS:HA   | 3        | 0.19          |
| (1,1681) | 1:40:A:SER:HA    | 1:41:A:ALA:HB1  | 6        | 0.19          |
| (1,1671) | 1:78:A:TYR:HA    | 1:28:A:ILE:HG12 | 1        | 0.19          |
| (1,1671) | 1:78:A:TYR:HA    | 1:28:A:ILE:HG12 | 6        | 0.19          |
| (1,1671) | 1:78:A:TYR:HA    | 1:28:A:ILE:HG12 | 9        | 0.19          |
| (1,1671) | 1:78:A:TYR:HA    | 1:28:A:ILE:HG12 | 12       | 0.19          |
| (1,1671) | 1:78:A:TYR:HA    | 1:28:A:ILE:HG12 | 14       | 0.19          |
| (1,1660) | 1:27:A:VAL:HA    | 1:27:A:VAL:HG12 | 7        | 0.19          |
| (1,1629) | 1:116:A:GLN:HG3  | 1:113:A:ALA:HB3 | 11       | 0.19          |
| (1,1629) | 1:116:A:GLN:HG3  | 1:113:A:ALA:HB3 | 15       | 0.19          |
| (1,1628) | 1:87:A:GLY:HA3   | 1:113:A:ALA:HB1 | 4        | 0.19          |
| (1,1628) | 1:87:A:GLY:HA3   | 1:113:A:ALA:HB2 | 12       | 0.19          |
| (1,1628) | 1:87:A:GLY:HA3   | 1:113:A:ALA:HB1 | 17       | 0.19          |
| (1,1616) | 1:109:A:HIS:HB2  | 1:108:A:GLN:H   | 13       | 0.19          |
| (1,1599) | 1:53:A:PHE:HB3   | 1:75:A:LEU:HD21 | 11       | 0.19          |
| (1,1588) | 1:74:A:ALA:HB3   | 1:74:A:ALA:HA   | 10       | 0.19          |
| (1,1556) | 1:59:A:ARG:HB2   | 1:58:A:ASP:HB2  | 3        | 0.19          |
| (1,1556) | 1:59:A:ARG:HB2   | 1:58:A:ASP:HB2  | 4        | 0.19          |
| (1,1556) | 1:59:A:ARG:HB2   | 1:58:A:ASP:HB2  | 5        | 0.19          |
| (1,1556) | 1:59:A:ARG:HB2   | 1:58:A:ASP:HB2  | 6        | 0.19          |
| (1,1556) | 1:59:A:ARG:HB2   | 1:58:A:ASP:HB2  | 7        | 0.19          |
| (1,1556) | 1:59:A:ARG:HB2   | 1:58:A:ASP:HB2  | 8        | 0.19          |
| (1,1556) | 1:59:A:ARG:HB2   | 1:58:A:ASP:HB2  | 9        | 0.19          |
| (1,1556) | 1:59:A:ARG:HB2   | 1:58:A:ASP:HB2  | 13       | 0.19          |
| (1,1556) | 1:59:A:ARG:HB2   | 1:58:A:ASP:HB2  | 17       | 0.19          |
| (1,1552) | 1:124:A:VAL:HG11 | 1:124:A:VAL:HB  | 11       | 0.19          |
| (1,1513) | 1:52:A:ILE:HG23  | 1:53:A:PHE:HB3  | 11       | 0.19          |
| (1,1511) | 1:28:A:ILE:HA    | 1:28:A:ILE:HG23 | 12       | 0.19          |
| (1,1511) | 1:28:A:ILE:HA    | 1:28:A:ILE:HG22 | 17       | 0.19          |
| (1,1508) | 1:29:A:ALA:H     | 1:28:A:ILE:HG23 | 4        | 0.19          |
| (1,1508) | 1:29:A:ALA:H     | 1:28:A:ILE:HG23 | 6        | 0.19          |
| (1,1508) | 1:29:A:ALA:H     | 1:28:A:ILE:HG21 | 7        | 0.19          |
| (1,1508) | 1:29:A:ALA:H     | 1:28:A:ILE:HG23 | 8        | 0.19          |
| (1,1480) | 1:64:A:MET:HE3   | 1:63:A:GLU:H    | 12       | 0.19          |
| (1,1480) | 1:64:A:MET:HE1   | 1:63:A:GLU:H    | 14       | 0.19          |
| (1,1456) | 1:57:A:VAL:HA    | 1:60:A:VAL:HB   | 1        | 0.19          |
| (1,1456) | 1:57:A:VAL:HA    | 1:60:A:VAL:HB   | 3        | 0.19          |
| (1,1456) | 1:57:A:VAL:HA    | 1:60:A:VAL:HB   | 5        | 0.19          |
| (1,1456) | 1:57:A:VAL:HA    | 1:60:A:VAL:HB   | 8        | 0.19          |
| (1,1456) | 1:57:A:VAL:HA    | 1:60:A:VAL:HB   | 10       | 0.19          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1456) | 1:57:A:VAL:HA    | 1:60:A:VAL:HB   | 11       | 0.19          |
| (1,1456) | 1:57:A:VAL:HA    | 1:60:A:VAL:HB   | 13       | 0.19          |
| (1,1456) | 1:57:A:VAL:HA    | 1:60:A:VAL:HB   | 15       | 0.19          |
| (1,1456) | 1:57:A:VAL:HA    | 1:60:A:VAL:HB   | 17       | 0.19          |
| (1,1428) | 1:93:A:THR:HG21  | 1:101:A:PRO:HB3 | 1        | 0.19          |
| (1,1428) | 1:93:A:THR:HG22  | 1:101:A:PRO:HB3 | 9        | 0.19          |
| (1,1419) | 1:77:A:LEU:HD12  | 1:25:A:LYS:HA   | 7        | 0.19          |
| (1,1419) | 1:77:A:LEU:HD12  | 1:25:A:LYS:HA   | 9        | 0.19          |
| (1,1419) | 1:77:A:LEU:HD12  | 1:25:A:LYS:HA   | 10       | 0.19          |
| (1,1419) | 1:77:A:LEU:HD12  | 1:25:A:LYS:HA   | 12       | 0.19          |
| (1,1419) | 1:77:A:LEU:HD11  | 1:25:A:LYS:HA   | 13       | 0.19          |
| (1,1410) | 1:110:A:VAL:HG21 | 1:108:A:GLN:H   | 5        | 0.19          |
| (1,1409) | 1:57:A:VAL:HG21  | 1:57:A:VAL:HG12 | 5        | 0.19          |
| (1,1409) | 1:57:A:VAL:HG23  | 1:57:A:VAL:HG12 | 10       | 0.19          |
| (1,1409) | 1:57:A:VAL:HG21  | 1:57:A:VAL:HG11 | 15       | 0.19          |
| (1,1409) | 1:57:A:VAL:HG22  | 1:57:A:VAL:HG11 | 16       | 0.19          |
| (1,1403) | 1:95:A:VAL:HG21  | 1:95:A:VAL:HG12 | 8        | 0.19          |
| (1,1399) | 1:95:A:VAL:HG22  | 1:95:A:VAL:H    | 9        | 0.19          |
| (1,1397) | 1:31:A:LEU:HD21  | 1:60:A:VAL:HG11 | 6        | 0.19          |
| (1,1397) | 1:31:A:LEU:HD22  | 1:60:A:VAL:HG12 | 8        | 0.19          |
| (1,1397) | 1:31:A:LEU:HD21  | 1:60:A:VAL:HG13 | 10       | 0.19          |
| (1,1382) | 1:57:A:VAL:HG23  | 1:53:A:PHE:HE1  | 7        | 0.19          |
| (1,1382) | 1:57:A:VAL:HG23  | 1:53:A:PHE:HE1  | 10       | 0.19          |
| (1,1382) | 1:57:A:VAL:HG23  | 1:53:A:PHE:HE1  | 17       | 0.19          |
| (1,1353) | 1:61:A:ALA:HB2   | 1:62:A:GLY:H    | 3        | 0.19          |
| (1,1350) | 1:129:A:ALA:HB3  | 1:129:A:ALA:H   | 10       | 0.19          |
| (1,1350) | 1:129:A:ALA:HB2  | 1:129:A:ALA:H   | 11       | 0.19          |
| (1,1337) | 1:78:A:TYR:HD2   | 1:28:A:ILE:HD11 | 1        | 0.19          |
| (1,1337) | 1:78:A:TYR:HD1   | 1:28:A:ILE:HD11 | 7        | 0.19          |
| (1,1337) | 1:78:A:TYR:HD1   | 1:28:A:ILE:HD11 | 10       | 0.19          |
| (1,1337) | 1:78:A:TYR:HD1   | 1:28:A:ILE:HD13 | 17       | 0.19          |
| (1,1331) | 1:78:A:TYR:HE1   | 1:84:A:TYR:HD2  | 3        | 0.19          |
| (1,1331) | 1:78:A:TYR:HE1   | 1:84:A:TYR:HD1  | 12       | 0.19          |
| (1,1325) | 1:53:A:PHE:HE2   | 1:75:A:LEU:HB3  | 10       | 0.19          |
| (1,1325) | 1:53:A:PHE:HE2   | 1:75:A:LEU:HB3  | 12       | 0.19          |
| (1,1321) | 1:124:A:VAL:HG12 | 1:125:A:GLN:H   | 1        | 0.19          |
| (1,1321) | 1:124:A:VAL:HG11 | 1:125:A:GLN:H   | 2        | 0.19          |
| (1,1321) | 1:124:A:VAL:HG12 | 1:125:A:GLN:H   | 4        | 0.19          |
| (1,1321) | 1:124:A:VAL:HG13 | 1:125:A:GLN:H   | 5        | 0.19          |
| (1,1321) | 1:124:A:VAL:HG12 | 1:125:A:GLN:H   | 6        | 0.19          |
| (1,1321) | 1:124:A:VAL:HG13 | 1:125:A:GLN:H   | 12       | 0.19          |
| (1,1321) | 1:124:A:VAL:HG13 | 1:125:A:GLN:H   | 13       | 0.19          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1321) | 1:124:A:VAL:HG11 | 1:125:A:GLN:H   | 15       | 0.19          |
| (1,1321) | 1:124:A:VAL:HG11 | 1:125:A:GLN:H   | 16       | 0.19          |
| (1,1303) | 1:97:A:LEU:HD13  | 1:35:A:PHE:HE2  | 3        | 0.19          |
| (1,1273) | 1:45:A:ALA:HB3   | 1:84:A:TYR:HB3  | 1        | 0.19          |
| (1,1253) | 1:47:A:PRO:HB3   | 1:87:A:GLY:HA2  | 2        | 0.19          |
| (1,1253) | 1:47:A:PRO:HB3   | 1:87:A:GLY:HA2  | 8        | 0.19          |
| (1,1253) | 1:47:A:PRO:HB3   | 1:87:A:GLY:HA2  | 10       | 0.19          |
| (1,1206) | 1:117:A:LEU:HD11 | 1:86:A:TYR:HB2  | 6        | 0.19          |
| (1,1167) | 1:34:A:ARG:HB3   | 1:30:A:PHE:HD2  | 13       | 0.19          |
| (1,1136) | 1:31:A:LEU:HD12  | 1:35:A:PHE:HD2  | 4        | 0.19          |
| (1,1136) | 1:31:A:LEU:HD11  | 1:35:A:PHE:HD1  | 16       | 0.19          |
| (1,1126) | 1:86:A:TYR:HE2   | 1:86:A:TYR:HB3  | 8        | 0.19          |
| (1,1126) | 1:86:A:TYR:HE1   | 1:86:A:TYR:HB3  | 16       | 0.19          |
| (1,1108) | 1:56:A:LEU:HD13  | 1:52:A:ILE:HG12 | 1        | 0.19          |
| (1,1108) | 1:56:A:LEU:HD13  | 1:52:A:ILE:HG12 | 11       | 0.19          |
| (1,1080) | 1:105:A:LEU:HD13 | 1:92:A:ALA:H    | 14       | 0.19          |
| (1,1049) | 1:59:A:ARG:HB2   | 1:60:A:VAL:HG13 | 2        | 0.19          |
| (1,1049) | 1:59:A:ARG:HB2   | 1:60:A:VAL:HG13 | 6        | 0.19          |
| (1,1049) | 1:59:A:ARG:HB2   | 1:60:A:VAL:HG11 | 8        | 0.19          |
| (1,1049) | 1:59:A:ARG:HB2   | 1:60:A:VAL:HG11 | 12       | 0.19          |
| (1,1049) | 1:59:A:ARG:HB2   | 1:60:A:VAL:HG13 | 14       | 0.19          |
| (1,1049) | 1:59:A:ARG:HB2   | 1:60:A:VAL:HG13 | 16       | 0.19          |
| (1,1032) | 1:85:A:LEU:H     | 1:84:A:TYR:HE2  | 4        | 0.19          |
| (1,895)  | 1:129:A:ALA:HB3  | 1:129:A:ALA:HA  | 11       | 0.19          |
| (1,852)  | 1:65:A:ASN:HB3   | 1:65:A:ASN:HD21 | 1        | 0.19          |
| (1,852)  | 1:65:A:ASN:HB3   | 1:65:A:ASN:HD21 | 5        | 0.19          |
| (1,852)  | 1:65:A:ASN:HB3   | 1:65:A:ASN:HD21 | 15       | 0.19          |
| (1,827)  | 1:45:A:ALA:HB1   | 1:45:A:ALA:H    | 5        | 0.19          |
| (1,827)  | 1:45:A:ALA:HB1   | 1:45:A:ALA:H    | 16       | 0.19          |
| (1,753)  | 1:92:A:ALA:HB3   | 1:91:A:GLY:H    | 7        | 0.19          |
| (1,635)  | 1:127:A:GLN:H    | 1:127:A:GLN:HB3 | 6        | 0.19          |
| (1,478)  | 1:27:A:VAL:HG22  | 1:29:A:ALA:H    | 4        | 0.19          |
| (1,478)  | 1:27:A:VAL:HG23  | 1:29:A:ALA:H    | 16       | 0.19          |
| (1,477)  | 1:31:A:LEU:H     | 1:31:A:LEU:HD11 | 1        | 0.19          |
| (1,477)  | 1:31:A:LEU:H     | 1:31:A:LEU:HD12 | 8        | 0.19          |
| (1,397)  | 1:57:A:VAL:H     | 1:56:A:LEU:HB3  | 14       | 0.19          |
| (1,263)  | 1:110:A:VAL:HG23 | 1:91:A:GLY:H    | 14       | 0.19          |
| (1,234)  | 1:95:A:VAL:HG23  | 1:99:A:GLY:H    | 4        | 0.19          |
| (1,234)  | 1:95:A:VAL:HG21  | 1:99:A:GLY:H    | 7        | 0.19          |
| (1,156)  | 1:126:A:ALA:HB1  | 1:126:A:ALA:H   | 2        | 0.19          |
| (1,154)  | 1:130:A:GLU:H    | 1:129:A:ALA:HB3 | 1        | 0.19          |
| (1,128)  | 1:35:A:PHE:HD1   | 1:39:A:PHE:H    | 13       | 0.19          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,100)  | 1:35:A:PHE:HE2  | 1:35:A:PHE:H    | 3        | 0.19          |
| (1,100)  | 1:35:A:PHE:HE1  | 1:35:A:PHE:H    | 6        | 0.19          |
| (1,100)  | 1:35:A:PHE:HE1  | 1:35:A:PHE:H    | 11       | 0.19          |
| (1,100)  | 1:35:A:PHE:HE2  | 1:35:A:PHE:H    | 15       | 0.19          |
| (1,80)   | 1:30:A:PHE:HD2  | 1:30:A:PHE:H    | 4        | 0.19          |
| (1,80)   | 1:30:A:PHE:HD2  | 1:30:A:PHE:H    | 5        | 0.19          |
| (1,80)   | 1:30:A:PHE:HD2  | 1:30:A:PHE:H    | 9        | 0.19          |
| (1,56)   | 1:84:A:TYR:H    | 1:84:A:TYR:HD1  | 7        | 0.19          |
| (1,56)   | 1:84:A:TYR:H    | 1:84:A:TYR:HD1  | 15       | 0.19          |
| (3,148)  | 1:22:A:ASN:H    | 1:65:A:ASN:HB3  | 6        | 0.18          |
| (3,135)  | 1:123:A:ARG:HB3 | 1:120:A:ALA:HA  | 12       | 0.18          |
| (3,111)  | 1:111:A:GLU:HG2 | 1:112:A:HIS:HA  | 7        | 0.18          |
| (3,111)  | 1:111:A:GLU:HG2 | 1:112:A:HIS:HA  | 10       | 0.18          |
| (3,94)   | 1:56:A:LEU:HB2  | 1:75:A:LEU:HD11 | 15       | 0.18          |
| (3,94)   | 1:56:A:LEU:HB2  | 1:75:A:LEU:HD11 | 16       | 0.18          |
| (3,54)   | 1:71:A:LEU:HB3  | 1:75:A:LEU:HD12 | 17       | 0.18          |
| (3,41)   | 1:52:A:ILE:HD11 | 1:56:A:LEU:HA   | 6        | 0.18          |
| (3,38)   | 1:32:A:ALA:HB2  | 1:33:A:GLU:HG2  | 15       | 0.18          |
| (3,34)   | 1:97:A:LEU:HD23 | 1:31:A:LEU:HD13 | 15       | 0.18          |
| (3,14)   | 1:82:A:TRP:HA   | 1:85:A:LEU:HB2  | 7        | 0.18          |
| (1,4345) | 1:117:A:LEU:HA  | 1:121:A:LYS:H   | 1        | 0.18          |
| (1,4345) | 1:117:A:LEU:HA  | 1:121:A:LYS:H   | 5        | 0.18          |
| (1,4345) | 1:117:A:LEU:HA  | 1:121:A:LYS:H   | 10       | 0.18          |
| (1,4345) | 1:117:A:LEU:HA  | 1:121:A:LYS:H   | 13       | 0.18          |
| (1,4343) | 1:118:A:GLU:H   | 1:119:A:GLU:H   | 1        | 0.18          |
| (1,4343) | 1:118:A:GLU:H   | 1:119:A:GLU:H   | 9        | 0.18          |
| (1,4326) | 1:65:A:ASN:HA   | 1:66:A:LEU:H    | 7        | 0.18          |
| (1,4326) | 1:65:A:ASN:HA   | 1:66:A:LEU:H    | 9        | 0.18          |
| (1,4323) | 1:62:A:GLY:H    | 1:68:A:LYS:HD2  | 6        | 0.18          |
| (1,4323) | 1:62:A:GLY:H    | 1:68:A:LYS:HD2  | 11       | 0.18          |
| (1,4320) | 1:62:A:GLY:H    | 1:66:A:LEU:H    | 5        | 0.18          |
| (1,4317) | 1:93:A:THR:HB   | 1:102:A:CYS:H   | 2        | 0.18          |
| (1,4317) | 1:93:A:THR:HB   | 1:102:A:CYS:H   | 6        | 0.18          |
| (1,4301) | 1:97:A:LEU:HB2  | 1:97:A:LEU:H    | 15       | 0.18          |
| (1,4270) | 1:75:A:LEU:HB3  | 1:74:A:ALA:H    | 6        | 0.18          |
| (1,4270) | 1:75:A:LEU:HB3  | 1:74:A:ALA:H    | 9        | 0.18          |
| (1,4241) | 1:17:A:ASN:H    | 1:18:A:GLN:H    | 10       | 0.18          |
| (1,4225) | 1:122:A:ALA:HB2 | 1:123:A:ARG:H   | 7        | 0.18          |
| (1,4225) | 1:122:A:ALA:HB1 | 1:123:A:ARG:H   | 12       | 0.18          |
| (1,4225) | 1:122:A:ALA:HB3 | 1:123:A:ARG:H   | 14       | 0.18          |
| (1,4225) | 1:122:A:ALA:HB2 | 1:123:A:ARG:H   | 16       | 0.18          |
| (1,4198) | 1:127:A:GLN:HA  | 1:127:A:GLN:H   | 15       | 0.18          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,4195) | 1:61:A:ALA:HB1  | 1:67:A:SER:H    | 13       | 0.18          |
| (1,4194) | 1:107:A:GLU:H   | 1:106:A:ASP:HA  | 10       | 0.18          |
| (1,4193) | 1:69:A:THR:HB   | 1:72:A:ARG:H    | 15       | 0.18          |
| (1,4176) | 1:97:A:LEU:HD12 | 1:97:A:LEU:H    | 11       | 0.18          |
| (1,4172) | 1:105:A:LEU:H   | 1:92:A:ALA:H    | 7        | 0.18          |
| (1,4133) | 1:82:A:TRP:HE1  | 1:82:A:TRP:HD1  | 4        | 0.18          |
| (1,4133) | 1:82:A:TRP:HE1  | 1:82:A:TRP:HD1  | 6        | 0.18          |
| (1,4133) | 1:82:A:TRP:HE1  | 1:82:A:TRP:HD1  | 10       | 0.18          |
| (1,4133) | 1:82:A:TRP:HE1  | 1:82:A:TRP:HD1  | 13       | 0.18          |
| (1,4133) | 1:82:A:TRP:HE1  | 1:82:A:TRP:HD1  | 16       | 0.18          |
| (1,4114) | 1:65:A:ASN:H    | 1:65:A:ASN:HD21 | 10       | 0.18          |
| (1,4109) | 1:97:A:LEU:HD11 | 1:98:A:ASP:H    | 1        | 0.18          |
| (1,4036) | 1:31:A:LEU:H    | 1:31:A:LEU:HD11 | 2        | 0.18          |
| (1,4036) | 1:31:A:LEU:H    | 1:31:A:LEU:HD11 | 11       | 0.18          |
| (1,4036) | 1:31:A:LEU:H    | 1:31:A:LEU:HD13 | 12       | 0.18          |
| (1,4036) | 1:31:A:LEU:H    | 1:31:A:LEU:HD13 | 13       | 0.18          |
| (1,4019) | 1:33:A:GLU:HB3  | 1:34:A:ARG:H    | 2        | 0.18          |
| (1,4019) | 1:33:A:GLU:HB3  | 1:34:A:ARG:H    | 12       | 0.18          |
| (1,4017) | 1:32:A:ALA:HB2  | 1:35:A:PHE:H    | 2        | 0.18          |
| (1,4017) | 1:32:A:ALA:HB2  | 1:35:A:PHE:H    | 7        | 0.18          |
| (1,4017) | 1:32:A:ALA:HB2  | 1:35:A:PHE:H    | 13       | 0.18          |
| (1,4016) | 1:15:A:MET:HA   | 1:15:A:MET:H    | 5        | 0.18          |
| (1,3987) | 1:50:A:ILE:HG22 | 1:50:A:ILE:H    | 14       | 0.18          |
| (1,3961) | 1:57:A:VAL:H    | 1:56:A:LEU:HB3  | 1        | 0.18          |
| (1,3961) | 1:57:A:VAL:H    | 1:56:A:LEU:HB3  | 4        | 0.18          |
| (1,3942) | 1:66:A:LEU:HD12 | 1:63:A:GLU:H    | 1        | 0.18          |
| (1,3940) | 1:62:A:GLY:HA3  | 1:63:A:GLU:H    | 7        | 0.18          |
| (1,3940) | 1:62:A:GLY:HA3  | 1:63:A:GLU:H    | 16       | 0.18          |
| (1,3917) | 1:74:A:ALA:HA   | 1:75:A:LEU:H    | 16       | 0.18          |
| (1,3917) | 1:74:A:ALA:HA   | 1:75:A:LEU:H    | 17       | 0.18          |
| (1,3916) | 1:71:A:LEU:HA   | 1:74:A:ALA:H    | 12       | 0.18          |
| (1,3907) | 1:76:A:ARG:HD2  | 1:77:A:LEU:H    | 8        | 0.18          |
| (1,3901) | 1:79:A:THR:H    | 1:77:A:LEU:HB2  | 4        | 0.18          |
| (1,3901) | 1:79:A:THR:H    | 1:77:A:LEU:HB2  | 11       | 0.18          |
| (1,3845) | 1:95:A:VAL:HG12 | 1:96:A:ASP:H    | 13       | 0.18          |
| (1,3830) | 1:101:A:PRO:HD3 | 1:100:A:ASN:H   | 12       | 0.18          |
| (1,3781) | 1:119:A:GLU:HA  | 1:119:A:GLU:H   | 3        | 0.18          |
| (1,3781) | 1:119:A:GLU:HA  | 1:119:A:GLU:H   | 11       | 0.18          |
| (1,3781) | 1:119:A:GLU:HA  | 1:119:A:GLU:H   | 12       | 0.18          |
| (1,3781) | 1:119:A:GLU:HA  | 1:119:A:GLU:H   | 15       | 0.18          |
| (1,3771) | 1:126:A:ALA:HB2 | 1:126:A:ALA:H   | 1        | 0.18          |
| (1,3770) | 1:130:A:GLU:HG3 | 1:130:A:GLU:H   | 14       | 0.18          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3768) | 1:130:A:GLU:H    | 1:130:A:GLU:HA  | 6        | 0.18          |
| (1,3767) | 1:129:A:ALA:HA   | 1:129:A:ALA:H   | 11       | 0.18          |
| (1,3766) | 1:128:A:ARG:HB3  | 1:129:A:ALA:H   | 13       | 0.18          |
| (1,3744) | 1:35:A:PHE:HD2   | 1:39:A:PHE:H    | 3        | 0.18          |
| (1,3717) | 1:35:A:PHE:H     | 1:39:A:PHE:HE1  | 5        | 0.18          |
| (1,3717) | 1:35:A:PHE:H     | 1:39:A:PHE:HE2  | 6        | 0.18          |
| (1,3717) | 1:35:A:PHE:H     | 1:39:A:PHE:HE1  | 8        | 0.18          |
| (1,3717) | 1:35:A:PHE:H     | 1:39:A:PHE:HE2  | 11       | 0.18          |
| (1,3698) | 1:30:A:PHE:HD2   | 1:30:A:PHE:H    | 11       | 0.18          |
| (1,3673) | 1:49:A:LYS:H     | 1:50:A:ILE:H    | 5        | 0.18          |
| (1,3673) | 1:49:A:LYS:H     | 1:50:A:ILE:H    | 9        | 0.18          |
| (1,3673) | 1:49:A:LYS:H     | 1:50:A:ILE:H    | 11       | 0.18          |
| (1,3673) | 1:49:A:LYS:H     | 1:50:A:ILE:H    | 13       | 0.18          |
| (1,3673) | 1:49:A:LYS:H     | 1:50:A:ILE:H    | 16       | 0.18          |
| (1,3662) | 1:83:A:ARG:H     | 1:82:A:TRP:HD1  | 1        | 0.18          |
| (1,3662) | 1:83:A:ARG:H     | 1:82:A:TRP:HD1  | 13       | 0.18          |
| (1,3600) | 1:113:A:ALA:HB3  | 1:92:A:ALA:HA   | 10       | 0.18          |
| (1,3595) | 1:108:A:GLN:HA   | 1:111:A:GLU:HB3 | 1        | 0.18          |
| (1,3595) | 1:108:A:GLN:HA   | 1:111:A:GLU:HB3 | 3        | 0.18          |
| (1,3595) | 1:108:A:GLN:HA   | 1:111:A:GLU:HB3 | 5        | 0.18          |
| (1,3595) | 1:108:A:GLN:HA   | 1:111:A:GLU:HB3 | 7        | 0.18          |
| (1,3595) | 1:108:A:GLN:HA   | 1:111:A:GLU:HB3 | 8        | 0.18          |
| (1,3595) | 1:108:A:GLN:HA   | 1:111:A:GLU:HB3 | 10       | 0.18          |
| (1,3595) | 1:108:A:GLN:HA   | 1:111:A:GLU:HB3 | 11       | 0.18          |
| (1,3595) | 1:108:A:GLN:HA   | 1:111:A:GLU:HB3 | 17       | 0.18          |
| (1,3583) | 1:112:A:HIS:H    | 1:109:A:HIS:HA  | 11       | 0.18          |
| (1,3552) | 1:123:A:ARG:HG2  | 1:124:A:VAL:HA  | 4        | 0.18          |
| (1,3520) | 1:100:A:ASN:HD22 | 1:98:A:ASP:HB3  | 8        | 0.18          |
| (1,3520) | 1:100:A:ASN:HD22 | 1:98:A:ASP:HB3  | 13       | 0.18          |
| (1,3519) | 1:65:A:ASN:H     | 1:65:A:ASN:HB3  | 5        | 0.18          |
| (1,3516) | 1:21:A:LEU:HG    | 1:65:A:ASN:HB3  | 7        | 0.18          |
| (1,3515) | 1:102:A:CYS:HB3  | 1:49:A:LYS:HA   | 11       | 0.18          |
| (1,3511) | 1:50:A:ILE:HG13  | 1:49:A:LYS:HA   | 8        | 0.18          |
| (1,3508) | 1:113:A:ALA:HB2  | 1:88:A:VAL:HA   | 10       | 0.18          |
| (1,3506) | 1:60:A:VAL:HG12  | 1:35:A:PHE:HZ   | 10       | 0.18          |
| (1,3506) | 1:60:A:VAL:HG11  | 1:35:A:PHE:HZ   | 12       | 0.18          |
| (1,3506) | 1:60:A:VAL:HG11  | 1:35:A:PHE:HZ   | 17       | 0.18          |
| (1,3501) | 1:27:A:VAL:HG22  | 1:28:A:ILE:HA   | 14       | 0.18          |
| (1,3477) | 1:15:A:MET:HG3   | 1:15:A:MET:HB2  | 8        | 0.18          |
| (1,3477) | 1:15:A:MET:HG3   | 1:15:A:MET:HB2  | 10       | 0.18          |
| (1,3441) | 1:21:A:LEU:HG    | 1:21:A:LEU:HB3  | 12       | 0.18          |
| (1,3437) | 1:21:A:LEU:HB2   | 1:21:A:LEU:HD13 | 1        | 0.18          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3437) | 1:21:A:LEU:HB2  | 1:21:A:LEU:HD11  | 7        | 0.18          |
| (1,3433) | 1:27:A:VAL:HA   | 1:21:A:LEU:HD13  | 7        | 0.18          |
| (1,3430) | 1:45:A:ALA:HB3  | 1:84:A:TYR:HA    | 1        | 0.18          |
| (1,3430) | 1:45:A:ALA:HB3  | 1:84:A:TYR:HA    | 7        | 0.18          |
| (1,3422) | 1:77:A:LEU:HG   | 1:77:A:LEU:HD22  | 4        | 0.18          |
| (1,3422) | 1:77:A:LEU:HG   | 1:77:A:LEU:HD21  | 5        | 0.18          |
| (1,3422) | 1:77:A:LEU:HG   | 1:77:A:LEU:HD22  | 6        | 0.18          |
| (1,3415) | 1:117:A:LEU:HA  | 1:117:A:LEU:HD12 | 9        | 0.18          |
| (1,3415) | 1:117:A:LEU:HA  | 1:117:A:LEU:HD13 | 11       | 0.18          |
| (1,3414) | 1:86:A:TYR:H    | 1:117:A:LEU:HD13 | 1        | 0.18          |
| (1,3414) | 1:86:A:TYR:H    | 1:117:A:LEU:HD11 | 4        | 0.18          |
| (1,3396) | 1:71:A:LEU:HA   | 1:74:A:ALA:HB2   | 6        | 0.18          |
| (1,3378) | 1:67:A:SER:HB3  | 1:66:A:LEU:HA    | 1        | 0.18          |
| (1,3378) | 1:67:A:SER:HB3  | 1:66:A:LEU:HA    | 4        | 0.18          |
| (1,3378) | 1:67:A:SER:HB3  | 1:66:A:LEU:HA    | 8        | 0.18          |
| (1,3378) | 1:67:A:SER:HB3  | 1:66:A:LEU:HA    | 9        | 0.18          |
| (1,3378) | 1:67:A:SER:HB3  | 1:66:A:LEU:HA    | 12       | 0.18          |
| (1,3378) | 1:67:A:SER:HB3  | 1:66:A:LEU:HA    | 13       | 0.18          |
| (1,3370) | 1:24:A:SER:HA   | 1:27:A:VAL:HG11  | 2        | 0.18          |
| (1,3348) | 1:79:A:THR:HG22 | 1:84:A:TYR:HE1   | 6        | 0.18          |
| (1,3336) | 1:71:A:LEU:HD21 | 1:74:A:ALA:H     | 3        | 0.18          |
| (1,3322) | 1:30:A:PHE:HD1  | 1:66:A:LEU:HD21  | 7        | 0.18          |
| (1,3322) | 1:30:A:PHE:HD2  | 1:66:A:LEU:HD21  | 10       | 0.18          |
| (1,3322) | 1:30:A:PHE:HD2  | 1:66:A:LEU:HD21  | 15       | 0.18          |
| (1,3320) | 1:27:A:VAL:HA   | 1:66:A:LEU:HD23  | 2        | 0.18          |
| (1,3320) | 1:27:A:VAL:HA   | 1:66:A:LEU:HD21  | 13       | 0.18          |
| (1,3320) | 1:27:A:VAL:HA   | 1:66:A:LEU:HD23  | 16       | 0.18          |
| (1,3282) | 1:44:A:GLU:HG2  | 1:45:A:ALA:HB3   | 2        | 0.18          |
| (1,3282) | 1:44:A:GLU:HG2  | 1:45:A:ALA:HB1   | 5        | 0.18          |
| (1,3269) | 1:33:A:GLU:HB3  | 1:17:A:ASN:HB2   | 4        | 0.18          |
| (1,3260) | 1:121:A:LYS:HG2 | 1:121:A:LYS:HB2  | 8        | 0.18          |
| (1,3241) | 1:52:A:ILE:HG13 | 1:97:A:LEU:HD21  | 4        | 0.18          |
| (1,3241) | 1:52:A:ILE:HG13 | 1:97:A:LEU:HD21  | 8        | 0.18          |
| (1,3240) | 1:52:A:ILE:HG13 | 1:48:A:LEU:HD12  | 5        | 0.18          |
| (1,3232) | 1:92:A:ALA:H    | 1:105:A:LEU:HB2  | 2        | 0.18          |
| (1,3232) | 1:92:A:ALA:H    | 1:105:A:LEU:HB2  | 3        | 0.18          |
| (1,3210) | 1:128:A:ARG:HA  | 1:128:A:ARG:HB3  | 15       | 0.18          |
| (1,3200) | 1:116:A:GLN:HG3 | 1:113:A:ALA:HB3  | 2        | 0.18          |
| (1,3197) | 1:87:A:GLY:HA3  | 1:113:A:ALA:HB2  | 9        | 0.18          |
| (1,3185) | 1:109:A:HIS:HB2 | 1:108:A:GLN:H    | 1        | 0.18          |
| (1,3181) | 1:108:A:GLN:HG3 | 1:108:A:GLN:HA   | 8        | 0.18          |
| (1,3180) | 1:111:A:GLU:HG2 | 1:111:A:GLU:HA   | 2        | 0.18          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3180) | 1:111:A:GLU:HG2 | 1:111:A:GLU:HA  | 13       | 0.18          |
| (1,3165) | 1:126:A:ALA:HB1 | 1:125:A:GLN:HG3 | 4        | 0.18          |
| (1,3165) | 1:126:A:ALA:HB2 | 1:125:A:GLN:HG3 | 5        | 0.18          |
| (1,3165) | 1:126:A:ALA:HB2 | 1:125:A:GLN:HG3 | 11       | 0.18          |
| (1,3165) | 1:126:A:ALA:HB1 | 1:125:A:GLN:HG3 | 12       | 0.18          |
| (1,3165) | 1:126:A:ALA:HB3 | 1:125:A:GLN:HG3 | 17       | 0.18          |
| (1,3160) | 1:74:A:ALA:HB1  | 1:74:A:ALA:HA   | 7        | 0.18          |
| (1,3134) | 1:15:A:MET:HB2  | 1:15:A:MET:HG2  | 16       | 0.18          |
| (1,3130) | 1:123:A:ARG:HG2 | 1:123:A:ARG:H   | 13       | 0.18          |
| (1,3118) | 1:58:A:ASP:HA   | 1:58:A:ASP:HB2  | 7        | 0.18          |
| (1,3080) | 1:125:A:GLN:HB2 | 1:125:A:GLN:HA  | 5        | 0.18          |
| (1,3068) | 1:52:A:ILE:HG23 | 1:53:A:PHE:HB2  | 4        | 0.18          |
| (1,3068) | 1:52:A:ILE:HG21 | 1:53:A:PHE:HB2  | 9        | 0.18          |
| (1,3066) | 1:30:A:PHE:HB3  | 1:29:A:ALA:HB1  | 4        | 0.18          |
| (1,3059) | 1:28:A:ILE:HB   | 1:28:A:ILE:HG21 | 2        | 0.18          |
| (1,3059) | 1:28:A:ILE:HB   | 1:28:A:ILE:HG23 | 4        | 0.18          |
| (1,3053) | 1:29:A:ALA:H    | 1:28:A:ILE:HG22 | 14       | 0.18          |
| (1,3053) | 1:29:A:ALA:H    | 1:28:A:ILE:HG23 | 17       | 0.18          |
| (1,3052) | 1:39:A:PHE:HZ   | 1:52:A:ILE:HG23 | 14       | 0.18          |
| (1,3032) | 1:121:A:LYS:HG3 | 1:121:A:LYS:HE3 | 9        | 0.18          |
| (1,3028) | 1:71:A:LEU:HD13 | 1:72:A:ARG:HA   | 11       | 0.18          |
| (1,3021) | 1:64:A:MET:HE1  | 1:63:A:GLU:H    | 13       | 0.18          |
| (1,2995) | 1:60:A:VAL:H    | 1:60:A:VAL:HB   | 16       | 0.18          |
| (1,2992) | 1:20:A:LYS:HB3  | 1:20:A:LYS:H    | 8        | 0.18          |
| (1,2992) | 1:20:A:LYS:HB3  | 1:20:A:LYS:H    | 11       | 0.18          |
| (1,2969) | 1:93:A:THR:HG21 | 1:101:A:PRO:HB3 | 4        | 0.18          |
| (1,2969) | 1:93:A:THR:HG23 | 1:101:A:PRO:HB3 | 6        | 0.18          |
| (1,2969) | 1:93:A:THR:HG22 | 1:101:A:PRO:HB3 | 13       | 0.18          |
| (1,2969) | 1:93:A:THR:HG21 | 1:101:A:PRO:HB3 | 16       | 0.18          |
| (1,2969) | 1:93:A:THR:HG23 | 1:101:A:PRO:HB3 | 17       | 0.18          |
| (1,2960) | 1:77:A:LEU:HD13 | 1:25:A:LYS:HA   | 3        | 0.18          |
| (1,2960) | 1:77:A:LEU:HD11 | 1:25:A:LYS:HA   | 6        | 0.18          |
| (1,2937) | 1:95:A:VAL:HG22 | 1:95:A:VAL:HG12 | 17       | 0.18          |
| (1,2927) | 1:31:A:LEU:HD22 | 1:39:A:PHE:HD2  | 6        | 0.18          |
| (1,2927) | 1:31:A:LEU:HD22 | 1:39:A:PHE:HD1  | 10       | 0.18          |
| (1,2927) | 1:31:A:LEU:HD21 | 1:39:A:PHE:HD1  | 12       | 0.18          |
| (1,2927) | 1:31:A:LEU:HD22 | 1:39:A:PHE:HD1  | 14       | 0.18          |
| (1,2927) | 1:31:A:LEU:HD22 | 1:39:A:PHE:HD2  | 17       | 0.18          |
| (1,2899) | 1:28:A:ILE:HD11 | 1:75:A:LEU:H    | 10       | 0.18          |
| (1,2893) | 1:50:A:ILE:HB   | 1:50:A:ILE:HG22 | 1        | 0.18          |
| (1,2893) | 1:50:A:ILE:HB   | 1:50:A:ILE:HG22 | 5        | 0.18          |
| (1,2891) | 1:32:A:ALA:HB3  | 1:28:A:ILE:HG23 | 15       | 0.18          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2888) | 1:29:A:ALA:HA    | 1:32:A:ALA:HB3  | 2        | 0.18          |
| (1,2888) | 1:29:A:ALA:HA    | 1:32:A:ALA:HB3  | 7        | 0.18          |
| (1,2888) | 1:29:A:ALA:HA    | 1:32:A:ALA:HB1  | 13       | 0.18          |
| (1,2888) | 1:29:A:ALA:HA    | 1:32:A:ALA:HB1  | 16       | 0.18          |
| (1,2881) | 1:74:A:ALA:HB2   | 1:31:A:LEU:HD11 | 6        | 0.18          |
| (1,2855) | 1:78:A:TYR:HD1   | 1:28:A:ILE:HD13 | 14       | 0.18          |
| (1,2804) | 1:66:A:LEU:HB3   | 1:60:A:VAL:HB   | 13       | 0.18          |
| (1,2804) | 1:66:A:LEU:HB3   | 1:60:A:VAL:HB   | 15       | 0.18          |
| (1,2800) | 1:48:A:LEU:HD23  | 1:48:A:LEU:HB3  | 17       | 0.18          |
| (1,2754) | 1:60:A:VAL:HG13  | 1:59:A:ARG:HD3  | 2        | 0.18          |
| (1,2754) | 1:60:A:VAL:HG13  | 1:59:A:ARG:HD3  | 6        | 0.18          |
| (1,2754) | 1:60:A:VAL:HG11  | 1:59:A:ARG:HD3  | 8        | 0.18          |
| (1,2754) | 1:60:A:VAL:HG11  | 1:59:A:ARG:HD3  | 12       | 0.18          |
| (1,2754) | 1:60:A:VAL:HG11  | 1:59:A:ARG:HD3  | 17       | 0.18          |
| (1,2753) | 1:97:A:LEU:HD11  | 1:59:A:ARG:HD3  | 6        | 0.18          |
| (1,2740) | 1:57:A:VAL:HG22  | 1:58:A:ASP:HB2  | 11       | 0.18          |
| (1,2712) | 1:39:A:PHE:HB3   | 1:35:A:PHE:HB3  | 1        | 0.18          |
| (1,2712) | 1:39:A:PHE:HB3   | 1:35:A:PHE:HB3  | 3        | 0.18          |
| (1,2712) | 1:39:A:PHE:HB3   | 1:35:A:PHE:HB3  | 7        | 0.18          |
| (1,2712) | 1:39:A:PHE:HB3   | 1:35:A:PHE:HB3  | 12       | 0.18          |
| (1,2711) | 1:35:A:PHE:HB2   | 1:35:A:PHE:HE2  | 4        | 0.18          |
| (1,2711) | 1:35:A:PHE:HB2   | 1:35:A:PHE:HE1  | 16       | 0.18          |
| (1,2694) | 1:73:A:SER:HB2   | 1:74:A:ALA:H    | 14       | 0.18          |
| (1,2639) | 1:71:A:LEU:HD12  | 1:71:A:LEU:HB2  | 10       | 0.18          |
| (1,2639) | 1:71:A:LEU:HD12  | 1:71:A:LEU:HB2  | 12       | 0.18          |
| (1,2639) | 1:71:A:LEU:HD12  | 1:71:A:LEU:HB2  | 13       | 0.18          |
| (1,2629) | 1:53:A:PHE:HZ    | 1:71:A:LEU:HB2  | 7        | 0.18          |
| (1,2629) | 1:53:A:PHE:HZ    | 1:71:A:LEU:HB2  | 8        | 0.18          |
| (1,2629) | 1:53:A:PHE:HZ    | 1:71:A:LEU:HB2  | 10       | 0.18          |
| (1,2621) | 1:105:A:LEU:HD11 | 1:92:A:ALA:H    | 1        | 0.18          |
| (1,2621) | 1:105:A:LEU:HD12 | 1:92:A:ALA:H    | 3        | 0.18          |
| (1,2621) | 1:105:A:LEU:HD13 | 1:92:A:ALA:H    | 9        | 0.18          |
| (1,2621) | 1:105:A:LEU:HD13 | 1:92:A:ALA:H    | 13       | 0.18          |
| (1,2621) | 1:105:A:LEU:HD13 | 1:92:A:ALA:H    | 16       | 0.18          |
| (1,2619) | 1:48:A:LEU:HD23  | 1:84:A:TYR:HE1  | 4        | 0.18          |
| (1,2618) | 1:34:A:ARG:HG3   | 1:34:A:ARG:H    | 11       | 0.18          |
| (1,2560) | 1:86:A:TYR:HE2   | 1:86:A:TYR:HD2  | 3        | 0.18          |
| (1,2559) | 1:86:A:TYR:HE1   | 1:86:A:TYR:HB2  | 13       | 0.18          |
| (1,2530) | 1:33:A:GLU:HA    | 1:34:A:ARG:H    | 6        | 0.18          |
| (1,2530) | 1:33:A:GLU:HA    | 1:34:A:ARG:H    | 14       | 0.18          |
| (1,2530) | 1:33:A:GLU:HA    | 1:34:A:ARG:H    | 17       | 0.18          |
| (1,2514) | 1:120:A:ALA:H    | 1:120:A:ALA:HA  | 8        | 0.18          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2514) | 1:120:A:ALA:H    | 1:120:A:ALA:HA  | 13       | 0.18          |
| (1,2489) | 1:28:A:ILE:HA    | 1:28:A:ILE:HG21 | 1        | 0.18          |
| (1,2489) | 1:28:A:ILE:HA    | 1:28:A:ILE:HG21 | 9        | 0.18          |
| (1,2489) | 1:28:A:ILE:HA    | 1:28:A:ILE:HG22 | 15       | 0.18          |
| (1,2489) | 1:28:A:ILE:HA    | 1:28:A:ILE:HG22 | 17       | 0.18          |
| (1,2424) | 1:64:A:MET:HE1   | 1:30:A:PHE:HD2  | 17       | 0.18          |
| (1,2367) | 1:52:A:ILE:H     | 1:52:A:ILE:HD11 | 7        | 0.18          |
| (1,2367) | 1:52:A:ILE:H     | 1:52:A:ILE:HD12 | 14       | 0.18          |
| (1,2351) | 1:110:A:VAL:HG21 | 1:109:A:HIS:HA  | 4        | 0.18          |
| (1,2351) | 1:110:A:VAL:HG21 | 1:109:A:HIS:HA  | 17       | 0.18          |
| (1,2341) | 1:66:A:LEU:HD23  | 1:70:A:GLN:H    | 10       | 0.18          |
| (1,2336) | 1:64:A:MET:HE2   | 1:31:A:LEU:HA   | 13       | 0.18          |
| (1,2299) | 1:55:A:ASP:HB3   | 1:96:A:ASP:HA   | 6        | 0.18          |
| (1,2299) | 1:55:A:ASP:HB3   | 1:96:A:ASP:HA   | 14       | 0.18          |
| (1,2295) | 1:121:A:LYS:HG2  | 1:121:A:LYS:HD3 | 8        | 0.18          |
| (1,2295) | 1:121:A:LYS:HG2  | 1:121:A:LYS:HD3 | 13       | 0.18          |
| (1,2288) | 1:70:A:GLN:HA    | 1:70:A:GLN:HG3  | 15       | 0.18          |
| (1,2288) | 1:70:A:GLN:HA    | 1:70:A:GLN:HG3  | 16       | 0.18          |
| (1,2221) | 1:31:A:LEU:HA    | 1:60:A:VAL:HB   | 13       | 0.18          |
| (1,2221) | 1:31:A:LEU:HA    | 1:60:A:VAL:HB   | 14       | 0.18          |
| (1,2221) | 1:31:A:LEU:HA    | 1:60:A:VAL:HB   | 15       | 0.18          |
| (1,2197) | 1:39:A:PHE:HD2   | 1:56:A:LEU:HA   | 11       | 0.18          |
| (1,2197) | 1:39:A:PHE:HD1   | 1:56:A:LEU:HA   | 12       | 0.18          |
| (1,2169) | 1:22:A:ASN:HB3   | 1:22:A:ASN:H    | 4        | 0.18          |
| (1,2169) | 1:22:A:ASN:HB3   | 1:22:A:ASN:H    | 7        | 0.18          |
| (1,2169) | 1:22:A:ASN:HB3   | 1:22:A:ASN:H    | 12       | 0.18          |
| (1,2164) | 1:120:A:ALA:HA   | 1:121:A:LYS:H   | 8        | 0.18          |
| (1,2164) | 1:120:A:ALA:HA   | 1:121:A:LYS:H   | 13       | 0.18          |
| (1,2149) | 1:21:A:LEU:HD21  | 1:30:A:PHE:HD2  | 10       | 0.18          |
| (1,2094) | 1:95:A:VAL:HG21  | 1:97:A:LEU:HD21 | 3        | 0.18          |
| (1,2045) | 1:77:A:LEU:H     | 1:78:A:TYR:H    | 5        | 0.18          |
| (1,2037) | 1:57:A:VAL:HG23  | 1:57:A:VAL:HG13 | 7        | 0.18          |
| (1,2037) | 1:57:A:VAL:HG22  | 1:57:A:VAL:HG12 | 8        | 0.18          |
| (1,2037) | 1:57:A:VAL:HG23  | 1:57:A:VAL:HG12 | 11       | 0.18          |
| (1,2035) | 1:52:A:ILE:HG13  | 1:97:A:LEU:HD23 | 3        | 0.18          |
| (1,1992) | 1:52:A:ILE:HG21  | 1:51:A:GLY:H    | 6        | 0.18          |
| (1,1955) | 1:92:A:ALA:HB3   | 1:113:A:ALA:HB1 | 5        | 0.18          |
| (1,1947) | 1:93:A:THR:HB    | 1:88:A:VAL:HG11 | 16       | 0.18          |
| (1,1928) | 1:105:A:LEU:HB3  | 1:109:A:HIS:HB2 | 3        | 0.18          |
| (1,1928) | 1:105:A:LEU:HB3  | 1:109:A:HIS:HB2 | 5        | 0.18          |
| (1,1928) | 1:105:A:LEU:HB3  | 1:109:A:HIS:HB2 | 6        | 0.18          |
| (1,1928) | 1:105:A:LEU:HB3  | 1:109:A:HIS:HB2 | 7        | 0.18          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1928) | 1:105:A:LEU:HB3  | 1:109:A:HIS:HB2  | 9        | 0.18          |
| (1,1928) | 1:105:A:LEU:HB3  | 1:109:A:HIS:HB2  | 14       | 0.18          |
| (1,1928) | 1:105:A:LEU:HB3  | 1:109:A:HIS:HB2  | 16       | 0.18          |
| (1,1890) | 1:100:A:ASN:HD22 | 1:98:A:ASP:HB3   | 1        | 0.18          |
| (1,1889) | 1:65:A:ASN:H     | 1:65:A:ASN:HB3   | 2        | 0.18          |
| (1,1883) | 1:64:A:MET:HE3   | 1:21:A:LEU:H     | 8        | 0.18          |
| (1,1881) | 1:113:A:ALA:HB3  | 1:88:A:VAL:HA    | 6        | 0.18          |
| (1,1877) | 1:27:A:VAL:HG21  | 1:27:A:VAL:H     | 2        | 0.18          |
| (1,1877) | 1:27:A:VAL:HG21  | 1:27:A:VAL:H     | 9        | 0.18          |
| (1,1877) | 1:27:A:VAL:HG23  | 1:27:A:VAL:H     | 11       | 0.18          |
| (1,1877) | 1:27:A:VAL:HG21  | 1:27:A:VAL:H     | 15       | 0.18          |
| (1,1812) | 1:117:A:LEU:HA   | 1:117:A:LEU:HD12 | 2        | 0.18          |
| (1,1811) | 1:86:A:TYR:H     | 1:117:A:LEU:HD11 | 13       | 0.18          |
| (1,1775) | 1:88:A:VAL:HA    | 1:47:A:PRO:HB3   | 12       | 0.18          |
| (1,1726) | 1:66:A:LEU:HD12  | 1:66:A:LEU:HA    | 2        | 0.18          |
| (1,1726) | 1:66:A:LEU:HD12  | 1:66:A:LEU:HA    | 4        | 0.18          |
| (1,1726) | 1:66:A:LEU:HD12  | 1:66:A:LEU:HA    | 10       | 0.18          |
| (1,1726) | 1:66:A:LEU:HD13  | 1:66:A:LEU:HA    | 17       | 0.18          |
| (1,1725) | 1:71:A:LEU:HD13  | 1:71:A:LEU:HG    | 12       | 0.18          |
| (1,1713) | 1:20:A:LYS:H     | 1:20:A:LYS:HD3   | 10       | 0.18          |
| (1,1690) | 1:42:A:GLU:HG2   | 1:41:A:ALA:HB1   | 14       | 0.18          |
| (1,1681) | 1:40:A:SER:HA    | 1:41:A:ALA:HB1   | 16       | 0.18          |
| (1,1671) | 1:78:A:TYR:HA    | 1:28:A:ILE:HG12  | 3        | 0.18          |
| (1,1671) | 1:78:A:TYR:HA    | 1:28:A:ILE:HG12  | 4        | 0.18          |
| (1,1671) | 1:78:A:TYR:HA    | 1:28:A:ILE:HG12  | 5        | 0.18          |
| (1,1671) | 1:78:A:TYR:HA    | 1:28:A:ILE:HG12  | 7        | 0.18          |
| (1,1671) | 1:78:A:TYR:HA    | 1:28:A:ILE:HG12  | 8        | 0.18          |
| (1,1671) | 1:78:A:TYR:HA    | 1:28:A:ILE:HG12  | 10       | 0.18          |
| (1,1671) | 1:78:A:TYR:HA    | 1:28:A:ILE:HG12  | 13       | 0.18          |
| (1,1671) | 1:78:A:TYR:HA    | 1:28:A:ILE:HG12  | 15       | 0.18          |
| (1,1671) | 1:78:A:TYR:HA    | 1:28:A:ILE:HG12  | 17       | 0.18          |
| (1,1660) | 1:27:A:VAL:HA    | 1:27:A:VAL:HG12  | 4        | 0.18          |
| (1,1629) | 1:116:A:GLN:HG3  | 1:113:A:ALA:HB3  | 4        | 0.18          |
| (1,1628) | 1:87:A:GLY:HA3   | 1:113:A:ALA:HB3  | 13       | 0.18          |
| (1,1616) | 1:109:A:HIS:HB2  | 1:108:A:GLN:H    | 15       | 0.18          |
| (1,1592) | 1:126:A:ALA:HB2  | 1:125:A:GLN:HG3  | 1        | 0.18          |
| (1,1588) | 1:74:A:ALA:HB1   | 1:74:A:ALA:HA    | 1        | 0.18          |
| (1,1588) | 1:74:A:ALA:HB3   | 1:74:A:ALA:HA    | 6        | 0.18          |
| (1,1588) | 1:74:A:ALA:HB3   | 1:74:A:ALA:HA    | 11       | 0.18          |
| (1,1560) | 1:76:A:ARG:HB2   | 1:77:A:LEU:H     | 11       | 0.18          |
| (1,1556) | 1:59:A:ARG:HB2   | 1:58:A:ASP:HB2   | 1        | 0.18          |
| (1,1556) | 1:59:A:ARG:HB2   | 1:58:A:ASP:HB2   | 2        | 0.18          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1556) | 1:59:A:ARG:HB2   | 1:58:A:ASP:HB2  | 10       | 0.18          |
| (1,1556) | 1:59:A:ARG:HB2   | 1:58:A:ASP:HB2  | 12       | 0.18          |
| (1,1556) | 1:59:A:ARG:HB2   | 1:58:A:ASP:HB2  | 14       | 0.18          |
| (1,1556) | 1:59:A:ARG:HB2   | 1:58:A:ASP:HB2  | 15       | 0.18          |
| (1,1556) | 1:59:A:ARG:HB2   | 1:58:A:ASP:HB2  | 16       | 0.18          |
| (1,1553) | 1:57:A:VAL:HG12  | 1:61:A:ALA:H    | 4        | 0.18          |
| (1,1513) | 1:52:A:ILE:HG23  | 1:53:A:PHE:HB3  | 8        | 0.18          |
| (1,1513) | 1:52:A:ILE:HG23  | 1:53:A:PHE:HB3  | 15       | 0.18          |
| (1,1511) | 1:28:A:ILE:HA    | 1:28:A:ILE:HG21 | 1        | 0.18          |
| (1,1511) | 1:28:A:ILE:HA    | 1:28:A:ILE:HG21 | 9        | 0.18          |
| (1,1511) | 1:28:A:ILE:HA    | 1:28:A:ILE:HG22 | 15       | 0.18          |
| (1,1508) | 1:29:A:ALA:H     | 1:28:A:ILE:HG23 | 3        | 0.18          |
| (1,1440) | 1:105:A:LEU:H    | 1:101:A:PRO:HD3 | 12       | 0.18          |
| (1,1440) | 1:105:A:LEU:H    | 1:101:A:PRO:HD3 | 16       | 0.18          |
| (1,1419) | 1:77:A:LEU:HD12  | 1:25:A:LYS:HA   | 8        | 0.18          |
| (1,1419) | 1:77:A:LEU:HD13  | 1:25:A:LYS:HA   | 11       | 0.18          |
| (1,1409) | 1:57:A:VAL:HG22  | 1:57:A:VAL:HG11 | 6        | 0.18          |
| (1,1397) | 1:31:A:LEU:HD21  | 1:60:A:VAL:HG12 | 13       | 0.18          |
| (1,1371) | 1:28:A:ILE:HD12  | 1:75:A:LEU:H    | 3        | 0.18          |
| (1,1371) | 1:28:A:ILE:HD12  | 1:75:A:LEU:H    | 4        | 0.18          |
| (1,1366) | 1:50:A:ILE:HG12  | 1:50:A:ILE:HG22 | 17       | 0.18          |
| (1,1365) | 1:32:A:ALA:HB3   | 1:28:A:ILE:HG21 | 12       | 0.18          |
| (1,1352) | 1:122:A:ALA:HB1  | 1:122:A:ALA:H   | 2        | 0.18          |
| (1,1350) | 1:129:A:ALA:HB2  | 1:129:A:ALA:H   | 17       | 0.18          |
| (1,1337) | 1:78:A:TYR:HD1   | 1:28:A:ILE:HD12 | 3        | 0.18          |
| (1,1337) | 1:78:A:TYR:HD1   | 1:28:A:ILE:HD11 | 11       | 0.18          |
| (1,1331) | 1:78:A:TYR:HE1   | 1:84:A:TYR:HD1  | 14       | 0.18          |
| (1,1325) | 1:53:A:PHE:HE1   | 1:75:A:LEU:HB3  | 8        | 0.18          |
| (1,1321) | 1:124:A:VAL:HG12 | 1:125:A:GLN:H   | 8        | 0.18          |
| (1,1315) | 1:95:A:VAL:HG22  | 1:97:A:LEU:HD22 | 8        | 0.18          |
| (1,1253) | 1:47:A:PRO:HB3   | 1:87:A:GLY:HA2  | 6        | 0.18          |
| (1,1253) | 1:47:A:PRO:HB3   | 1:87:A:GLY:HA2  | 11       | 0.18          |
| (1,1253) | 1:47:A:PRO:HB3   | 1:87:A:GLY:HA2  | 14       | 0.18          |
| (1,1239) | 1:79:A:THR:H     | 1:78:A:TYR:HE1  | 2        | 0.18          |
| (1,1206) | 1:117:A:LEU:HD13 | 1:86:A:TYR:HB2  | 1        | 0.18          |
| (1,1167) | 1:34:A:ARG:HB3   | 1:30:A:PHE:HD1  | 5        | 0.18          |
| (1,1167) | 1:34:A:ARG:HB3   | 1:30:A:PHE:HD1  | 6        | 0.18          |
| (1,1136) | 1:31:A:LEU:HD11  | 1:35:A:PHE:HD2  | 17       | 0.18          |
| (1,1126) | 1:86:A:TYR:HE1   | 1:86:A:TYR:HB3  | 1        | 0.18          |
| (1,1108) | 1:56:A:LEU:HD13  | 1:52:A:ILE:HG12 | 2        | 0.18          |
| (1,1108) | 1:56:A:LEU:HD13  | 1:52:A:ILE:HG12 | 3        | 0.18          |
| (1,1080) | 1:105:A:LEU:HD11 | 1:92:A:ALA:H    | 5        | 0.18          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1074) | 1:34:A:ARG:HG2   | 1:35:A:PHE:HD2   | 5        | 0.18          |
| (1,1073) | 1:97:A:LEU:HD13  | 1:97:A:LEU:H     | 9        | 0.18          |
| (1,1049) | 1:59:A:ARG:HB2   | 1:60:A:VAL:HG12  | 10       | 0.18          |
| (1,1049) | 1:59:A:ARG:HB2   | 1:60:A:VAL:HG11  | 17       | 0.18          |
| (1,993)  | 1:79:A:THR:HG22  | 1:75:A:LEU:HA    | 12       | 0.18          |
| (1,853)  | 1:65:A:ASN:HB2   | 1:65:A:ASN:HD21  | 11       | 0.18          |
| (1,838)  | 1:64:A:MET:HE1   | 1:30:A:PHE:HD1   | 10       | 0.18          |
| (1,830)  | 1:129:A:ALA:HB3  | 1:127:A:GLN:HB3  | 15       | 0.18          |
| (1,635)  | 1:127:A:GLN:H    | 1:127:A:GLN:HB3  | 3        | 0.18          |
| (1,635)  | 1:127:A:GLN:H    | 1:127:A:GLN:HB3  | 7        | 0.18          |
| (1,614)  | 1:97:A:LEU:HD13  | 1:97:A:LEU:H     | 9        | 0.18          |
| (1,580)  | 1:98:A:ASP:HB2   | 1:100:A:ASN:HD21 | 14       | 0.18          |
| (1,580)  | 1:98:A:ASP:HB2   | 1:100:A:ASN:HD21 | 16       | 0.18          |
| (1,557)  | 1:66:A:LEU:HB2   | 1:70:A:GLN:HE22  | 15       | 0.18          |
| (1,549)  | 1:97:A:LEU:HD12  | 1:98:A:ASP:H     | 17       | 0.18          |
| (1,527)  | 1:65:A:ASN:HB3   | 1:65:A:ASN:HD21  | 1        | 0.18          |
| (1,527)  | 1:65:A:ASN:HB3   | 1:65:A:ASN:HD21  | 11       | 0.18          |
| (1,523)  | 1:21:A:LEU:HA    | 1:22:A:ASN:HD22  | 1        | 0.18          |
| (1,512)  | 1:13:A:ASP:HB2   | 1:13:A:ASP:H     | 2        | 0.18          |
| (1,512)  | 1:13:A:ASP:HB2   | 1:13:A:ASP:H     | 7        | 0.18          |
| (1,512)  | 1:13:A:ASP:HB2   | 1:13:A:ASP:H     | 8        | 0.18          |
| (1,477)  | 1:31:A:LEU:H     | 1:31:A:LEU:HD13  | 3        | 0.18          |
| (1,477)  | 1:31:A:LEU:H     | 1:31:A:LEU:HD11  | 15       | 0.18          |
| (1,451)  | 1:32:A:ALA:HB1   | 1:35:A:PHE:H     | 1        | 0.18          |
| (1,397)  | 1:57:A:VAL:H     | 1:56:A:LEU:HB3   | 2        | 0.18          |
| (1,397)  | 1:57:A:VAL:H     | 1:56:A:LEU:HB3   | 15       | 0.18          |
| (1,397)  | 1:57:A:VAL:H     | 1:56:A:LEU:HB3   | 16       | 0.18          |
| (1,311)  | 1:79:A:THR:H     | 1:77:A:LEU:HB2   | 14       | 0.18          |
| (1,263)  | 1:110:A:VAL:HG22 | 1:91:A:GLY:H     | 11       | 0.18          |
| (1,241)  | 1:95:A:VAL:HG11  | 1:96:A:ASP:H     | 16       | 0.18          |
| (1,134)  | 1:123:A:ARG:H    | 1:121:A:LYS:H    | 1        | 0.18          |
| (1,100)  | 1:35:A:PHE:HE1   | 1:35:A:PHE:H     | 8        | 0.18          |
| (1,100)  | 1:35:A:PHE:HE1   | 1:35:A:PHE:H     | 13       | 0.18          |
| (1,80)   | 1:30:A:PHE:HD2   | 1:30:A:PHE:H     | 6        | 0.18          |
| (1,80)   | 1:30:A:PHE:HD2   | 1:30:A:PHE:H     | 8        | 0.18          |
| (1,80)   | 1:30:A:PHE:HD1   | 1:30:A:PHE:H     | 13       | 0.18          |
| (1,56)   | 1:84:A:TYR:H     | 1:84:A:TYR:HD2   | 5        | 0.18          |
| (1,56)   | 1:84:A:TYR:H     | 1:84:A:TYR:HD2   | 10       | 0.18          |
| (1,56)   | 1:84:A:TYR:H     | 1:84:A:TYR:HD2   | 11       | 0.18          |
| (1,56)   | 1:84:A:TYR:H     | 1:84:A:TYR:HD2   | 14       | 0.18          |
| (3,122)  | 1:27:A:VAL:HG21  | 1:28:A:ILE:HD11  | 5        | 0.17          |
| (3,122)  | 1:27:A:VAL:HG21  | 1:28:A:ILE:HD12  | 15       | 0.17          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (3,111)  | 1:111:A:GLU:HG2 | 1:112:A:HIS:HA   | 17       | 0.17          |
| (3,106)  | 1:68:A:LYS:HD2  | 1:68:A:LYS:HA    | 7        | 0.17          |
| (3,106)  | 1:68:A:LYS:HD2  | 1:68:A:LYS:HA    | 15       | 0.17          |
| (3,94)   | 1:56:A:LEU:HB2  | 1:75:A:LEU:HD13  | 3        | 0.17          |
| (3,94)   | 1:56:A:LEU:HB2  | 1:75:A:LEU:HD12  | 11       | 0.17          |
| (3,92)   | 1:88:A:VAL:HG23 | 1:87:A:GLY:HA2   | 15       | 0.17          |
| (3,81)   | 1:77:A:LEU:HA   | 1:77:A:LEU:HD11  | 1        | 0.17          |
| (3,34)   | 1:97:A:LEU:HD21 | 1:31:A:LEU:HD12  | 4        | 0.17          |
| (3,14)   | 1:82:A:TRP:HA   | 1:85:A:LEU:HB2   | 3        | 0.17          |
| (1,4345) | 1:117:A:LEU:HA  | 1:121:A:LYS:H    | 14       | 0.17          |
| (1,4344) | 1:120:A:ALA:H   | 1:119:A:GLU:HG2  | 14       | 0.17          |
| (1,4343) | 1:118:A:GLU:H   | 1:119:A:GLU:H    | 6        | 0.17          |
| (1,4343) | 1:118:A:GLU:H   | 1:119:A:GLU:H    | 16       | 0.17          |
| (1,4326) | 1:65:A:ASN:HA   | 1:66:A:LEU:H     | 4        | 0.17          |
| (1,4325) | 1:62:A:GLY:HA3  | 1:66:A:LEU:H     | 5        | 0.17          |
| (1,4325) | 1:62:A:GLY:HA3  | 1:66:A:LEU:H     | 11       | 0.17          |
| (1,4323) | 1:62:A:GLY:H    | 1:68:A:LYS:HD2   | 4        | 0.17          |
| (1,4320) | 1:62:A:GLY:H    | 1:66:A:LEU:H     | 15       | 0.17          |
| (1,4317) | 1:93:A:THR:HB   | 1:102:A:CYS:H    | 4        | 0.17          |
| (1,4317) | 1:93:A:THR:HB   | 1:102:A:CYS:H    | 5        | 0.17          |
| (1,4317) | 1:93:A:THR:HB   | 1:102:A:CYS:H    | 15       | 0.17          |
| (1,4316) | 1:95:A:VAL:H    | 1:94:A:ARG:HB3   | 11       | 0.17          |
| (1,4316) | 1:95:A:VAL:H    | 1:94:A:ARG:HB3   | 17       | 0.17          |
| (1,4301) | 1:97:A:LEU:HB2  | 1:97:A:LEU:H     | 10       | 0.17          |
| (1,4301) | 1:97:A:LEU:HB2  | 1:97:A:LEU:H     | 12       | 0.17          |
| (1,4300) | 1:92:A:ALA:H    | 1:105:A:LEU:HD22 | 7        | 0.17          |
| (1,4270) | 1:75:A:LEU:HB3  | 1:74:A:ALA:H     | 14       | 0.17          |
| (1,4225) | 1:122:A:ALA:HB3 | 1:123:A:ARG:H    | 5        | 0.17          |
| (1,4212) | 1:115:A:LYS:HE3 | 1:115:A:LYS:H    | 11       | 0.17          |
| (1,4212) | 1:115:A:LYS:HE3 | 1:115:A:LYS:H    | 12       | 0.17          |
| (1,4202) | 1:127:A:GLN:H   | 1:127:A:GLN:HB3  | 1        | 0.17          |
| (1,4202) | 1:127:A:GLN:H   | 1:127:A:GLN:HB3  | 2        | 0.17          |
| (1,4198) | 1:127:A:GLN:HA  | 1:127:A:GLN:H    | 4        | 0.17          |
| (1,4193) | 1:69:A:THR:HB   | 1:72:A:ARG:H     | 4        | 0.17          |
| (1,4193) | 1:69:A:THR:HB   | 1:72:A:ARG:H     | 5        | 0.17          |
| (1,4193) | 1:69:A:THR:HB   | 1:72:A:ARG:H     | 7        | 0.17          |
| (1,4193) | 1:69:A:THR:HB   | 1:72:A:ARG:H     | 12       | 0.17          |
| (1,4193) | 1:69:A:THR:HB   | 1:72:A:ARG:H     | 16       | 0.17          |
| (1,4193) | 1:69:A:THR:HB   | 1:72:A:ARG:H     | 17       | 0.17          |
| (1,4170) | 1:49:A:LYS:HB2  | 1:49:A:LYS:H     | 15       | 0.17          |
| (1,4153) | 1:18:A:GLN:HB3  | 1:18:A:GLN:H     | 8        | 0.17          |
| (1,4150) | 1:17:A:ASN:HB3  | 1:18:A:GLN:H     | 17       | 0.17          |

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| Key      | Atom-1           | Atom-2         | Model ID | Violation (Å) |
|----------|------------------|----------------|----------|---------------|
| (1,4143) | 1:37:A:HIS:HA    | 1:39:A:PHE:H   | 6        | 0.17          |
| (1,4133) | 1:82:A:TRP:HE1   | 1:82:A:TRP:HD1 | 1        | 0.17          |
| (1,4133) | 1:82:A:TRP:HE1   | 1:82:A:TRP:HD1 | 3        | 0.17          |
| (1,4133) | 1:82:A:TRP:HE1   | 1:82:A:TRP:HD1 | 7        | 0.17          |
| (1,4133) | 1:82:A:TRP:HE1   | 1:82:A:TRP:HD1 | 8        | 0.17          |
| (1,4133) | 1:82:A:TRP:HE1   | 1:82:A:TRP:HD1 | 15       | 0.17          |
| (1,4127) | 1:34:A:ARG:HE    | 1:30:A:PHE:HD2 | 14       | 0.17          |
| (1,4069) | 1:13:A:ASP:HB2   | 1:13:A:ASP:H   | 4        | 0.17          |
| (1,4019) | 1:33:A:GLU:HB3   | 1:34:A:ARG:H   | 1        | 0.17          |
| (1,4019) | 1:33:A:GLU:HB3   | 1:34:A:ARG:H   | 14       | 0.17          |
| (1,4016) | 1:15:A:MET:HA    | 1:15:A:MET:H   | 1        | 0.17          |
| (1,4016) | 1:15:A:MET:HA    | 1:15:A:MET:H   | 3        | 0.17          |
| (1,4016) | 1:15:A:MET:HA    | 1:15:A:MET:H   | 10       | 0.17          |
| (1,3979) | 1:50:A:ILE:HA    | 1:51:A:GLY:H   | 2        | 0.17          |
| (1,3979) | 1:50:A:ILE:HA    | 1:51:A:GLY:H   | 8        | 0.17          |
| (1,3961) | 1:57:A:VAL:H     | 1:56:A:LEU:HB3 | 5        | 0.17          |
| (1,3961) | 1:57:A:VAL:H     | 1:56:A:LEU:HB3 | 9        | 0.17          |
| (1,3935) | 1:63:A:GLU:HB3   | 1:65:A:ASN:H   | 6        | 0.17          |
| (1,3935) | 1:63:A:GLU:HB3   | 1:65:A:ASN:H   | 13       | 0.17          |
| (1,3935) | 1:63:A:GLU:HB3   | 1:65:A:ASN:H   | 16       | 0.17          |
| (1,3933) | 1:65:A:ASN:HB2   | 1:65:A:ASN:H   | 3        | 0.17          |
| (1,3917) | 1:74:A:ALA:HA    | 1:75:A:LEU:H   | 3        | 0.17          |
| (1,3917) | 1:74:A:ALA:HA    | 1:75:A:LEU:H   | 4        | 0.17          |
| (1,3917) | 1:74:A:ALA:HA    | 1:75:A:LEU:H   | 7        | 0.17          |
| (1,3917) | 1:74:A:ALA:HA    | 1:75:A:LEU:H   | 10       | 0.17          |
| (1,3917) | 1:74:A:ALA:HA    | 1:75:A:LEU:H   | 12       | 0.17          |
| (1,3917) | 1:74:A:ALA:HA    | 1:75:A:LEU:H   | 13       | 0.17          |
| (1,3916) | 1:71:A:LEU:HA    | 1:74:A:ALA:H   | 3        | 0.17          |
| (1,3916) | 1:71:A:LEU:HA    | 1:74:A:ALA:H   | 6        | 0.17          |
| (1,3916) | 1:71:A:LEU:HA    | 1:74:A:ALA:H   | 17       | 0.17          |
| (1,3907) | 1:76:A:ARG:HD2   | 1:77:A:LEU:H   | 1        | 0.17          |
| (1,3907) | 1:76:A:ARG:HD2   | 1:77:A:LEU:H   | 2        | 0.17          |
| (1,3887) | 1:81:A:SER:HB2   | 1:82:A:TRP:H   | 11       | 0.17          |
| (1,3861) | 1:110:A:VAL:HG21 | 1:91:A:GLY:H   | 6        | 0.17          |
| (1,3830) | 1:101:A:PRO:HD3  | 1:100:A:ASN:H  | 5        | 0.17          |
| (1,3830) | 1:101:A:PRO:HD3  | 1:100:A:ASN:H  | 8        | 0.17          |
| (1,3830) | 1:101:A:PRO:HD3  | 1:100:A:ASN:H  | 10       | 0.17          |
| (1,3798) | 1:43:A:GLY:HA3   | 1:44:A:GLU:H   | 15       | 0.17          |
| (1,3781) | 1:119:A:GLU:HA   | 1:119:A:GLU:H  | 2        | 0.17          |
| (1,3781) | 1:119:A:GLU:HA   | 1:119:A:GLU:H  | 13       | 0.17          |
| (1,3781) | 1:119:A:GLU:HA   | 1:119:A:GLU:H  | 17       | 0.17          |
| (1,3768) | 1:130:A:GLU:H    | 1:130:A:GLU:HA | 11       | 0.17          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3768) | 1:130:A:GLU:H    | 1:130:A:GLU:HA  | 13       | 0.17          |
| (1,3744) | 1:35:A:PHE:HD2   | 1:39:A:PHE:H    | 10       | 0.17          |
| (1,3744) | 1:35:A:PHE:HD2   | 1:39:A:PHE:H    | 15       | 0.17          |
| (1,3698) | 1:30:A:PHE:HD1   | 1:30:A:PHE:H    | 1        | 0.17          |
| (1,3698) | 1:30:A:PHE:HD2   | 1:30:A:PHE:H    | 10       | 0.17          |
| (1,3698) | 1:30:A:PHE:HD1   | 1:30:A:PHE:H    | 12       | 0.17          |
| (1,3698) | 1:30:A:PHE:HD1   | 1:30:A:PHE:H    | 14       | 0.17          |
| (1,3673) | 1:49:A:LYS:H     | 1:50:A:ILE:H    | 1        | 0.17          |
| (1,3673) | 1:49:A:LYS:H     | 1:50:A:ILE:H    | 10       | 0.17          |
| (1,3673) | 1:49:A:LYS:H     | 1:50:A:ILE:H    | 14       | 0.17          |
| (1,3673) | 1:49:A:LYS:H     | 1:50:A:ILE:H    | 15       | 0.17          |
| (1,3595) | 1:108:A:GLN:HA   | 1:111:A:GLU:HB3 | 15       | 0.17          |
| (1,3591) | 1:93:A:THR:HB    | 1:88:A:VAL:HG12 | 8        | 0.17          |
| (1,3591) | 1:93:A:THR:HB    | 1:88:A:VAL:HG12 | 12       | 0.17          |
| (1,3583) | 1:112:A:HIS:H    | 1:109:A:HIS:HA  | 1        | 0.17          |
| (1,3582) | 1:110:A:VAL:H    | 1:109:A:HIS:HA  | 10       | 0.17          |
| (1,3582) | 1:110:A:VAL:H    | 1:109:A:HIS:HA  | 17       | 0.17          |
| (1,3539) | 1:63:A:GLU:HG3   | 1:63:A:GLU:H    | 15       | 0.17          |
| (1,3537) | 1:51:A:GLY:HA2   | 1:54:A:GLN:HB2  | 6        | 0.17          |
| (1,3537) | 1:51:A:GLY:HA2   | 1:54:A:GLN:HB2  | 7        | 0.17          |
| (1,3537) | 1:51:A:GLY:HA2   | 1:54:A:GLN:HB2  | 13       | 0.17          |
| (1,3536) | 1:66:A:LEU:HB3   | 1:62:A:GLY:HA3  | 15       | 0.17          |
| (1,3520) | 1:100:A:ASN:HD22 | 1:98:A:ASP:HB3  | 10       | 0.17          |
| (1,3520) | 1:100:A:ASN:HD22 | 1:98:A:ASP:HB3  | 12       | 0.17          |
| (1,3519) | 1:65:A:ASN:H     | 1:65:A:ASN:HB3  | 11       | 0.17          |
| (1,3515) | 1:102:A:CYS:HB3  | 1:49:A:LYS:HA   | 1        | 0.17          |
| (1,3506) | 1:60:A:VAL:HG12  | 1:35:A:PHE:HZ   | 1        | 0.17          |
| (1,3506) | 1:60:A:VAL:HG13  | 1:35:A:PHE:HZ   | 14       | 0.17          |
| (1,3502) | 1:27:A:VAL:HG21  | 1:27:A:VAL:H    | 7        | 0.17          |
| (1,3501) | 1:27:A:VAL:HG23  | 1:28:A:ILE:HA   | 9        | 0.17          |
| (1,3500) | 1:27:A:VAL:HG23  | 1:31:A:LEU:HD12 | 9        | 0.17          |
| (1,3497) | 1:27:A:VAL:HA    | 1:27:A:VAL:HG11 | 8        | 0.17          |
| (1,3479) | 1:45:A:ALA:HB1   | 1:44:A:GLU:HB3  | 16       | 0.17          |
| (1,3477) | 1:15:A:MET:HG3   | 1:15:A:MET:HB2  | 7        | 0.17          |
| (1,3477) | 1:15:A:MET:HG3   | 1:15:A:MET:HB2  | 17       | 0.17          |
| (1,3476) | 1:107:A:GLU:HG2  | 1:108:A:GLN:H   | 15       | 0.17          |
| (1,3457) | 1:20:A:LYS:HE3   | 1:19:A:PRO:HA   | 15       | 0.17          |
| (1,3441) | 1:21:A:LEU:HG    | 1:21:A:LEU:HB3  | 5        | 0.17          |
| (1,3441) | 1:21:A:LEU:HG    | 1:21:A:LEU:HB3  | 10       | 0.17          |
| (1,3441) | 1:21:A:LEU:HG    | 1:21:A:LEU:HB3  | 14       | 0.17          |
| (1,3441) | 1:21:A:LEU:HG    | 1:21:A:LEU:HB3  | 17       | 0.17          |
| (1,3436) | 1:64:A:MET:HE3   | 1:21:A:LEU:HD11 | 9        | 0.17          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3422) | 1:77:A:LEU:HG   | 1:77:A:LEU:HD22  | 3        | 0.17          |
| (1,3422) | 1:77:A:LEU:HG   | 1:77:A:LEU:HD22  | 13       | 0.17          |
| (1,3415) | 1:117:A:LEU:HA  | 1:117:A:LEU:HD12 | 12       | 0.17          |
| (1,3412) | 1:82:A:TRP:HZ3  | 1:117:A:LEU:HD12 | 1        | 0.17          |
| (1,3412) | 1:82:A:TRP:HZ3  | 1:117:A:LEU:HD13 | 8        | 0.17          |
| (1,3398) | 1:117:A:LEU:HA  | 1:120:A:ALA:HB1  | 15       | 0.17          |
| (1,3396) | 1:71:A:LEU:HA   | 1:74:A:ALA:HB2   | 11       | 0.17          |
| (1,3396) | 1:71:A:LEU:HA   | 1:74:A:ALA:HB2   | 12       | 0.17          |
| (1,3395) | 1:33:A:GLU:HB3  | 1:33:A:GLU:HA    | 16       | 0.17          |
| (1,3378) | 1:67:A:SER:HB3  | 1:66:A:LEU:HA    | 2        | 0.17          |
| (1,3378) | 1:67:A:SER:HB3  | 1:66:A:LEU:HA    | 3        | 0.17          |
| (1,3378) | 1:67:A:SER:HB3  | 1:66:A:LEU:HA    | 6        | 0.17          |
| (1,3378) | 1:67:A:SER:HB3  | 1:66:A:LEU:HA    | 7        | 0.17          |
| (1,3378) | 1:67:A:SER:HB3  | 1:66:A:LEU:HA    | 10       | 0.17          |
| (1,3378) | 1:67:A:SER:HB3  | 1:66:A:LEU:HA    | 11       | 0.17          |
| (1,3378) | 1:67:A:SER:HB3  | 1:66:A:LEU:HA    | 15       | 0.17          |
| (1,3378) | 1:67:A:SER:HB3  | 1:66:A:LEU:HA    | 16       | 0.17          |
| (1,3322) | 1:30:A:PHE:HD2  | 1:66:A:LEU:HD23  | 3        | 0.17          |
| (1,3322) | 1:30:A:PHE:HD1  | 1:66:A:LEU:HD22  | 17       | 0.17          |
| (1,3320) | 1:27:A:VAL:HA   | 1:66:A:LEU:HD22  | 8        | 0.17          |
| (1,3315) | 1:66:A:LEU:HD12 | 1:66:A:LEU:HA    | 3        | 0.17          |
| (1,3314) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HG    | 10       | 0.17          |
| (1,3306) | 1:128:A:ARG:HG2 | 1:128:A:ARG:HD2  | 1        | 0.17          |
| (1,3299) | 1:20:A:LYS:H    | 1:20:A:LYS:HD3   | 17       | 0.17          |
| (1,3270) | 1:42:A:GLU:HG2  | 1:41:A:ALA:HB1   | 6        | 0.17          |
| (1,3264) | 1:121:A:LYS:HG2 | 1:121:A:LYS:H    | 2        | 0.17          |
| (1,3255) | 1:40:A:SER:HA   | 1:41:A:ALA:HB1   | 13       | 0.17          |
| (1,3250) | 1:41:A:ALA:HA   | 1:41:A:ALA:HB1   | 4        | 0.17          |
| (1,3250) | 1:41:A:ALA:HA   | 1:41:A:ALA:HB3   | 5        | 0.17          |
| (1,3241) | 1:52:A:ILE:HG13 | 1:97:A:LEU:HD21  | 9        | 0.17          |
| (1,3241) | 1:52:A:ILE:HG13 | 1:97:A:LEU:HD23  | 12       | 0.17          |
| (1,3241) | 1:52:A:ILE:HG13 | 1:97:A:LEU:HD21  | 13       | 0.17          |
| (1,3241) | 1:52:A:ILE:HG13 | 1:97:A:LEU:HD23  | 17       | 0.17          |
| (1,3240) | 1:52:A:ILE:HG13 | 1:48:A:LEU:HD12  | 14       | 0.17          |
| (1,3232) | 1:92:A:ALA:H    | 1:105:A:LEU:HB2  | 4        | 0.17          |
| (1,3232) | 1:92:A:ALA:H    | 1:105:A:LEU:HB2  | 10       | 0.17          |
| (1,3232) | 1:92:A:ALA:H    | 1:105:A:LEU:HB2  | 12       | 0.17          |
| (1,3232) | 1:92:A:ALA:H    | 1:105:A:LEU:HB2  | 13       | 0.17          |
| (1,3232) | 1:92:A:ALA:H    | 1:105:A:LEU:HB2  | 16       | 0.17          |
| (1,3230) | 1:68:A:LYS:HB2  | 1:68:A:LYS:HA    | 16       | 0.17          |
| (1,3210) | 1:128:A:ARG:HA  | 1:128:A:ARG:HB3  | 14       | 0.17          |
| (1,3200) | 1:116:A:GLN:HG3 | 1:113:A:ALA:HB2  | 8        | 0.17          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3200) | 1:116:A:GLN:HG3 | 1:113:A:ALA:HB2 | 14       | 0.17          |
| (1,3197) | 1:87:A:GLY:HA3  | 1:113:A:ALA:HB1 | 2        | 0.17          |
| (1,3197) | 1:87:A:GLY:HA3  | 1:113:A:ALA:HB1 | 11       | 0.17          |
| (1,3197) | 1:87:A:GLY:HA3  | 1:113:A:ALA:HB3 | 14       | 0.17          |
| (1,3197) | 1:87:A:GLY:HA3  | 1:113:A:ALA:HB1 | 15       | 0.17          |
| (1,3197) | 1:87:A:GLY:HA3  | 1:113:A:ALA:HB1 | 16       | 0.17          |
| (1,3185) | 1:109:A:HIS:HB2 | 1:108:A:GLN:H   | 3        | 0.17          |
| (1,3185) | 1:109:A:HIS:HB2 | 1:108:A:GLN:H   | 14       | 0.17          |
| (1,3160) | 1:74:A:ALA:HB3  | 1:74:A:ALA:HA   | 3        | 0.17          |
| (1,3160) | 1:74:A:ALA:HB1  | 1:74:A:ALA:HA   | 5        | 0.17          |
| (1,3160) | 1:74:A:ALA:HB1  | 1:74:A:ALA:HA   | 17       | 0.17          |
| (1,3134) | 1:15:A:MET:HB2  | 1:15:A:MET:HG2  | 15       | 0.17          |
| (1,3130) | 1:123:A:ARG:HG2 | 1:123:A:ARG:H   | 8        | 0.17          |
| (1,3130) | 1:123:A:ARG:HG2 | 1:123:A:ARG:H   | 12       | 0.17          |
| (1,3068) | 1:52:A:ILE:HG21 | 1:53:A:PHE:HB2  | 2        | 0.17          |
| (1,3059) | 1:28:A:ILE:HB   | 1:28:A:ILE:HG21 | 7        | 0.17          |
| (1,3053) | 1:29:A:ALA:H    | 1:28:A:ILE:HG21 | 2        | 0.17          |
| (1,3053) | 1:29:A:ALA:H    | 1:28:A:ILE:HG23 | 5        | 0.17          |
| (1,3053) | 1:29:A:ALA:H    | 1:28:A:ILE:HG22 | 9        | 0.17          |
| (1,3053) | 1:29:A:ALA:H    | 1:28:A:ILE:HG22 | 11       | 0.17          |
| (1,3053) | 1:29:A:ALA:H    | 1:28:A:ILE:HG21 | 12       | 0.17          |
| (1,3053) | 1:29:A:ALA:H    | 1:28:A:ILE:HG23 | 16       | 0.17          |
| (1,3052) | 1:39:A:PHE:HZ   | 1:52:A:ILE:HG21 | 5        | 0.17          |
| (1,3040) | 1:52:A:ILE:HA   | 1:52:A:ILE:HG12 | 6        | 0.17          |
| (1,3032) | 1:121:A:LYS:HG3 | 1:121:A:LYS:HE3 | 3        | 0.17          |
| (1,3032) | 1:121:A:LYS:HG3 | 1:121:A:LYS:HE3 | 5        | 0.17          |
| (1,3032) | 1:121:A:LYS:HG3 | 1:121:A:LYS:HE3 | 12       | 0.17          |
| (1,3019) | 1:64:A:MET:HE3  | 1:66:A:LEU:H    | 14       | 0.17          |
| (1,3000) | 1:57:A:VAL:HA   | 1:60:A:VAL:HB   | 14       | 0.17          |
| (1,2995) | 1:60:A:VAL:H    | 1:60:A:VAL:HB   | 2        | 0.17          |
| (1,2995) | 1:60:A:VAL:H    | 1:60:A:VAL:HB   | 8        | 0.17          |
| (1,2995) | 1:60:A:VAL:H    | 1:60:A:VAL:HB   | 10       | 0.17          |
| (1,2995) | 1:60:A:VAL:H    | 1:60:A:VAL:HB   | 12       | 0.17          |
| (1,2995) | 1:60:A:VAL:H    | 1:60:A:VAL:HB   | 14       | 0.17          |
| (1,2995) | 1:60:A:VAL:H    | 1:60:A:VAL:HB   | 17       | 0.17          |
| (1,2992) | 1:20:A:LYS:HB3  | 1:20:A:LYS:H    | 9        | 0.17          |
| (1,2992) | 1:20:A:LYS:HB3  | 1:20:A:LYS:H    | 15       | 0.17          |
| (1,2992) | 1:20:A:LYS:HB3  | 1:20:A:LYS:H    | 17       | 0.17          |
| (1,2979) | 1:53:A:PHE:HZ   | 1:68:A:LYS:HB2  | 17       | 0.17          |
| (1,2969) | 1:93:A:THR:HG23 | 1:101:A:PRO:HB3 | 3        | 0.17          |
| (1,2960) | 1:77:A:LEU:HD13 | 1:25:A:LYS:HA   | 5        | 0.17          |
| (1,2960) | 1:77:A:LEU:HD12 | 1:25:A:LYS:HA   | 17       | 0.17          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2950) | 1:75:A:LEU:HD12  | 1:75:A:LEU:H    | 4        | 0.17          |
| (1,2950) | 1:75:A:LEU:HD13  | 1:75:A:LEU:H    | 12       | 0.17          |
| (1,2937) | 1:95:A:VAL:HG21  | 1:95:A:VAL:HG12 | 8        | 0.17          |
| (1,2893) | 1:50:A:ILE:HB    | 1:50:A:ILE:HG22 | 14       | 0.17          |
| (1,2881) | 1:74:A:ALA:HB3   | 1:31:A:LEU:HD12 | 5        | 0.17          |
| (1,2871) | 1:129:A:ALA:HB3  | 1:129:A:ALA:H   | 10       | 0.17          |
| (1,2855) | 1:78:A:TYR:HD2   | 1:28:A:ILE:HD12 | 4        | 0.17          |
| (1,2855) | 1:78:A:TYR:HD2   | 1:28:A:ILE:HD13 | 8        | 0.17          |
| (1,2855) | 1:78:A:TYR:HD2   | 1:28:A:ILE:HD13 | 13       | 0.17          |
| (1,2840) | 1:124:A:VAL:HG13 | 1:125:A:GLN:H   | 3        | 0.17          |
| (1,2840) | 1:124:A:VAL:HG13 | 1:125:A:GLN:H   | 7        | 0.17          |
| (1,2840) | 1:124:A:VAL:HG11 | 1:125:A:GLN:H   | 14       | 0.17          |
| (1,2840) | 1:124:A:VAL:HG11 | 1:125:A:GLN:H   | 17       | 0.17          |
| (1,2836) | 1:95:A:VAL:HG23  | 1:97:A:LEU:HD22 | 11       | 0.17          |
| (1,2804) | 1:66:A:LEU:HB3   | 1:60:A:VAL:HB   | 1        | 0.17          |
| (1,2804) | 1:66:A:LEU:HB3   | 1:60:A:VAL:HB   | 2        | 0.17          |
| (1,2804) | 1:66:A:LEU:HB3   | 1:60:A:VAL:HB   | 4        | 0.17          |
| (1,2804) | 1:66:A:LEU:HB3   | 1:60:A:VAL:HB   | 8        | 0.17          |
| (1,2804) | 1:66:A:LEU:HB3   | 1:60:A:VAL:HB   | 10       | 0.17          |
| (1,2804) | 1:66:A:LEU:HB3   | 1:60:A:VAL:HB   | 12       | 0.17          |
| (1,2804) | 1:66:A:LEU:HB3   | 1:60:A:VAL:HB   | 16       | 0.17          |
| (1,2774) | 1:91:A:GLY:HA3   | 1:90:A:PRO:HB2  | 1        | 0.17          |
| (1,2774) | 1:91:A:GLY:HA3   | 1:90:A:PRO:HB2  | 3        | 0.17          |
| (1,2767) | 1:43:A:GLY:HA2   | 1:44:A:GLU:H    | 17       | 0.17          |
| (1,2754) | 1:60:A:VAL:HG12  | 1:59:A:ARG:HD3  | 3        | 0.17          |
| (1,2754) | 1:60:A:VAL:HG11  | 1:59:A:ARG:HD3  | 4        | 0.17          |
| (1,2754) | 1:60:A:VAL:HG11  | 1:59:A:ARG:HD3  | 9        | 0.17          |
| (1,2754) | 1:60:A:VAL:HG11  | 1:59:A:ARG:HD3  | 13       | 0.17          |
| (1,2753) | 1:97:A:LEU:HD12  | 1:59:A:ARG:HD3  | 8        | 0.17          |
| (1,2712) | 1:39:A:PHE:HB3   | 1:35:A:PHE:HB3  | 2        | 0.17          |
| (1,2712) | 1:39:A:PHE:HB3   | 1:35:A:PHE:HB3  | 4        | 0.17          |
| (1,2712) | 1:39:A:PHE:HB3   | 1:35:A:PHE:HB3  | 5        | 0.17          |
| (1,2712) | 1:39:A:PHE:HB3   | 1:35:A:PHE:HB3  | 9        | 0.17          |
| (1,2712) | 1:39:A:PHE:HB3   | 1:35:A:PHE:HB3  | 10       | 0.17          |
| (1,2712) | 1:39:A:PHE:HB3   | 1:35:A:PHE:HB3  | 11       | 0.17          |
| (1,2712) | 1:39:A:PHE:HB3   | 1:35:A:PHE:HB3  | 15       | 0.17          |
| (1,2712) | 1:39:A:PHE:HB3   | 1:35:A:PHE:HB3  | 16       | 0.17          |
| (1,2712) | 1:39:A:PHE:HB3   | 1:35:A:PHE:HB3  | 17       | 0.17          |
| (1,2711) | 1:35:A:PHE:HB2   | 1:35:A:PHE:HE2  | 3        | 0.17          |
| (1,2711) | 1:35:A:PHE:HB2   | 1:35:A:PHE:HE2  | 10       | 0.17          |
| (1,2711) | 1:35:A:PHE:HB2   | 1:35:A:PHE:HE1  | 13       | 0.17          |
| (1,2711) | 1:35:A:PHE:HB2   | 1:35:A:PHE:HE2  | 17       | 0.17          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2694) | 1:73:A:SER:HB2   | 1:74:A:ALA:H    | 1        | 0.17          |
| (1,2694) | 1:73:A:SER:HB2   | 1:74:A:ALA:H    | 8        | 0.17          |
| (1,2672) | 1:31:A:LEU:HD12  | 1:35:A:PHE:HD2  | 7        | 0.17          |
| (1,2639) | 1:71:A:LEU:HD13  | 1:71:A:LEU:HB2  | 2        | 0.17          |
| (1,2639) | 1:71:A:LEU:HD13  | 1:71:A:LEU:HB2  | 3        | 0.17          |
| (1,2639) | 1:71:A:LEU:HD12  | 1:71:A:LEU:HB2  | 4        | 0.17          |
| (1,2639) | 1:71:A:LEU:HD11  | 1:71:A:LEU:HB2  | 6        | 0.17          |
| (1,2639) | 1:71:A:LEU:HD13  | 1:71:A:LEU:HB2  | 7        | 0.17          |
| (1,2637) | 1:71:A:LEU:HB3   | 1:71:A:LEU:HG   | 6        | 0.17          |
| (1,2637) | 1:71:A:LEU:HB3   | 1:71:A:LEU:HG   | 17       | 0.17          |
| (1,2629) | 1:53:A:PHE:HZ    | 1:71:A:LEU:HB2  | 4        | 0.17          |
| (1,2629) | 1:53:A:PHE:HZ    | 1:71:A:LEU:HB2  | 9        | 0.17          |
| (1,2629) | 1:53:A:PHE:HZ    | 1:71:A:LEU:HB2  | 11       | 0.17          |
| (1,2629) | 1:53:A:PHE:HZ    | 1:71:A:LEU:HB2  | 12       | 0.17          |
| (1,2621) | 1:105:A:LEU:HD11 | 1:92:A:ALA:H    | 2        | 0.17          |
| (1,2621) | 1:105:A:LEU:HD12 | 1:92:A:ALA:H    | 4        | 0.17          |
| (1,2621) | 1:105:A:LEU:HD13 | 1:92:A:ALA:H    | 8        | 0.17          |
| (1,2621) | 1:105:A:LEU:HD11 | 1:92:A:ALA:H    | 10       | 0.17          |
| (1,2621) | 1:105:A:LEU:HD11 | 1:92:A:ALA:H    | 12       | 0.17          |
| (1,2612) | 1:30:A:PHE:HD1   | 1:34:A:ARG:HG2  | 11       | 0.17          |
| (1,2587) | 1:68:A:LYS:HB2   | 1:69:A:THR:HG23 | 3        | 0.17          |
| (1,2530) | 1:33:A:GLU:HA    | 1:34:A:ARG:H    | 2        | 0.17          |
| (1,2530) | 1:33:A:GLU:HA    | 1:34:A:ARG:H    | 4        | 0.17          |
| (1,2530) | 1:33:A:GLU:HA    | 1:34:A:ARG:H    | 5        | 0.17          |
| (1,2530) | 1:33:A:GLU:HA    | 1:34:A:ARG:H    | 15       | 0.17          |
| (1,2529) | 1:79:A:THR:HG22  | 1:75:A:LEU:HA   | 2        | 0.17          |
| (1,2514) | 1:120:A:ALA:H    | 1:120:A:ALA:HA  | 4        | 0.17          |
| (1,2514) | 1:120:A:ALA:H    | 1:120:A:ALA:HA  | 5        | 0.17          |
| (1,2514) | 1:120:A:ALA:H    | 1:120:A:ALA:HA  | 7        | 0.17          |
| (1,2514) | 1:120:A:ALA:H    | 1:120:A:ALA:HA  | 10       | 0.17          |
| (1,2514) | 1:120:A:ALA:H    | 1:120:A:ALA:HA  | 16       | 0.17          |
| (1,2505) | 1:126:A:ALA:HA   | 1:126:A:ALA:H   | 16       | 0.17          |
| (1,2489) | 1:28:A:ILE:HA    | 1:28:A:ILE:HG23 | 2        | 0.17          |
| (1,2489) | 1:28:A:ILE:HA    | 1:28:A:ILE:HG22 | 8        | 0.17          |
| (1,2469) | 1:53:A:PHE:HZ    | 1:72:A:ARG:HG3  | 3        | 0.17          |
| (1,2469) | 1:53:A:PHE:HZ    | 1:72:A:ARG:HG3  | 7        | 0.17          |
| (1,2469) | 1:53:A:PHE:HZ    | 1:72:A:ARG:HG3  | 11       | 0.17          |
| (1,2416) | 1:45:A:ALA:HB2   | 1:45:A:ALA:H    | 8        | 0.17          |
| (1,2416) | 1:45:A:ALA:HB2   | 1:45:A:ALA:H    | 14       | 0.17          |
| (1,2408) | 1:52:A:ILE:HD13  | 1:96:A:ASP:HA   | 6        | 0.17          |
| (1,2351) | 1:110:A:VAL:HG23 | 1:109:A:HIS:HA  | 8        | 0.17          |
| (1,2351) | 1:110:A:VAL:HG21 | 1:109:A:HIS:HA  | 12       | 0.17          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2336) | 1:64:A:MET:HE3  | 1:31:A:LEU:HA   | 12       | 0.17          |
| (1,2299) | 1:55:A:ASP:HB3  | 1:96:A:ASP:HA   | 2        | 0.17          |
| (1,2299) | 1:55:A:ASP:HB3  | 1:96:A:ASP:HA   | 9        | 0.17          |
| (1,2299) | 1:55:A:ASP:HB3  | 1:96:A:ASP:HA   | 11       | 0.17          |
| (1,2299) | 1:55:A:ASP:HB3  | 1:96:A:ASP:HA   | 12       | 0.17          |
| (1,2295) | 1:121:A:LYS:HG2 | 1:121:A:LYS:HD3 | 14       | 0.17          |
| (1,2288) | 1:70:A:GLN:HA   | 1:70:A:GLN:HG3  | 6        | 0.17          |
| (1,2288) | 1:70:A:GLN:HA   | 1:70:A:GLN:HG3  | 7        | 0.17          |
| (1,2288) | 1:70:A:GLN:HA   | 1:70:A:GLN:HG3  | 11       | 0.17          |
| (1,2221) | 1:31:A:LEU:HA   | 1:60:A:VAL:HB   | 9        | 0.17          |
| (1,2197) | 1:39:A:PHE:HD1  | 1:56:A:LEU:HA   | 10       | 0.17          |
| (1,2185) | 1:53:A:PHE:H    | 1:97:A:LEU:HD21 | 11       | 0.17          |
| (1,2169) | 1:22:A:ASN:HB3  | 1:22:A:ASN:H    | 3        | 0.17          |
| (1,2169) | 1:22:A:ASN:HB3  | 1:22:A:ASN:H    | 5        | 0.17          |
| (1,2169) | 1:22:A:ASN:HB3  | 1:22:A:ASN:H    | 6        | 0.17          |
| (1,2169) | 1:22:A:ASN:HB3  | 1:22:A:ASN:H    | 15       | 0.17          |
| (1,2149) | 1:21:A:LEU:HD23 | 1:30:A:PHE:HD1  | 12       | 0.17          |
| (1,2079) | 1:66:A:LEU:HD12 | 1:62:A:GLY:H    | 1        | 0.17          |
| (1,2079) | 1:66:A:LEU:HD13 | 1:62:A:GLY:H    | 4        | 0.17          |
| (1,2052) | 1:65:A:ASN:H    | 1:66:A:LEU:H    | 16       | 0.17          |
| (1,2045) | 1:77:A:LEU:H    | 1:78:A:TYR:H    | 3        | 0.17          |
| (1,2045) | 1:77:A:LEU:H    | 1:78:A:TYR:H    | 13       | 0.17          |
| (1,2042) | 1:15:A:MET:H    | 1:16:A:GLU:H    | 4        | 0.17          |
| (1,2037) | 1:57:A:VAL:HG21 | 1:57:A:VAL:HG11 | 2        | 0.17          |
| (1,2035) | 1:52:A:ILE:HG13 | 1:97:A:LEU:HD23 | 7        | 0.17          |
| (1,2025) | 1:97:A:LEU:HD21 | 1:35:A:PHE:HD2  | 1        | 0.17          |
| (1,1939) | 1:33:A:GLU:HB3  | 1:30:A:PHE:HA   | 12       | 0.17          |
| (1,1928) | 1:105:A:LEU:HB3 | 1:109:A:HIS:HB2 | 1        | 0.17          |
| (1,1928) | 1:105:A:LEU:HB3 | 1:109:A:HIS:HB2 | 2        | 0.17          |
| (1,1928) | 1:105:A:LEU:HB3 | 1:109:A:HIS:HB2 | 8        | 0.17          |
| (1,1928) | 1:105:A:LEU:HB3 | 1:109:A:HIS:HB2 | 10       | 0.17          |
| (1,1928) | 1:105:A:LEU:HB3 | 1:109:A:HIS:HB2 | 11       | 0.17          |
| (1,1928) | 1:105:A:LEU:HB3 | 1:109:A:HIS:HB2 | 12       | 0.17          |
| (1,1928) | 1:105:A:LEU:HB3 | 1:109:A:HIS:HB2 | 13       | 0.17          |
| (1,1889) | 1:65:A:ASN:H    | 1:65:A:ASN:HB3  | 8        | 0.17          |
| (1,1885) | 1:83:A:ARG:HG3  | 1:84:A:TYR:H    | 16       | 0.17          |
| (1,1883) | 1:64:A:MET:HE1  | 1:21:A:LEU:H    | 16       | 0.17          |
| (1,1881) | 1:113:A:ALA:HB2 | 1:88:A:VAL:HA   | 8        | 0.17          |
| (1,1877) | 1:27:A:VAL:HG23 | 1:27:A:VAL:H    | 4        | 0.17          |
| (1,1877) | 1:27:A:VAL:HG22 | 1:27:A:VAL:H    | 12       | 0.17          |
| (1,1877) | 1:27:A:VAL:HG23 | 1:27:A:VAL:H    | 16       | 0.17          |
| (1,1877) | 1:27:A:VAL:HG21 | 1:27:A:VAL:H    | 17       | 0.17          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1845) | 1:95:A:VAL:HG22  | 1:96:A:ASP:HA    | 6        | 0.17          |
| (1,1845) | 1:95:A:VAL:HG23  | 1:96:A:ASP:HA    | 8        | 0.17          |
| (1,1818) | 1:118:A:GLU:HA   | 1:122:A:ALA:H    | 8        | 0.17          |
| (1,1817) | 1:77:A:LEU:HG    | 1:77:A:LEU:HD21  | 1        | 0.17          |
| (1,1817) | 1:77:A:LEU:HG    | 1:77:A:LEU:HD21  | 14       | 0.17          |
| (1,1811) | 1:86:A:TYR:H     | 1:117:A:LEU:HD12 | 14       | 0.17          |
| (1,1811) | 1:86:A:TYR:H     | 1:117:A:LEU:HD11 | 16       | 0.17          |
| (1,1801) | 1:117:A:LEU:HA   | 1:120:A:ALA:HB3  | 3        | 0.17          |
| (1,1801) | 1:117:A:LEU:HA   | 1:120:A:ALA:HB3  | 7        | 0.17          |
| (1,1801) | 1:117:A:LEU:HA   | 1:120:A:ALA:HB2  | 17       | 0.17          |
| (1,1776) | 1:88:A:VAL:HA    | 1:88:A:VAL:HG13  | 11       | 0.17          |
| (1,1775) | 1:88:A:VAL:HA    | 1:47:A:PRO:HB3   | 6        | 0.17          |
| (1,1775) | 1:88:A:VAL:HA    | 1:47:A:PRO:HB3   | 7        | 0.17          |
| (1,1775) | 1:88:A:VAL:HA    | 1:47:A:PRO:HB3   | 14       | 0.17          |
| (1,1775) | 1:88:A:VAL:HA    | 1:47:A:PRO:HB3   | 15       | 0.17          |
| (1,1753) | 1:113:A:ALA:HB2  | 1:89:A:LYS:H     | 3        | 0.17          |
| (1,1753) | 1:113:A:ALA:HB3  | 1:89:A:LYS:H     | 4        | 0.17          |
| (1,1753) | 1:113:A:ALA:HB3  | 1:89:A:LYS:H     | 15       | 0.17          |
| (1,1726) | 1:66:A:LEU:HD13  | 1:66:A:LEU:HA    | 14       | 0.17          |
| (1,1725) | 1:71:A:LEU:HD13  | 1:71:A:LEU:HG    | 16       | 0.17          |
| (1,1671) | 1:78:A:TYR:HA    | 1:28:A:ILE:HG12  | 16       | 0.17          |
| (1,1668) | 1:52:A:ILE:HG13  | 1:48:A:LEU:HD12  | 7        | 0.17          |
| (1,1638) | 1:124:A:VAL:HG11 | 1:124:A:VAL:HA   | 1        | 0.17          |
| (1,1638) | 1:124:A:VAL:HG11 | 1:124:A:VAL:HA   | 4        | 0.17          |
| (1,1638) | 1:124:A:VAL:HG11 | 1:124:A:VAL:HA   | 8        | 0.17          |
| (1,1638) | 1:124:A:VAL:HG13 | 1:124:A:VAL:HA   | 17       | 0.17          |
| (1,1629) | 1:116:A:GLN:HG3  | 1:113:A:ALA:HB2  | 10       | 0.17          |
| (1,1628) | 1:87:A:GLY:HA3   | 1:113:A:ALA:HB3  | 8        | 0.17          |
| (1,1628) | 1:87:A:GLY:HA3   | 1:113:A:ALA:HB3  | 10       | 0.17          |
| (1,1616) | 1:109:A:HIS:HB2  | 1:108:A:GLN:H    | 11       | 0.17          |
| (1,1613) | 1:124:A:VAL:HG21 | 1:121:A:LYS:HA   | 16       | 0.17          |
| (1,1588) | 1:74:A:ALA:HB1   | 1:74:A:ALA:HA    | 8        | 0.17          |
| (1,1553) | 1:57:A:VAL:HG12  | 1:61:A:ALA:H     | 9        | 0.17          |
| (1,1513) | 1:52:A:ILE:HG23  | 1:53:A:PHE:HB3   | 4        | 0.17          |
| (1,1511) | 1:28:A:ILE:HA    | 1:28:A:ILE:HG23  | 2        | 0.17          |
| (1,1511) | 1:28:A:ILE:HA    | 1:28:A:ILE:HG22  | 8        | 0.17          |
| (1,1511) | 1:28:A:ILE:HA    | 1:28:A:ILE:HG22  | 13       | 0.17          |
| (1,1511) | 1:28:A:ILE:HA    | 1:28:A:ILE:HG21  | 14       | 0.17          |
| (1,1478) | 1:64:A:MET:HE1   | 1:66:A:LEU:H     | 3        | 0.17          |
| (1,1440) | 1:105:A:LEU:H    | 1:101:A:PRO:HD3  | 1        | 0.17          |
| (1,1440) | 1:105:A:LEU:H    | 1:101:A:PRO:HD3  | 2        | 0.17          |
| (1,1440) | 1:105:A:LEU:H    | 1:101:A:PRO:HD3  | 6        | 0.17          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1440) | 1:105:A:LEU:H    | 1:101:A:PRO:HD3 | 8        | 0.17          |
| (1,1440) | 1:105:A:LEU:H    | 1:101:A:PRO:HD3 | 9        | 0.17          |
| (1,1440) | 1:105:A:LEU:H    | 1:101:A:PRO:HD3 | 13       | 0.17          |
| (1,1440) | 1:105:A:LEU:H    | 1:101:A:PRO:HD3 | 17       | 0.17          |
| (1,1412) | 1:39:A:PHE:HZ    | 1:75:A:LEU:HD12 | 2        | 0.17          |
| (1,1412) | 1:39:A:PHE:HZ    | 1:75:A:LEU:HD13 | 4        | 0.17          |
| (1,1410) | 1:110:A:VAL:HG21 | 1:108:A:GLN:H   | 3        | 0.17          |
| (1,1409) | 1:57:A:VAL:HG21  | 1:57:A:VAL:HG11 | 2        | 0.17          |
| (1,1409) | 1:57:A:VAL:HG23  | 1:57:A:VAL:HG13 | 7        | 0.17          |
| (1,1409) | 1:57:A:VAL:HG22  | 1:57:A:VAL:HG12 | 8        | 0.17          |
| (1,1409) | 1:57:A:VAL:HG23  | 1:57:A:VAL:HG12 | 11       | 0.17          |
| (1,1397) | 1:31:A:LEU:HD23  | 1:60:A:VAL:HG12 | 12       | 0.17          |
| (1,1382) | 1:57:A:VAL:HG21  | 1:53:A:PHE:HE2  | 5        | 0.17          |
| (1,1382) | 1:57:A:VAL:HG21  | 1:53:A:PHE:HE1  | 11       | 0.17          |
| (1,1363) | 1:29:A:ALA:HA    | 1:32:A:ALA:HB2  | 12       | 0.17          |
| (1,1363) | 1:29:A:ALA:HA    | 1:32:A:ALA:HB1  | 17       | 0.17          |
| (1,1352) | 1:122:A:ALA:HB3  | 1:122:A:ALA:H   | 11       | 0.17          |
| (1,1350) | 1:129:A:ALA:HB3  | 1:129:A:ALA:H   | 15       | 0.17          |
| (1,1337) | 1:78:A:TYR:HD1   | 1:28:A:ILE:HD11 | 2        | 0.17          |
| (1,1337) | 1:78:A:TYR:HD2   | 1:28:A:ILE:HD11 | 9        | 0.17          |
| (1,1325) | 1:53:A:PHE:HE2   | 1:75:A:LEU:HB3  | 3        | 0.17          |
| (1,1325) | 1:53:A:PHE:HE2   | 1:75:A:LEU:HB3  | 7        | 0.17          |
| (1,1325) | 1:53:A:PHE:HE2   | 1:75:A:LEU:HB3  | 13       | 0.17          |
| (1,1325) | 1:53:A:PHE:HE1   | 1:75:A:LEU:HB3  | 15       | 0.17          |
| (1,1325) | 1:53:A:PHE:HE1   | 1:75:A:LEU:HB3  | 16       | 0.17          |
| (1,1321) | 1:124:A:VAL:HG11 | 1:125:A:GLN:H   | 10       | 0.17          |
| (1,1253) | 1:47:A:PRO:HB3   | 1:87:A:GLY:HA2  | 3        | 0.17          |
| (1,1253) | 1:47:A:PRO:HB3   | 1:87:A:GLY:HA2  | 7        | 0.17          |
| (1,1253) | 1:47:A:PRO:HB3   | 1:87:A:GLY:HA2  | 9        | 0.17          |
| (1,1253) | 1:47:A:PRO:HB3   | 1:87:A:GLY:HA2  | 13       | 0.17          |
| (1,1253) | 1:47:A:PRO:HB3   | 1:87:A:GLY:HA2  | 15       | 0.17          |
| (1,1206) | 1:117:A:LEU:HD12 | 1:86:A:TYR:HB2  | 17       | 0.17          |
| (1,1126) | 1:86:A:TYR:HE2   | 1:86:A:TYR:HB3  | 13       | 0.17          |
| (1,1108) | 1:56:A:LEU:HD11  | 1:52:A:ILE:HG12 | 4        | 0.17          |
| (1,1108) | 1:56:A:LEU:HD13  | 1:52:A:ILE:HG12 | 5        | 0.17          |
| (1,1108) | 1:56:A:LEU:HD13  | 1:52:A:ILE:HG12 | 6        | 0.17          |
| (1,1108) | 1:56:A:LEU:HD13  | 1:52:A:ILE:HG12 | 8        | 0.17          |
| (1,1108) | 1:56:A:LEU:HD13  | 1:52:A:ILE:HG12 | 9        | 0.17          |
| (1,1078) | 1:48:A:LEU:HD22  | 1:84:A:TYR:HE2  | 2        | 0.17          |
| (1,1074) | 1:34:A:ARG:HG2   | 1:35:A:PHE:HD1  | 13       | 0.17          |
| (1,1073) | 1:97:A:LEU:HD11  | 1:97:A:LEU:H    | 13       | 0.17          |
| (1,1061) | 1:21:A:LEU:HD23  | 1:27:A:VAL:HG12 | 4        | 0.17          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1049) | 1:59:A:ARG:HB2  | 1:60:A:VAL:HG12 | 1        | 0.17          |
| (1,1049) | 1:59:A:ARG:HB2  | 1:60:A:VAL:HG11 | 13       | 0.17          |
| (1,1032) | 1:85:A:LEU:H    | 1:84:A:TYR:HE1  | 17       | 0.17          |
| (1,1030) | 1:86:A:TYR:HE1  | 1:86:A:TYR:HB2  | 14       | 0.17          |
| (1,993)  | 1:79:A:THR:HG23 | 1:75:A:LEU:HA   | 5        | 0.17          |
| (1,959)  | 1:30:A:PHE:HD1  | 1:31:A:LEU:HA   | 1        | 0.17          |
| (1,856)  | 1:13:A:ASP:HB3  | 1:14:A:PRO:HD3  | 8        | 0.17          |
| (1,827)  | 1:45:A:ALA:HB1  | 1:45:A:ALA:H    | 11       | 0.17          |
| (1,755)  | 1:95:A:VAL:H    | 1:94:A:ARG:HB3  | 15       | 0.17          |
| (1,753)  | 1:92:A:ALA:HB3  | 1:91:A:GLY:H    | 3        | 0.17          |
| (1,665)  | 1:122:A:ALA:HB2 | 1:123:A:ARG:H   | 13       | 0.17          |
| (1,635)  | 1:127:A:GLN:H   | 1:127:A:GLN:HB3 | 5        | 0.17          |
| (1,614)  | 1:97:A:LEU:HD11 | 1:97:A:LEU:H    | 13       | 0.17          |
| (1,605)  | 1:40:A:SER:HA   | 1:43:A:GLY:H    | 12       | 0.17          |
| (1,557)  | 1:66:A:LEU:HB2  | 1:70:A:GLN:HE22 | 16       | 0.17          |
| (1,527)  | 1:65:A:ASN:HB3  | 1:65:A:ASN:HD21 | 5        | 0.17          |
| (1,527)  | 1:65:A:ASN:HB3  | 1:65:A:ASN:HD21 | 15       | 0.17          |
| (1,512)  | 1:13:A:ASP:HB2  | 1:13:A:ASP:H    | 3        | 0.17          |
| (1,512)  | 1:13:A:ASP:HB2  | 1:13:A:ASP:H    | 9        | 0.17          |
| (1,512)  | 1:13:A:ASP:HB2  | 1:13:A:ASP:H    | 12       | 0.17          |
| (1,512)  | 1:13:A:ASP:HB2  | 1:13:A:ASP:H    | 14       | 0.17          |
| (1,512)  | 1:13:A:ASP:HB2  | 1:13:A:ASP:H    | 16       | 0.17          |
| (1,477)  | 1:31:A:LEU:H    | 1:31:A:LEU:HD13 | 14       | 0.17          |
| (1,451)  | 1:32:A:ALA:HB2  | 1:35:A:PHE:H    | 3        | 0.17          |
| (1,451)  | 1:32:A:ALA:HB3  | 1:35:A:PHE:H    | 14       | 0.17          |
| (1,311)  | 1:79:A:THR:H    | 1:77:A:LEU:HB2  | 1        | 0.17          |
| (1,311)  | 1:79:A:THR:H    | 1:77:A:LEU:HB2  | 2        | 0.17          |
| (1,234)  | 1:95:A:VAL:HG22 | 1:99:A:GLY:H    | 2        | 0.17          |
| (1,234)  | 1:95:A:VAL:HG22 | 1:99:A:GLY:H    | 10       | 0.17          |
| (1,234)  | 1:95:A:VAL:HG23 | 1:99:A:GLY:H    | 12       | 0.17          |
| (1,234)  | 1:95:A:VAL:HG21 | 1:99:A:GLY:H    | 14       | 0.17          |
| (1,156)  | 1:126:A:ALA:HB3 | 1:126:A:ALA:H   | 9        | 0.17          |
| (1,156)  | 1:126:A:ALA:HB3 | 1:126:A:ALA:H   | 14       | 0.17          |
| (1,134)  | 1:123:A:ARG:H   | 1:121:A:LYS:H   | 2        | 0.17          |
| (1,134)  | 1:123:A:ARG:H   | 1:121:A:LYS:H   | 4        | 0.17          |
| (1,134)  | 1:123:A:ARG:H   | 1:121:A:LYS:H   | 5        | 0.17          |
| (1,134)  | 1:123:A:ARG:H   | 1:121:A:LYS:H   | 8        | 0.17          |
| (1,134)  | 1:123:A:ARG:H   | 1:121:A:LYS:H   | 10       | 0.17          |
| (1,134)  | 1:123:A:ARG:H   | 1:121:A:LYS:H   | 16       | 0.17          |
| (1,100)  | 1:35:A:PHE:HE2  | 1:35:A:PHE:H    | 4        | 0.17          |
| (1,80)   | 1:30:A:PHE:HD1  | 1:30:A:PHE:H    | 7        | 0.17          |
| (1,56)   | 1:84:A:TYR:H    | 1:84:A:TYR:HD2  | 8        | 0.17          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,56)   | 1:84:A:TYR:H    | 1:84:A:TYR:HD2   | 9        | 0.17          |
| (1,12)   | 1:100:A:ASN:H   | 1:100:A:ASN:HD21 | 6        | 0.17          |
| (3,122)  | 1:27:A:VAL:HG23 | 1:28:A:ILE:HD11  | 14       | 0.16          |
| (3,111)  | 1:111:A:GLU:HG2 | 1:112:A:HIS:HA   | 8        | 0.16          |
| (3,94)   | 1:56:A:LEU:HB2  | 1:75:A:LEU:HD13  | 2        | 0.16          |
| (3,94)   | 1:56:A:LEU:HB2  | 1:75:A:LEU:HD11  | 4        | 0.16          |
| (3,92)   | 1:88:A:VAL:HG23 | 1:87:A:GLY:HA2   | 6        | 0.16          |
| (3,92)   | 1:88:A:VAL:HG21 | 1:87:A:GLY:HA2   | 12       | 0.16          |
| (3,83)   | 1:114:A:ARG:HB2 | 1:113:A:ALA:HB2  | 7        | 0.16          |
| (3,54)   | 1:71:A:LEU:HB3  | 1:75:A:LEU:HD12  | 16       | 0.16          |
| (3,52)   | 1:95:A:VAL:HG23 | 1:37:A:HIS:HB2   | 11       | 0.16          |
| (3,18)   | 1:58:A:ASP:HB3  | 1:60:A:VAL:HG12  | 1        | 0.16          |
| (1,4345) | 1:117:A:LEU:HA  | 1:121:A:LYS:H    | 4        | 0.16          |
| (1,4345) | 1:117:A:LEU:HA  | 1:121:A:LYS:H    | 16       | 0.16          |
| (1,4343) | 1:118:A:GLU:H   | 1:119:A:GLU:H    | 3        | 0.16          |
| (1,4339) | 1:116:A:GLN:HG3 | 1:115:A:LYS:H    | 12       | 0.16          |
| (1,4331) | 1:104:A:GLU:HG2 | 1:104:A:GLU:H    | 7        | 0.16          |
| (1,4323) | 1:62:A:GLY:H    | 1:68:A:LYS:HD2   | 7        | 0.16          |
| (1,4323) | 1:62:A:GLY:H    | 1:68:A:LYS:HD2   | 9        | 0.16          |
| (1,4320) | 1:62:A:GLY:H    | 1:66:A:LEU:H     | 3        | 0.16          |
| (1,4301) | 1:97:A:LEU:HB2  | 1:97:A:LEU:H     | 8        | 0.16          |
| (1,4278) | 1:12:A:GLN:HA   | 1:13:A:ASP:H     | 10       | 0.16          |
| (1,4270) | 1:75:A:LEU:HB3  | 1:74:A:ALA:H     | 2        | 0.16          |
| (1,4225) | 1:122:A:ALA:HB2 | 1:123:A:ARG:H    | 3        | 0.16          |
| (1,4225) | 1:122:A:ALA:HB3 | 1:123:A:ARG:H    | 10       | 0.16          |
| (1,4212) | 1:115:A:LYS:HE3 | 1:115:A:LYS:H    | 2        | 0.16          |
| (1,4212) | 1:115:A:LYS:HE3 | 1:115:A:LYS:H    | 3        | 0.16          |
| (1,4212) | 1:115:A:LYS:HE3 | 1:115:A:LYS:H    | 4        | 0.16          |
| (1,4212) | 1:115:A:LYS:HE3 | 1:115:A:LYS:H    | 14       | 0.16          |
| (1,4212) | 1:115:A:LYS:HE3 | 1:115:A:LYS:H    | 15       | 0.16          |
| (1,4212) | 1:115:A:LYS:HE3 | 1:115:A:LYS:H    | 16       | 0.16          |
| (1,4212) | 1:115:A:LYS:HE3 | 1:115:A:LYS:H    | 17       | 0.16          |
| (1,4198) | 1:127:A:GLN:HA  | 1:127:A:GLN:H    | 5        | 0.16          |
| (1,4198) | 1:127:A:GLN:HA  | 1:127:A:GLN:H    | 7        | 0.16          |
| (1,4198) | 1:127:A:GLN:HA  | 1:127:A:GLN:H    | 16       | 0.16          |
| (1,4198) | 1:127:A:GLN:HA  | 1:127:A:GLN:H    | 17       | 0.16          |
| (1,4193) | 1:69:A:THR:HB   | 1:72:A:ARG:H     | 6        | 0.16          |
| (1,4193) | 1:69:A:THR:HB   | 1:72:A:ARG:H     | 10       | 0.16          |
| (1,4193) | 1:69:A:THR:HB   | 1:72:A:ARG:H     | 13       | 0.16          |
| (1,4193) | 1:69:A:THR:HB   | 1:72:A:ARG:H     | 14       | 0.16          |
| (1,4180) | 1:95:A:VAL:H    | 1:48:A:LEU:HD11  | 14       | 0.16          |
| (1,4176) | 1:97:A:LEU:HD11 | 1:97:A:LEU:H     | 4        | 0.16          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,4154) | 1:17:A:ASN:HA   | 1:18:A:GLN:H    | 10       | 0.16          |
| (1,4153) | 1:18:A:GLN:HB3  | 1:18:A:GLN:H    | 17       | 0.16          |
| (1,4150) | 1:17:A:ASN:HB3  | 1:18:A:GLN:H    | 2        | 0.16          |
| (1,4144) | 1:21:A:LEU:H    | 1:65:A:ASN:HB3  | 3        | 0.16          |
| (1,4133) | 1:82:A:TRP:HE1  | 1:82:A:TRP:HD1  | 9        | 0.16          |
| (1,4133) | 1:82:A:TRP:HE1  | 1:82:A:TRP:HD1  | 12       | 0.16          |
| (1,4126) | 1:59:A:ARG:HE   | 1:97:A:LEU:HD11 | 3        | 0.16          |
| (1,4109) | 1:97:A:LEU:HD12 | 1:98:A:ASP:H    | 10       | 0.16          |
| (1,4109) | 1:97:A:LEU:HD13 | 1:98:A:ASP:H    | 12       | 0.16          |
| (1,4109) | 1:97:A:LEU:HD11 | 1:98:A:ASP:H    | 13       | 0.16          |
| (1,4069) | 1:13:A:ASP:HB2  | 1:13:A:ASP:H    | 1        | 0.16          |
| (1,4040) | 1:25:A:LYS:HG3  | 1:25:A:LYS:H    | 3        | 0.16          |
| (1,4040) | 1:25:A:LYS:HG3  | 1:25:A:LYS:H    | 4        | 0.16          |
| (1,4040) | 1:25:A:LYS:HG3  | 1:25:A:LYS:H    | 6        | 0.16          |
| (1,4040) | 1:25:A:LYS:HG3  | 1:25:A:LYS:H    | 7        | 0.16          |
| (1,4040) | 1:25:A:LYS:HG3  | 1:25:A:LYS:H    | 9        | 0.16          |
| (1,4040) | 1:25:A:LYS:HG3  | 1:25:A:LYS:H    | 10       | 0.16          |
| (1,4040) | 1:25:A:LYS:HG3  | 1:25:A:LYS:H    | 11       | 0.16          |
| (1,4040) | 1:25:A:LYS:HG3  | 1:25:A:LYS:H    | 13       | 0.16          |
| (1,4040) | 1:25:A:LYS:HG3  | 1:25:A:LYS:H    | 15       | 0.16          |
| (1,4040) | 1:25:A:LYS:HG3  | 1:25:A:LYS:H    | 16       | 0.16          |
| (1,4040) | 1:25:A:LYS:HG3  | 1:25:A:LYS:H    | 17       | 0.16          |
| (1,4037) | 1:27:A:VAL:HG22 | 1:29:A:ALA:H    | 1        | 0.16          |
| (1,4019) | 1:33:A:GLU:HB3  | 1:34:A:ARG:H    | 7        | 0.16          |
| (1,4019) | 1:33:A:GLU:HB3  | 1:34:A:ARG:H    | 11       | 0.16          |
| (1,4016) | 1:15:A:MET:HA   | 1:15:A:MET:H    | 9        | 0.16          |
| (1,3987) | 1:50:A:ILE:HG21 | 1:50:A:ILE:H    | 11       | 0.16          |
| (1,3979) | 1:50:A:ILE:HA   | 1:51:A:GLY:H    | 17       | 0.16          |
| (1,3961) | 1:57:A:VAL:H    | 1:56:A:LEU:HB3  | 3        | 0.16          |
| (1,3961) | 1:57:A:VAL:H    | 1:56:A:LEU:HB3  | 7        | 0.16          |
| (1,3940) | 1:62:A:GLY:HA3  | 1:63:A:GLU:H    | 9        | 0.16          |
| (1,3940) | 1:62:A:GLY:HA3  | 1:63:A:GLU:H    | 13       | 0.16          |
| (1,3940) | 1:62:A:GLY:HA3  | 1:63:A:GLU:H    | 15       | 0.16          |
| (1,3935) | 1:63:A:GLU:HB3  | 1:65:A:ASN:H    | 2        | 0.16          |
| (1,3935) | 1:63:A:GLU:HB3  | 1:65:A:ASN:H    | 8        | 0.16          |
| (1,3935) | 1:63:A:GLU:HB3  | 1:65:A:ASN:H    | 12       | 0.16          |
| (1,3917) | 1:74:A:ALA:HA   | 1:75:A:LEU:H    | 2        | 0.16          |
| (1,3917) | 1:74:A:ALA:HA   | 1:75:A:LEU:H    | 5        | 0.16          |
| (1,3917) | 1:74:A:ALA:HA   | 1:75:A:LEU:H    | 6        | 0.16          |
| (1,3917) | 1:74:A:ALA:HA   | 1:75:A:LEU:H    | 8        | 0.16          |
| (1,3917) | 1:74:A:ALA:HA   | 1:75:A:LEU:H    | 9        | 0.16          |
| (1,3917) | 1:74:A:ALA:HA   | 1:75:A:LEU:H    | 11       | 0.16          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3917) | 1:74:A:ALA:HA   | 1:75:A:LEU:H    | 14       | 0.16          |
| (1,3917) | 1:74:A:ALA:HA   | 1:75:A:LEU:H    | 15       | 0.16          |
| (1,3916) | 1:71:A:LEU:HA   | 1:74:A:ALA:H    | 9        | 0.16          |
| (1,3916) | 1:71:A:LEU:HA   | 1:74:A:ALA:H    | 10       | 0.16          |
| (1,3916) | 1:71:A:LEU:HA   | 1:74:A:ALA:H    | 14       | 0.16          |
| (1,3916) | 1:71:A:LEU:HA   | 1:74:A:ALA:H    | 16       | 0.16          |
| (1,3879) | 1:127:A:GLN:H   | 1:127:A:GLN:HG2 | 11       | 0.16          |
| (1,3879) | 1:127:A:GLN:H   | 1:127:A:GLN:HG2 | 14       | 0.16          |
| (1,3859) | 1:90:A:PRO:HB2  | 1:91:A:GLY:H    | 6        | 0.16          |
| (1,3830) | 1:101:A:PRO:HD3 | 1:100:A:ASN:H   | 1        | 0.16          |
| (1,3830) | 1:101:A:PRO:HD3 | 1:100:A:ASN:H   | 2        | 0.16          |
| (1,3830) | 1:101:A:PRO:HD3 | 1:100:A:ASN:H   | 16       | 0.16          |
| (1,3830) | 1:101:A:PRO:HD3 | 1:100:A:ASN:H   | 17       | 0.16          |
| (1,3824) | 1:102:A:CYS:H   | 1:100:A:ASN:HB3 | 6        | 0.16          |
| (1,3786) | 1:27:A:VAL:HG12 | 1:21:A:LEU:H    | 11       | 0.16          |
| (1,3781) | 1:119:A:GLU:HA  | 1:119:A:GLU:H   | 7        | 0.16          |
| (1,3781) | 1:119:A:GLU:HA  | 1:119:A:GLU:H   | 8        | 0.16          |
| (1,3771) | 1:126:A:ALA:HB1 | 1:126:A:ALA:H   | 4        | 0.16          |
| (1,3768) | 1:130:A:GLU:H   | 1:130:A:GLU:HA  | 14       | 0.16          |
| (1,3767) | 1:129:A:ALA:HA  | 1:129:A:ALA:H   | 1        | 0.16          |
| (1,3757) | 1:116:A:GLN:H   | 1:117:A:LEU:H   | 6        | 0.16          |
| (1,3757) | 1:116:A:GLN:H   | 1:117:A:LEU:H   | 9        | 0.16          |
| (1,3698) | 1:30:A:PHE:HD2  | 1:30:A:PHE:H    | 2        | 0.16          |
| (1,3698) | 1:30:A:PHE:HD1  | 1:30:A:PHE:H    | 16       | 0.16          |
| (1,3673) | 1:49:A:LYS:H    | 1:50:A:ILE:H    | 7        | 0.16          |
| (1,3591) | 1:93:A:THR:HB   | 1:88:A:VAL:HG12 | 7        | 0.16          |
| (1,3582) | 1:110:A:VAL:H   | 1:109:A:HIS:HA  | 1        | 0.16          |
| (1,3582) | 1:110:A:VAL:H   | 1:109:A:HIS:HA  | 2        | 0.16          |
| (1,3582) | 1:110:A:VAL:H   | 1:109:A:HIS:HA  | 3        | 0.16          |
| (1,3582) | 1:110:A:VAL:H   | 1:109:A:HIS:HA  | 4        | 0.16          |
| (1,3582) | 1:110:A:VAL:H   | 1:109:A:HIS:HA  | 5        | 0.16          |
| (1,3582) | 1:110:A:VAL:H   | 1:109:A:HIS:HA  | 8        | 0.16          |
| (1,3582) | 1:110:A:VAL:H   | 1:109:A:HIS:HA  | 9        | 0.16          |
| (1,3582) | 1:110:A:VAL:H   | 1:109:A:HIS:HA  | 11       | 0.16          |
| (1,3582) | 1:110:A:VAL:H   | 1:109:A:HIS:HA  | 12       | 0.16          |
| (1,3582) | 1:110:A:VAL:H   | 1:109:A:HIS:HA  | 13       | 0.16          |
| (1,3582) | 1:110:A:VAL:H   | 1:109:A:HIS:HA  | 15       | 0.16          |
| (1,3582) | 1:110:A:VAL:H   | 1:109:A:HIS:HA  | 16       | 0.16          |
| (1,3552) | 1:123:A:ARG:HG2 | 1:124:A:VAL:HA  | 1        | 0.16          |
| (1,3552) | 1:123:A:ARG:HG2 | 1:124:A:VAL:HA  | 2        | 0.16          |
| (1,3552) | 1:123:A:ARG:HG2 | 1:124:A:VAL:HA  | 5        | 0.16          |
| (1,3552) | 1:123:A:ARG:HG2 | 1:124:A:VAL:HA  | 9        | 0.16          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3552) | 1:123:A:ARG:HG2 | 1:124:A:VAL:HA   | 11       | 0.16          |
| (1,3552) | 1:123:A:ARG:HG2 | 1:124:A:VAL:HA   | 14       | 0.16          |
| (1,3552) | 1:123:A:ARG:HG2 | 1:124:A:VAL:HA   | 15       | 0.16          |
| (1,3539) | 1:63:A:GLU:HG3  | 1:63:A:GLU:H     | 16       | 0.16          |
| (1,3537) | 1:51:A:GLY:HA2  | 1:54:A:GLN:HB2   | 14       | 0.16          |
| (1,3537) | 1:51:A:GLY:HA2  | 1:54:A:GLN:HB2   | 15       | 0.16          |
| (1,3531) | 1:65:A:ASN:H    | 1:65:A:ASN:HA    | 14       | 0.16          |
| (1,3523) | 1:56:A:LEU:HG   | 1:56:A:LEU:HB3   | 1        | 0.16          |
| (1,3523) | 1:56:A:LEU:HG   | 1:56:A:LEU:HB3   | 12       | 0.16          |
| (1,3502) | 1:27:A:VAL:HG23 | 1:27:A:VAL:H     | 8        | 0.16          |
| (1,3500) | 1:27:A:VAL:HG23 | 1:31:A:LEU:HD11  | 6        | 0.16          |
| (1,3500) | 1:27:A:VAL:HG22 | 1:31:A:LEU:HD11  | 13       | 0.16          |
| (1,3497) | 1:27:A:VAL:HA   | 1:27:A:VAL:HG11  | 1        | 0.16          |
| (1,3477) | 1:15:A:MET:HG3  | 1:15:A:MET:HB2   | 1        | 0.16          |
| (1,3477) | 1:15:A:MET:HG3  | 1:15:A:MET:HB2   | 2        | 0.16          |
| (1,3477) | 1:15:A:MET:HG3  | 1:15:A:MET:HB2   | 5        | 0.16          |
| (1,3477) | 1:15:A:MET:HG3  | 1:15:A:MET:HB2   | 6        | 0.16          |
| (1,3477) | 1:15:A:MET:HG3  | 1:15:A:MET:HB2   | 11       | 0.16          |
| (1,3477) | 1:15:A:MET:HG3  | 1:15:A:MET:HB2   | 13       | 0.16          |
| (1,3456) | 1:95:A:VAL:HG22 | 1:96:A:ASP:HA    | 10       | 0.16          |
| (1,3433) | 1:27:A:VAL:HA   | 1:21:A:LEU:HD11  | 4        | 0.16          |
| (1,3430) | 1:45:A:ALA:HB3  | 1:84:A:TYR:HA    | 3        | 0.16          |
| (1,3430) | 1:45:A:ALA:HB3  | 1:84:A:TYR:HA    | 9        | 0.16          |
| (1,3430) | 1:45:A:ALA:HB1  | 1:84:A:TYR:HA    | 15       | 0.16          |
| (1,3414) | 1:86:A:TYR:H    | 1:117:A:LEU:HD12 | 5        | 0.16          |
| (1,3396) | 1:71:A:LEU:HA   | 1:74:A:ALA:HB3   | 5        | 0.16          |
| (1,3396) | 1:71:A:LEU:HA   | 1:74:A:ALA:HB2   | 15       | 0.16          |
| (1,3390) | 1:88:A:VAL:HG23 | 1:84:A:TYR:HA    | 4        | 0.16          |
| (1,3370) | 1:24:A:SER:HA   | 1:27:A:VAL:HG11  | 7        | 0.16          |
| (1,3370) | 1:24:A:SER:HA   | 1:27:A:VAL:HG11  | 10       | 0.16          |
| (1,3369) | 1:24:A:SER:HA   | 1:27:A:VAL:HG21  | 7        | 0.16          |
| (1,3369) | 1:24:A:SER:HA   | 1:27:A:VAL:HG21  | 9        | 0.16          |
| (1,3348) | 1:79:A:THR:HG23 | 1:84:A:TYR:HE1   | 12       | 0.16          |
| (1,3344) | 1:113:A:ALA:HB3 | 1:89:A:LYS:H     | 2        | 0.16          |
| (1,3344) | 1:113:A:ALA:HB1 | 1:89:A:LYS:H     | 12       | 0.16          |
| (1,3336) | 1:71:A:LEU:HD22 | 1:74:A:ALA:H     | 11       | 0.16          |
| (1,3322) | 1:30:A:PHE:HD1  | 1:66:A:LEU:HD21  | 13       | 0.16          |
| (1,3320) | 1:27:A:VAL:HA   | 1:66:A:LEU:HD23  | 5        | 0.16          |
| (1,3320) | 1:27:A:VAL:HA   | 1:66:A:LEU:HD22  | 12       | 0.16          |
| (1,3314) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HG    | 17       | 0.16          |
| (1,3306) | 1:128:A:ARG:HG2 | 1:128:A:ARG:HD2  | 16       | 0.16          |
| (1,3299) | 1:20:A:LYS:H    | 1:20:A:LYS:HD3   | 11       | 0.16          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3299) | 1:20:A:LYS:H    | 1:20:A:LYS:HD3  | 13       | 0.16          |
| (1,3250) | 1:41:A:ALA:HA   | 1:41:A:ALA:HB2  | 17       | 0.16          |
| (1,3241) | 1:52:A:ILE:HG13 | 1:97:A:LEU:HD23 | 15       | 0.16          |
| (1,3232) | 1:92:A:ALA:H    | 1:105:A:LEU:HB2 | 8        | 0.16          |
| (1,3232) | 1:92:A:ALA:H    | 1:105:A:LEU:HB2 | 17       | 0.16          |
| (1,3221) | 1:37:A:HIS:HB2  | 1:99:A:GLY:HA2  | 15       | 0.16          |
| (1,3210) | 1:128:A:ARG:HA  | 1:128:A:ARG:HB3 | 1        | 0.16          |
| (1,3210) | 1:128:A:ARG:HA  | 1:128:A:ARG:HB3 | 8        | 0.16          |
| (1,3197) | 1:87:A:GLY:HA3  | 1:113:A:ALA:HB3 | 3        | 0.16          |
| (1,3197) | 1:87:A:GLY:HA3  | 1:113:A:ALA:HB1 | 5        | 0.16          |
| (1,3197) | 1:87:A:GLY:HA3  | 1:113:A:ALA:HB1 | 6        | 0.16          |
| (1,3197) | 1:87:A:GLY:HA3  | 1:113:A:ALA:HB2 | 7        | 0.16          |
| (1,3185) | 1:109:A:HIS:HB2 | 1:108:A:GLN:H   | 4        | 0.16          |
| (1,3185) | 1:109:A:HIS:HB2 | 1:108:A:GLN:H   | 6        | 0.16          |
| (1,3185) | 1:109:A:HIS:HB2 | 1:108:A:GLN:H   | 9        | 0.16          |
| (1,3185) | 1:109:A:HIS:HB2 | 1:108:A:GLN:H   | 10       | 0.16          |
| (1,3185) | 1:109:A:HIS:HB2 | 1:108:A:GLN:H   | 16       | 0.16          |
| (1,3185) | 1:109:A:HIS:HB2 | 1:108:A:GLN:H   | 17       | 0.16          |
| (1,3181) | 1:108:A:GLN:HG3 | 1:108:A:GLN:HA  | 7        | 0.16          |
| (1,3165) | 1:126:A:ALA:HB3 | 1:125:A:GLN:HG3 | 10       | 0.16          |
| (1,3160) | 1:74:A:ALA:HB3  | 1:74:A:ALA:HA   | 6        | 0.16          |
| (1,3160) | 1:74:A:ALA:HB3  | 1:74:A:ALA:HA   | 10       | 0.16          |
| (1,3130) | 1:123:A:ARG:HG2 | 1:123:A:ARG:H   | 2        | 0.16          |
| (1,3130) | 1:123:A:ARG:HG2 | 1:123:A:ARG:H   | 14       | 0.16          |
| (1,3087) | 1:56:A:LEU:HG   | 1:56:A:LEU:HA   | 4        | 0.16          |
| (1,3087) | 1:56:A:LEU:HG   | 1:56:A:LEU:HA   | 7        | 0.16          |
| (1,3068) | 1:52:A:ILE:HG23 | 1:53:A:PHE:HB2  | 8        | 0.16          |
| (1,3068) | 1:52:A:ILE:HG21 | 1:53:A:PHE:HB2  | 14       | 0.16          |
| (1,3059) | 1:28:A:ILE:HB   | 1:28:A:ILE:HG23 | 8        | 0.16          |
| (1,3059) | 1:28:A:ILE:HB   | 1:28:A:ILE:HG23 | 17       | 0.16          |
| (1,3053) | 1:29:A:ALA:H    | 1:28:A:ILE:HG23 | 10       | 0.16          |
| (1,3040) | 1:52:A:ILE:HA   | 1:52:A:ILE:HG12 | 16       | 0.16          |
| (1,3032) | 1:121:A:LYS:HG3 | 1:121:A:LYS:HE3 | 4        | 0.16          |
| (1,3032) | 1:121:A:LYS:HG3 | 1:121:A:LYS:HE3 | 6        | 0.16          |
| (1,3032) | 1:121:A:LYS:HG3 | 1:121:A:LYS:HE3 | 7        | 0.16          |
| (1,3032) | 1:121:A:LYS:HG3 | 1:121:A:LYS:HE3 | 10       | 0.16          |
| (1,3032) | 1:121:A:LYS:HG3 | 1:121:A:LYS:HE3 | 15       | 0.16          |
| (1,3032) | 1:121:A:LYS:HG3 | 1:121:A:LYS:HE3 | 17       | 0.16          |
| (1,3022) | 1:64:A:MET:HE2  | 1:30:A:PHE:HA   | 11       | 0.16          |
| (1,3000) | 1:57:A:VAL:HA   | 1:60:A:VAL:HB   | 2        | 0.16          |
| (1,3000) | 1:57:A:VAL:HA   | 1:60:A:VAL:HB   | 4        | 0.16          |
| (1,3000) | 1:57:A:VAL:HA   | 1:60:A:VAL:HB   | 6        | 0.16          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3000) | 1:57:A:VAL:HA    | 1:60:A:VAL:HB   | 16       | 0.16          |
| (1,2995) | 1:60:A:VAL:H     | 1:60:A:VAL:HB   | 4        | 0.16          |
| (1,2995) | 1:60:A:VAL:H     | 1:60:A:VAL:HB   | 6        | 0.16          |
| (1,2995) | 1:60:A:VAL:H     | 1:60:A:VAL:HB   | 9        | 0.16          |
| (1,2995) | 1:60:A:VAL:H     | 1:60:A:VAL:HB   | 13       | 0.16          |
| (1,2995) | 1:60:A:VAL:H     | 1:60:A:VAL:HB   | 15       | 0.16          |
| (1,2992) | 1:20:A:LYS:HB3   | 1:20:A:LYS:H    | 2        | 0.16          |
| (1,2992) | 1:20:A:LYS:HB3   | 1:20:A:LYS:H    | 3        | 0.16          |
| (1,2969) | 1:93:A:THR:HG21  | 1:101:A:PRO:HB3 | 1        | 0.16          |
| (1,2969) | 1:93:A:THR:HG22  | 1:101:A:PRO:HB3 | 2        | 0.16          |
| (1,2969) | 1:93:A:THR:HG22  | 1:101:A:PRO:HB3 | 9        | 0.16          |
| (1,2961) | 1:56:A:LEU:HD22  | 1:52:A:ILE:HB   | 5        | 0.16          |
| (1,2960) | 1:77:A:LEU:HD12  | 1:25:A:LYS:HA   | 7        | 0.16          |
| (1,2960) | 1:77:A:LEU:HD12  | 1:25:A:LYS:HA   | 9        | 0.16          |
| (1,2960) | 1:77:A:LEU:HD12  | 1:25:A:LYS:HA   | 10       | 0.16          |
| (1,2960) | 1:77:A:LEU:HD12  | 1:25:A:LYS:HA   | 12       | 0.16          |
| (1,2960) | 1:77:A:LEU:HD11  | 1:25:A:LYS:HA   | 13       | 0.16          |
| (1,2950) | 1:75:A:LEU:HD11  | 1:75:A:LEU:H    | 2        | 0.16          |
| (1,2950) | 1:75:A:LEU:HD13  | 1:75:A:LEU:H    | 5        | 0.16          |
| (1,2943) | 1:110:A:VAL:HG22 | 1:108:A:GLN:H   | 11       | 0.16          |
| (1,2943) | 1:110:A:VAL:HG22 | 1:108:A:GLN:H   | 15       | 0.16          |
| (1,2932) | 1:95:A:VAL:HG22  | 1:95:A:VAL:H    | 17       | 0.16          |
| (1,2930) | 1:31:A:LEU:HD21  | 1:60:A:VAL:HG11 | 6        | 0.16          |
| (1,2930) | 1:31:A:LEU:HD22  | 1:60:A:VAL:HG12 | 8        | 0.16          |
| (1,2930) | 1:31:A:LEU:HD21  | 1:60:A:VAL:HG13 | 10       | 0.16          |
| (1,2899) | 1:28:A:ILE:HD11  | 1:75:A:LEU:H    | 7        | 0.16          |
| (1,2893) | 1:50:A:ILE:HB    | 1:50:A:ILE:HG21 | 6        | 0.16          |
| (1,2893) | 1:50:A:ILE:HB    | 1:50:A:ILE:HG21 | 10       | 0.16          |
| (1,2893) | 1:50:A:ILE:HB    | 1:50:A:ILE:HG23 | 13       | 0.16          |
| (1,2876) | 1:61:A:ALA:HB2   | 1:62:A:GLY:H    | 3        | 0.16          |
| (1,2876) | 1:61:A:ALA:HB2   | 1:62:A:GLY:H    | 5        | 0.16          |
| (1,2875) | 1:122:A:ALA:HB1  | 1:122:A:ALA:H   | 2        | 0.16          |
| (1,2871) | 1:129:A:ALA:HB2  | 1:129:A:ALA:H   | 11       | 0.16          |
| (1,2855) | 1:78:A:TYR:HD2   | 1:28:A:ILE:HD13 | 5        | 0.16          |
| (1,2855) | 1:78:A:TYR:HD1   | 1:28:A:ILE:HD11 | 10       | 0.16          |
| (1,2855) | 1:78:A:TYR:HD1   | 1:28:A:ILE:HD11 | 15       | 0.16          |
| (1,2840) | 1:124:A:VAL:HG12 | 1:125:A:GLN:H   | 1        | 0.16          |
| (1,2840) | 1:124:A:VAL:HG11 | 1:125:A:GLN:H   | 2        | 0.16          |
| (1,2840) | 1:124:A:VAL:HG12 | 1:125:A:GLN:H   | 4        | 0.16          |
| (1,2840) | 1:124:A:VAL:HG13 | 1:125:A:GLN:H   | 9        | 0.16          |
| (1,2840) | 1:124:A:VAL:HG13 | 1:125:A:GLN:H   | 12       | 0.16          |
| (1,2840) | 1:124:A:VAL:HG13 | 1:125:A:GLN:H   | 13       | 0.16          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2840) | 1:124:A:VAL:HG11 | 1:125:A:GLN:H   | 15       | 0.16          |
| (1,2819) | 1:97:A:LEU:HD13  | 1:35:A:PHE:HE2  | 4        | 0.16          |
| (1,2819) | 1:97:A:LEU:HD13  | 1:35:A:PHE:HE2  | 15       | 0.16          |
| (1,2804) | 1:66:A:LEU:HB3   | 1:60:A:VAL:HB   | 6        | 0.16          |
| (1,2804) | 1:66:A:LEU:HB3   | 1:60:A:VAL:HB   | 9        | 0.16          |
| (1,2804) | 1:66:A:LEU:HB3   | 1:60:A:VAL:HB   | 17       | 0.16          |
| (1,2775) | 1:47:A:PRO:HB3   | 1:87:A:GLY:HA2  | 5        | 0.16          |
| (1,2775) | 1:47:A:PRO:HB3   | 1:87:A:GLY:HA2  | 16       | 0.16          |
| (1,2774) | 1:91:A:GLY:HA3   | 1:90:A:PRO:HB2  | 4        | 0.16          |
| (1,2774) | 1:91:A:GLY:HA3   | 1:90:A:PRO:HB2  | 6        | 0.16          |
| (1,2774) | 1:91:A:GLY:HA3   | 1:90:A:PRO:HB2  | 9        | 0.16          |
| (1,2772) | 1:42:A:GLU:HB3   | 1:43:A:GLY:HA3  | 17       | 0.16          |
| (1,2771) | 1:42:A:GLU:HB3   | 1:43:A:GLY:HA2  | 17       | 0.16          |
| (1,2754) | 1:60:A:VAL:HG12  | 1:59:A:ARG:HD3  | 11       | 0.16          |
| (1,2719) | 1:117:A:LEU:HD11 | 1:86:A:TYR:HB2  | 4        | 0.16          |
| (1,2719) | 1:117:A:LEU:HD11 | 1:86:A:TYR:HB2  | 11       | 0.16          |
| (1,2719) | 1:117:A:LEU:HD11 | 1:86:A:TYR:HB2  | 13       | 0.16          |
| (1,2719) | 1:117:A:LEU:HD11 | 1:86:A:TYR:HB2  | 16       | 0.16          |
| (1,2712) | 1:39:A:PHE:HB3   | 1:35:A:PHE:HB3  | 8        | 0.16          |
| (1,2712) | 1:39:A:PHE:HB3   | 1:35:A:PHE:HB3  | 13       | 0.16          |
| (1,2712) | 1:39:A:PHE:HB3   | 1:35:A:PHE:HB3  | 14       | 0.16          |
| (1,2711) | 1:35:A:PHE:HB2   | 1:35:A:PHE:HE1  | 12       | 0.16          |
| (1,2672) | 1:31:A:LEU:HD13  | 1:35:A:PHE:HD1  | 2        | 0.16          |
| (1,2672) | 1:31:A:LEU:HD12  | 1:35:A:PHE:HD1  | 6        | 0.16          |
| (1,2672) | 1:31:A:LEU:HD13  | 1:35:A:PHE:HD2  | 15       | 0.16          |
| (1,2648) | 1:56:A:LEU:HD13  | 1:52:A:ILE:HG12 | 1        | 0.16          |
| (1,2648) | 1:56:A:LEU:HD13  | 1:52:A:ILE:HG12 | 11       | 0.16          |
| (1,2639) | 1:71:A:LEU:HD12  | 1:71:A:LEU:HB2  | 9        | 0.16          |
| (1,2639) | 1:71:A:LEU:HD13  | 1:71:A:LEU:HB2  | 17       | 0.16          |
| (1,2637) | 1:71:A:LEU:HB3   | 1:71:A:LEU:HG   | 2        | 0.16          |
| (1,2637) | 1:71:A:LEU:HB3   | 1:71:A:LEU:HG   | 7        | 0.16          |
| (1,2637) | 1:71:A:LEU:HB3   | 1:71:A:LEU:HG   | 8        | 0.16          |
| (1,2637) | 1:71:A:LEU:HB3   | 1:71:A:LEU:HG   | 9        | 0.16          |
| (1,2637) | 1:71:A:LEU:HB3   | 1:71:A:LEU:HG   | 14       | 0.16          |
| (1,2637) | 1:71:A:LEU:HB3   | 1:71:A:LEU:HG   | 16       | 0.16          |
| (1,2621) | 1:105:A:LEU:HD12 | 1:92:A:ALA:H    | 11       | 0.16          |
| (1,2621) | 1:105:A:LEU:HD13 | 1:92:A:ALA:H    | 15       | 0.16          |
| (1,2621) | 1:105:A:LEU:HD12 | 1:92:A:ALA:H    | 17       | 0.16          |
| (1,2612) | 1:30:A:PHE:HD1   | 1:34:A:ARG:HG2  | 3        | 0.16          |
| (1,2579) | 1:59:A:ARG:HB2   | 1:60:A:VAL:HG13 | 14       | 0.16          |
| (1,2560) | 1:86:A:TYR:HE2   | 1:86:A:TYR:HD2  | 1        | 0.16          |
| (1,2560) | 1:86:A:TYR:HE1   | 1:86:A:TYR:HD1  | 7        | 0.16          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2560) | 1:86:A:TYR:HE1   | 1:86:A:TYR:HD1  | 15       | 0.16          |
| (1,2530) | 1:33:A:GLU:HA    | 1:34:A:ARG:H    | 8        | 0.16          |
| (1,2530) | 1:33:A:GLU:HA    | 1:34:A:ARG:H    | 9        | 0.16          |
| (1,2530) | 1:33:A:GLU:HA    | 1:34:A:ARG:H    | 12       | 0.16          |
| (1,2530) | 1:33:A:GLU:HA    | 1:34:A:ARG:H    | 16       | 0.16          |
| (1,2514) | 1:120:A:ALA:H    | 1:120:A:ALA:HA  | 12       | 0.16          |
| (1,2514) | 1:120:A:ALA:H    | 1:120:A:ALA:HA  | 14       | 0.16          |
| (1,2514) | 1:120:A:ALA:H    | 1:120:A:ALA:HA  | 17       | 0.16          |
| (1,2489) | 1:28:A:ILE:HA    | 1:28:A:ILE:HG22 | 6        | 0.16          |
| (1,2489) | 1:28:A:ILE:HA    | 1:28:A:ILE:HG22 | 10       | 0.16          |
| (1,2489) | 1:28:A:ILE:HA    | 1:28:A:ILE:HG22 | 13       | 0.16          |
| (1,2489) | 1:28:A:ILE:HA    | 1:28:A:ILE:HG21 | 14       | 0.16          |
| (1,2480) | 1:71:A:LEU:HB2   | 1:27:A:VAL:HG12 | 16       | 0.16          |
| (1,2469) | 1:53:A:PHE:HZ    | 1:72:A:ARG:HG3  | 1        | 0.16          |
| (1,2469) | 1:53:A:PHE:HZ    | 1:72:A:ARG:HG3  | 10       | 0.16          |
| (1,2469) | 1:53:A:PHE:HZ    | 1:72:A:ARG:HG3  | 12       | 0.16          |
| (1,2436) | 1:13:A:ASP:HB3   | 1:33:A:GLU:HB3  | 1        | 0.16          |
| (1,2416) | 1:45:A:ALA:HB1   | 1:45:A:ALA:H    | 4        | 0.16          |
| (1,2416) | 1:45:A:ALA:HB1   | 1:45:A:ALA:H    | 5        | 0.16          |
| (1,2351) | 1:110:A:VAL:HG21 | 1:109:A:HIS:HA  | 3        | 0.16          |
| (1,2351) | 1:110:A:VAL:HG23 | 1:109:A:HIS:HA  | 6        | 0.16          |
| (1,2351) | 1:110:A:VAL:HG22 | 1:109:A:HIS:HA  | 13       | 0.16          |
| (1,2341) | 1:66:A:LEU:HD21  | 1:70:A:GLN:H    | 12       | 0.16          |
| (1,2299) | 1:55:A:ASP:HB3   | 1:96:A:ASP:HA   | 10       | 0.16          |
| (1,2288) | 1:70:A:GLN:HA    | 1:70:A:GLN:HG3  | 2        | 0.16          |
| (1,2288) | 1:70:A:GLN:HA    | 1:70:A:GLN:HG3  | 9        | 0.16          |
| (1,2288) | 1:70:A:GLN:HA    | 1:70:A:GLN:HG3  | 12       | 0.16          |
| (1,2283) | 1:33:A:GLU:HG2   | 1:33:A:GLU:HA   | 6        | 0.16          |
| (1,2221) | 1:31:A:LEU:HA    | 1:60:A:VAL:HB   | 6        | 0.16          |
| (1,2221) | 1:31:A:LEU:HA    | 1:60:A:VAL:HB   | 8        | 0.16          |
| (1,2221) | 1:31:A:LEU:HA    | 1:60:A:VAL:HB   | 16       | 0.16          |
| (1,2197) | 1:39:A:PHE:HD1   | 1:56:A:LEU:HA   | 15       | 0.16          |
| (1,2185) | 1:53:A:PHE:H     | 1:97:A:LEU:HD23 | 3        | 0.16          |
| (1,2170) | 1:22:A:ASN:H     | 1:22:A:ASN:HB2  | 11       | 0.16          |
| (1,2169) | 1:22:A:ASN:HB3   | 1:22:A:ASN:H    | 10       | 0.16          |
| (1,2169) | 1:22:A:ASN:HB3   | 1:22:A:ASN:H    | 14       | 0.16          |
| (1,2140) | 1:84:A:TYR:HB2   | 1:82:A:TRP:HA   | 3        | 0.16          |
| (1,2140) | 1:84:A:TYR:HB2   | 1:82:A:TRP:HA   | 5        | 0.16          |
| (1,2140) | 1:84:A:TYR:HB2   | 1:82:A:TRP:HA   | 9        | 0.16          |
| (1,2140) | 1:84:A:TYR:HB2   | 1:82:A:TRP:HA   | 11       | 0.16          |
| (1,2116) | 1:45:A:ALA:HB3   | 1:84:A:TYR:HA   | 5        | 0.16          |
| (1,2116) | 1:45:A:ALA:HB3   | 1:84:A:TYR:HA   | 11       | 0.16          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2094) | 1:95:A:VAL:HG22  | 1:97:A:LEU:HD22  | 4        | 0.16          |
| (1,2089) | 1:49:A:LYS:HB2   | 1:52:A:ILE:H     | 2        | 0.16          |
| (1,2079) | 1:66:A:LEU:HD13  | 1:62:A:GLY:H     | 2        | 0.16          |
| (1,2045) | 1:77:A:LEU:H     | 1:78:A:TYR:H     | 10       | 0.16          |
| (1,2045) | 1:77:A:LEU:H     | 1:78:A:TYR:H     | 14       | 0.16          |
| (1,2037) | 1:57:A:VAL:HG23  | 1:57:A:VAL:HG13  | 17       | 0.16          |
| (1,2035) | 1:52:A:ILE:HG13  | 1:97:A:LEU:HD23  | 2        | 0.16          |
| (1,2021) | 1:53:A:PHE:HE2   | 1:57:A:VAL:HG11  | 12       | 0.16          |
| (1,2005) | 1:95:A:VAL:HG23  | 1:48:A:LEU:HD11  | 13       | 0.16          |
| (1,1963) | 1:120:A:ALA:HB1  | 1:82:A:TRP:HE1   | 9        | 0.16          |
| (1,1963) | 1:120:A:ALA:HB2  | 1:82:A:TRP:HE1   | 11       | 0.16          |
| (1,1955) | 1:92:A:ALA:HB1   | 1:113:A:ALA:HB1  | 11       | 0.16          |
| (1,1952) | 1:112:A:HIS:HA   | 1:115:A:LYS:HB3  | 14       | 0.16          |
| (1,1939) | 1:33:A:GLU:HB3   | 1:30:A:PHE:HA    | 10       | 0.16          |
| (1,1928) | 1:105:A:LEU:HB3  | 1:109:A:HIS:HB2  | 4        | 0.16          |
| (1,1928) | 1:105:A:LEU:HB3  | 1:109:A:HIS:HB2  | 15       | 0.16          |
| (1,1928) | 1:105:A:LEU:HB3  | 1:109:A:HIS:HB2  | 17       | 0.16          |
| (1,1889) | 1:65:A:ASN:H     | 1:65:A:ASN:HB3   | 13       | 0.16          |
| (1,1889) | 1:65:A:ASN:H     | 1:65:A:ASN:HB3   | 16       | 0.16          |
| (1,1877) | 1:27:A:VAL:HG21  | 1:27:A:VAL:H     | 5        | 0.16          |
| (1,1877) | 1:27:A:VAL:HG23  | 1:27:A:VAL:H     | 14       | 0.16          |
| (1,1865) | 1:45:A:ALA:HB3   | 1:44:A:GLU:HB3   | 2        | 0.16          |
| (1,1824) | 1:27:A:VAL:HA    | 1:21:A:LEU:HD13  | 9        | 0.16          |
| (1,1817) | 1:77:A:LEU:HG    | 1:77:A:LEU:HD22  | 2        | 0.16          |
| (1,1811) | 1:86:A:TYR:H     | 1:117:A:LEU:HD11 | 8        | 0.16          |
| (1,1775) | 1:88:A:VAL:HA    | 1:47:A:PRO:HB3   | 9        | 0.16          |
| (1,1775) | 1:88:A:VAL:HA    | 1:47:A:PRO:HB3   | 13       | 0.16          |
| (1,1775) | 1:88:A:VAL:HA    | 1:47:A:PRO:HB3   | 16       | 0.16          |
| (1,1773) | 1:24:A:SER:HA    | 1:27:A:VAL:HG21  | 17       | 0.16          |
| (1,1727) | 1:66:A:LEU:HD11  | 1:30:A:PHE:HD2   | 5        | 0.16          |
| (1,1726) | 1:66:A:LEU:HD12  | 1:66:A:LEU:HA    | 12       | 0.16          |
| (1,1713) | 1:20:A:LYS:H     | 1:20:A:LYS:HD3   | 1        | 0.16          |
| (1,1709) | 1:72:A:ARG:HB3   | 1:53:A:PHE:HE2   | 17       | 0.16          |
| (1,1681) | 1:40:A:SER:HA    | 1:41:A:ALA:HB1   | 1        | 0.16          |
| (1,1638) | 1:124:A:VAL:HG12 | 1:124:A:VAL:HA   | 3        | 0.16          |
| (1,1638) | 1:124:A:VAL:HG11 | 1:124:A:VAL:HA   | 6        | 0.16          |
| (1,1638) | 1:124:A:VAL:HG12 | 1:124:A:VAL:HA   | 7        | 0.16          |
| (1,1638) | 1:124:A:VAL:HG12 | 1:124:A:VAL:HA   | 9        | 0.16          |
| (1,1638) | 1:124:A:VAL:HG13 | 1:124:A:VAL:HA   | 10       | 0.16          |
| (1,1638) | 1:124:A:VAL:HG13 | 1:124:A:VAL:HA   | 11       | 0.16          |
| (1,1638) | 1:124:A:VAL:HG12 | 1:124:A:VAL:HA   | 12       | 0.16          |
| (1,1638) | 1:124:A:VAL:HG13 | 1:124:A:VAL:HA   | 14       | 0.16          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1638) | 1:124:A:VAL:HG13 | 1:124:A:VAL:HA  | 15       | 0.16          |
| (1,1638) | 1:124:A:VAL:HG13 | 1:124:A:VAL:HA  | 16       | 0.16          |
| (1,1616) | 1:109:A:HIS:HB2  | 1:108:A:GLN:H   | 5        | 0.16          |
| (1,1613) | 1:124:A:VAL:HG22 | 1:121:A:LYS:HA  | 12       | 0.16          |
| (1,1599) | 1:53:A:PHE:HB3   | 1:75:A:LEU:HD23 | 1        | 0.16          |
| (1,1599) | 1:53:A:PHE:HB3   | 1:75:A:LEU:HD23 | 6        | 0.16          |
| (1,1599) | 1:53:A:PHE:HB3   | 1:75:A:LEU:HD21 | 16       | 0.16          |
| (1,1590) | 1:61:A:ALA:HB3   | 1:61:A:ALA:H    | 5        | 0.16          |
| (1,1580) | 1:97:A:LEU:HA    | 1:97:A:LEU:H    | 5        | 0.16          |
| (1,1580) | 1:97:A:LEU:HA    | 1:97:A:LEU:H    | 7        | 0.16          |
| (1,1580) | 1:97:A:LEU:HA    | 1:97:A:LEU:H    | 16       | 0.16          |
| (1,1553) | 1:57:A:VAL:HG12  | 1:61:A:ALA:H    | 1        | 0.16          |
| (1,1546) | 1:56:A:LEU:HD13  | 1:52:A:ILE:HG13 | 2        | 0.16          |
| (1,1546) | 1:56:A:LEU:HD13  | 1:52:A:ILE:HG13 | 5        | 0.16          |
| (1,1546) | 1:56:A:LEU:HD13  | 1:52:A:ILE:HG13 | 14       | 0.16          |
| (1,1513) | 1:52:A:ILE:HG21  | 1:53:A:PHE:HB3  | 2        | 0.16          |
| (1,1511) | 1:28:A:ILE:HA    | 1:28:A:ILE:HG22 | 5        | 0.16          |
| (1,1511) | 1:28:A:ILE:HA    | 1:28:A:ILE:HG22 | 6        | 0.16          |
| (1,1511) | 1:28:A:ILE:HA    | 1:28:A:ILE:HG22 | 10       | 0.16          |
| (1,1480) | 1:64:A:MET:HE2   | 1:63:A:GLU:H    | 16       | 0.16          |
| (1,1440) | 1:105:A:LEU:H    | 1:101:A:PRO:HD3 | 4        | 0.16          |
| (1,1440) | 1:105:A:LEU:H    | 1:101:A:PRO:HD3 | 5        | 0.16          |
| (1,1440) | 1:105:A:LEU:H    | 1:101:A:PRO:HD3 | 10       | 0.16          |
| (1,1440) | 1:105:A:LEU:H    | 1:101:A:PRO:HD3 | 14       | 0.16          |
| (1,1440) | 1:105:A:LEU:H    | 1:101:A:PRO:HD3 | 15       | 0.16          |
| (1,1439) | 1:103:A:GLY:HA3  | 1:101:A:PRO:HD3 | 7        | 0.16          |
| (1,1414) | 1:74:A:ALA:HB2   | 1:75:A:LEU:HD12 | 15       | 0.16          |
| (1,1412) | 1:39:A:PHE:HZ    | 1:75:A:LEU:HD13 | 17       | 0.16          |
| (1,1409) | 1:57:A:VAL:HG23  | 1:57:A:VAL:HG13 | 17       | 0.16          |
| (1,1403) | 1:95:A:VAL:HG23  | 1:95:A:VAL:HG12 | 9        | 0.16          |
| (1,1399) | 1:95:A:VAL:HG21  | 1:95:A:VAL:H    | 4        | 0.16          |
| (1,1397) | 1:31:A:LEU:HD22  | 1:60:A:VAL:HG13 | 3        | 0.16          |
| (1,1382) | 1:57:A:VAL:HG23  | 1:53:A:PHE:HE1  | 3        | 0.16          |
| (1,1371) | 1:28:A:ILE:HD12  | 1:75:A:LEU:H    | 6        | 0.16          |
| (1,1363) | 1:29:A:ALA:HA    | 1:32:A:ALA:HB2  | 14       | 0.16          |
| (1,1358) | 1:32:A:ALA:HB1   | 1:33:A:GLU:H    | 8        | 0.16          |
| (1,1356) | 1:61:A:ALA:HB3   | 1:57:A:VAL:HG12 | 3        | 0.16          |
| (1,1352) | 1:122:A:ALA:HB3  | 1:122:A:ALA:H   | 13       | 0.16          |
| (1,1352) | 1:122:A:ALA:HB1  | 1:122:A:ALA:H   | 17       | 0.16          |
| (1,1350) | 1:129:A:ALA:HB2  | 1:129:A:ALA:H   | 5        | 0.16          |
| (1,1331) | 1:78:A:TYR:HE1   | 1:84:A:TYR:HD1  | 11       | 0.16          |
| (1,1329) | 1:73:A:SER:HB3   | 1:74:A:ALA:H    | 1        | 0.16          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1329) | 1:73:A:SER:HB3   | 1:74:A:ALA:H    | 2        | 0.16          |
| (1,1329) | 1:73:A:SER:HB3   | 1:74:A:ALA:H    | 6        | 0.16          |
| (1,1329) | 1:73:A:SER:HB3   | 1:74:A:ALA:H    | 8        | 0.16          |
| (1,1329) | 1:73:A:SER:HB3   | 1:74:A:ALA:H    | 9        | 0.16          |
| (1,1329) | 1:73:A:SER:HB3   | 1:74:A:ALA:H    | 14       | 0.16          |
| (1,1325) | 1:53:A:PHE:HE1   | 1:75:A:LEU:HB3  | 1        | 0.16          |
| (1,1325) | 1:53:A:PHE:HE1   | 1:75:A:LEU:HB3  | 2        | 0.16          |
| (1,1325) | 1:53:A:PHE:HE2   | 1:75:A:LEU:HB3  | 4        | 0.16          |
| (1,1325) | 1:53:A:PHE:HE1   | 1:75:A:LEU:HB3  | 5        | 0.16          |
| (1,1325) | 1:53:A:PHE:HE2   | 1:75:A:LEU:HB3  | 17       | 0.16          |
| (1,1275) | 1:84:A:TYR:HE2   | 1:84:A:TYR:HB3  | 6        | 0.16          |
| (1,1253) | 1:47:A:PRO:HB3   | 1:87:A:GLY:HA2  | 12       | 0.16          |
| (1,1240) | 1:78:A:TYR:HE1   | 1:79:A:THR:HB   | 15       | 0.16          |
| (1,1239) | 1:79:A:THR:H     | 1:78:A:TYR:HE1  | 11       | 0.16          |
| (1,1224) | 1:13:A:ASP:HB2   | 1:16:A:GLU:H    | 8        | 0.16          |
| (1,1224) | 1:13:A:ASP:HB2   | 1:16:A:GLU:H    | 17       | 0.16          |
| (1,1206) | 1:117:A:LEU:HD13 | 1:86:A:TYR:HB2  | 3        | 0.16          |
| (1,1167) | 1:34:A:ARG:HB3   | 1:30:A:PHE:HD1  | 9        | 0.16          |
| (1,1167) | 1:34:A:ARG:HB3   | 1:30:A:PHE:HD1  | 15       | 0.16          |
| (1,1147) | 1:83:A:ARG:HB2   | 1:86:A:TYR:HD1  | 17       | 0.16          |
| (1,1108) | 1:56:A:LEU:HD12  | 1:52:A:ILE:HG12 | 16       | 0.16          |
| (1,1108) | 1:56:A:LEU:HD12  | 1:52:A:ILE:HG12 | 17       | 0.16          |
| (1,1078) | 1:48:A:LEU:HD22  | 1:84:A:TYR:HE2  | 17       | 0.16          |
| (1,1073) | 1:97:A:LEU:HD11  | 1:97:A:LEU:H    | 3        | 0.16          |
| (1,1053) | 1:93:A:THR:HG21  | 1:102:A:CYS:HA  | 2        | 0.16          |
| (1,1049) | 1:59:A:ARG:HB2   | 1:60:A:VAL:HG11 | 4        | 0.16          |
| (1,1049) | 1:59:A:ARG:HB2   | 1:60:A:VAL:HG11 | 9        | 0.16          |
| (1,1049) | 1:59:A:ARG:HB2   | 1:60:A:VAL:HG13 | 15       | 0.16          |
| (1,993)  | 1:79:A:THR:HG21  | 1:75:A:LEU:HA   | 6        | 0.16          |
| (1,993)  | 1:79:A:THR:HG21  | 1:75:A:LEU:HA   | 7        | 0.16          |
| (1,993)  | 1:79:A:THR:HG22  | 1:75:A:LEU:HA   | 13       | 0.16          |
| (1,993)  | 1:79:A:THR:HG21  | 1:75:A:LEU:HA   | 17       | 0.16          |
| (1,755)  | 1:95:A:VAL:H     | 1:94:A:ARG:HB3  | 5        | 0.16          |
| (1,753)  | 1:92:A:ALA:HB1   | 1:91:A:GLY:H    | 16       | 0.16          |
| (1,665)  | 1:122:A:ALA:HB3  | 1:123:A:ARG:H   | 2        | 0.16          |
| (1,665)  | 1:122:A:ALA:HB1  | 1:123:A:ARG:H   | 8        | 0.16          |
| (1,665)  | 1:122:A:ALA:HB2  | 1:123:A:ARG:H   | 11       | 0.16          |
| (1,665)  | 1:122:A:ALA:HB1  | 1:123:A:ARG:H   | 12       | 0.16          |
| (1,665)  | 1:122:A:ALA:HB3  | 1:123:A:ARG:H   | 15       | 0.16          |
| (1,665)  | 1:122:A:ALA:HB3  | 1:123:A:ARG:H   | 17       | 0.16          |
| (1,645)  | 1:115:A:LYS:HE3  | 1:115:A:LYS:H   | 6        | 0.16          |
| (1,645)  | 1:115:A:LYS:HE3  | 1:115:A:LYS:H   | 9        | 0.16          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,635) | 1:127:A:GLN:H   | 1:127:A:GLN:HB3 | 4        | 0.16          |
| (1,635) | 1:127:A:GLN:H   | 1:127:A:GLN:HB3 | 12       | 0.16          |
| (1,614) | 1:97:A:LEU:HD11 | 1:97:A:LEU:H    | 3        | 0.16          |
| (1,604) | 1:32:A:ALA:HB2  | 1:41:A:ALA:H    | 2        | 0.16          |
| (1,593) | 1:17:A:ASN:HA   | 1:18:A:GLN:H    | 12       | 0.16          |
| (1,549) | 1:97:A:LEU:HD11 | 1:98:A:ASP:H    | 15       | 0.16          |
| (1,512) | 1:13:A:ASP:HB2  | 1:13:A:ASP:H    | 5        | 0.16          |
| (1,511) | 1:13:A:ASP:HB3  | 1:13:A:ASP:H    | 17       | 0.16          |
| (1,478) | 1:27:A:VAL:HG21 | 1:29:A:ALA:H    | 2        | 0.16          |
| (1,477) | 1:31:A:LEU:H    | 1:31:A:LEU:HD13 | 4        | 0.16          |
| (1,477) | 1:31:A:LEU:H    | 1:31:A:LEU:HD13 | 6        | 0.16          |
| (1,451) | 1:32:A:ALA:HB2  | 1:35:A:PHE:H    | 11       | 0.16          |
| (1,423) | 1:50:A:ILE:HG21 | 1:50:A:ILE:H    | 10       | 0.16          |
| (1,397) | 1:57:A:VAL:H    | 1:56:A:LEU:HB3  | 13       | 0.16          |
| (1,351) | 1:63:A:GLU:HB3  | 1:65:A:ASN:H    | 1        | 0.16          |
| (1,348) | 1:65:A:ASN:HB2  | 1:65:A:ASN:H    | 14       | 0.16          |
| (1,287) | 1:127:A:GLN:H   | 1:127:A:GLN:HG2 | 13       | 0.16          |
| (1,234) | 1:95:A:VAL:HG22 | 1:99:A:GLY:H    | 13       | 0.16          |
| (1,156) | 1:126:A:ALA:HB2 | 1:126:A:ALA:H   | 1        | 0.16          |
| (1,153) | 1:129:A:ALA:HA  | 1:129:A:ALA:H   | 11       | 0.16          |
| (1,134) | 1:123:A:ARG:H   | 1:121:A:LYS:H   | 7        | 0.16          |
| (1,134) | 1:123:A:ARG:H   | 1:121:A:LYS:H   | 9        | 0.16          |
| (1,134) | 1:123:A:ARG:H   | 1:121:A:LYS:H   | 11       | 0.16          |
| (1,134) | 1:123:A:ARG:H   | 1:121:A:LYS:H   | 14       | 0.16          |
| (1,134) | 1:123:A:ARG:H   | 1:121:A:LYS:H   | 15       | 0.16          |
| (1,128) | 1:35:A:PHE:HD2  | 1:39:A:PHE:H    | 4        | 0.16          |
| (1,101) | 1:35:A:PHE:H    | 1:39:A:PHE:HE2  | 1        | 0.16          |
| (1,101) | 1:35:A:PHE:H    | 1:39:A:PHE:HE2  | 2        | 0.16          |
| (1,101) | 1:35:A:PHE:H    | 1:39:A:PHE:HE1  | 16       | 0.16          |
| (1,100) | 1:35:A:PHE:HE2  | 1:35:A:PHE:H    | 9        | 0.16          |
| (1,80)  | 1:30:A:PHE:HD2  | 1:30:A:PHE:H    | 15       | 0.16          |
| (3,137) | 1:123:A:ARG:H   | 1:123:A:ARG:HA  | 4        | 0.15          |
| (3,137) | 1:123:A:ARG:H   | 1:123:A:ARG:HA  | 15       | 0.15          |
| (3,135) | 1:123:A:ARG:HB3 | 1:120:A:ALA:HA  | 13       | 0.15          |
| (3,122) | 1:27:A:VAL:HG21 | 1:28:A:ILE:HD12 | 9        | 0.15          |
| (3,106) | 1:68:A:LYS:HD2  | 1:68:A:LYS:HA   | 10       | 0.15          |
| (3,106) | 1:68:A:LYS:HD2  | 1:68:A:LYS:HA   | 12       | 0.15          |
| (3,94)  | 1:56:A:LEU:HB2  | 1:75:A:LEU:HD11 | 8        | 0.15          |
| (3,92)  | 1:88:A:VAL:HG23 | 1:87:A:GLY:HA2  | 2        | 0.15          |
| (3,92)  | 1:88:A:VAL:HG21 | 1:87:A:GLY:HA2  | 5        | 0.15          |
| (3,62)  | 1:52:A:ILE:HG22 | 1:56:A:LEU:H    | 10       | 0.15          |
| (3,54)  | 1:71:A:LEU:HB3  | 1:75:A:LEU:HD12 | 4        | 0.15          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,54)   | 1:71:A:LEU:HB3  | 1:75:A:LEU:HD12 | 13       | 0.15          |
| (3,41)   | 1:52:A:ILE:HD11 | 1:56:A:LEU:HA   | 10       | 0.15          |
| (3,34)   | 1:97:A:LEU:HD23 | 1:31:A:LEU:HD12 | 3        | 0.15          |
| (3,34)   | 1:97:A:LEU:HD21 | 1:31:A:LEU:HD12 | 13       | 0.15          |
| (3,22)   | 1:48:A:LEU:HD11 | 1:97:A:LEU:H    | 6        | 0.15          |
| (3,22)   | 1:48:A:LEU:HD12 | 1:97:A:LEU:H    | 15       | 0.15          |
| (3,14)   | 1:82:A:TRP:HA   | 1:85:A:LEU:HB2  | 15       | 0.15          |
| (1,4344) | 1:120:A:ALA:H   | 1:119:A:GLU:HG2 | 2        | 0.15          |
| (1,4343) | 1:118:A:GLU:H   | 1:119:A:GLU:H   | 4        | 0.15          |
| (1,4343) | 1:118:A:GLU:H   | 1:119:A:GLU:H   | 15       | 0.15          |
| (1,4326) | 1:65:A:ASN:HA   | 1:66:A:LEU:H    | 15       | 0.15          |
| (1,4323) | 1:62:A:GLY:H    | 1:68:A:LYS:HD2  | 2        | 0.15          |
| (1,4320) | 1:62:A:GLY:H    | 1:66:A:LEU:H    | 8        | 0.15          |
| (1,4320) | 1:62:A:GLY:H    | 1:66:A:LEU:H    | 13       | 0.15          |
| (1,4317) | 1:93:A:THR:HB   | 1:102:A:CYS:H   | 8        | 0.15          |
| (1,4317) | 1:93:A:THR:HB   | 1:102:A:CYS:H   | 9        | 0.15          |
| (1,4317) | 1:93:A:THR:HB   | 1:102:A:CYS:H   | 11       | 0.15          |
| (1,4317) | 1:93:A:THR:HB   | 1:102:A:CYS:H   | 12       | 0.15          |
| (1,4317) | 1:93:A:THR:HB   | 1:102:A:CYS:H   | 13       | 0.15          |
| (1,4317) | 1:93:A:THR:HB   | 1:102:A:CYS:H   | 14       | 0.15          |
| (1,4316) | 1:95:A:VAL:H    | 1:94:A:ARG:HB3  | 4        | 0.15          |
| (1,4316) | 1:95:A:VAL:H    | 1:94:A:ARG:HB3  | 10       | 0.15          |
| (1,4301) | 1:97:A:LEU:HB2  | 1:97:A:LEU:H    | 6        | 0.15          |
| (1,4301) | 1:97:A:LEU:HB2  | 1:97:A:LEU:H    | 9        | 0.15          |
| (1,4301) | 1:97:A:LEU:HB2  | 1:97:A:LEU:H    | 11       | 0.15          |
| (1,4278) | 1:12:A:GLN:HA   | 1:13:A:ASP:H    | 15       | 0.15          |
| (1,4273) | 1:73:A:SER:HA   | 1:75:A:LEU:H    | 1        | 0.15          |
| (1,4273) | 1:73:A:SER:HA   | 1:75:A:LEU:H    | 6        | 0.15          |
| (1,4273) | 1:73:A:SER:HA   | 1:75:A:LEU:H    | 9        | 0.15          |
| (1,4273) | 1:73:A:SER:HA   | 1:75:A:LEU:H    | 14       | 0.15          |
| (1,4270) | 1:75:A:LEU:HB3  | 1:74:A:ALA:H    | 1        | 0.15          |
| (1,4270) | 1:75:A:LEU:HB3  | 1:74:A:ALA:H    | 8        | 0.15          |
| (1,4260) | 1:38:A:CYS:H    | 1:35:A:PHE:HD1  | 14       | 0.15          |
| (1,4260) | 1:38:A:CYS:H    | 1:35:A:PHE:HD2  | 16       | 0.15          |
| (1,4225) | 1:122:A:ALA:HB2 | 1:123:A:ARG:H   | 1        | 0.15          |
| (1,4212) | 1:115:A:LYS:HE3 | 1:115:A:LYS:H   | 1        | 0.15          |
| (1,4212) | 1:115:A:LYS:HE3 | 1:115:A:LYS:H   | 7        | 0.15          |
| (1,4212) | 1:115:A:LYS:HE3 | 1:115:A:LYS:H   | 10       | 0.15          |
| (1,4198) | 1:127:A:GLN:HA  | 1:127:A:GLN:H   | 3        | 0.15          |
| (1,4198) | 1:127:A:GLN:HA  | 1:127:A:GLN:H   | 12       | 0.15          |
| (1,4193) | 1:69:A:THR:HB   | 1:72:A:ARG:H    | 3        | 0.15          |
| (1,4193) | 1:69:A:THR:HB   | 1:72:A:ARG:H    | 9        | 0.15          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,4170) | 1:49:A:LYS:HB2  | 1:49:A:LYS:H    | 7        | 0.15          |
| (1,4170) | 1:49:A:LYS:HB2  | 1:49:A:LYS:H    | 10       | 0.15          |
| (1,4165) | 1:40:A:SER:HA   | 1:43:A:GLY:H    | 6        | 0.15          |
| (1,4148) | 1:25:A:LYS:HB2  | 1:26:A:GLU:H    | 3        | 0.15          |
| (1,4148) | 1:25:A:LYS:HB2  | 1:26:A:GLU:H    | 9        | 0.15          |
| (1,4148) | 1:25:A:LYS:HB2  | 1:26:A:GLU:H    | 10       | 0.15          |
| (1,4148) | 1:25:A:LYS:HB2  | 1:26:A:GLU:H    | 17       | 0.15          |
| (1,4133) | 1:82:A:TRP:HE1  | 1:82:A:TRP:HD1  | 11       | 0.15          |
| (1,4133) | 1:82:A:TRP:HE1  | 1:82:A:TRP:HD1  | 14       | 0.15          |
| (1,4119) | 1:66:A:LEU:HB2  | 1:70:A:GLN:HE22 | 4        | 0.15          |
| (1,4110) | 1:40:A:SER:HA   | 1:42:A:GLU:H    | 11       | 0.15          |
| (1,4084) | 1:20:A:LYS:HB3  | 1:22:A:ASN:HD22 | 7        | 0.15          |
| (1,4060) | 1:97:A:LEU:HD21 | 1:39:A:PHE:H    | 7        | 0.15          |
| (1,4041) | 1:21:A:LEU:HA   | 1:23:A:SER:H    | 8        | 0.15          |
| (1,4040) | 1:25:A:LYS:HG3  | 1:25:A:LYS:H    | 8        | 0.15          |
| (1,4019) | 1:33:A:GLU:HB3  | 1:34:A:ARG:H    | 5        | 0.15          |
| (1,3994) | 1:45:A:ALA:H    | 1:83:A:ARG:HB2  | 3        | 0.15          |
| (1,3987) | 1:50:A:ILE:HG21 | 1:50:A:ILE:H    | 7        | 0.15          |
| (1,3979) | 1:50:A:ILE:HA   | 1:51:A:GLY:H    | 4        | 0.15          |
| (1,3940) | 1:62:A:GLY:HA3  | 1:63:A:GLU:H    | 2        | 0.15          |
| (1,3940) | 1:62:A:GLY:HA3  | 1:63:A:GLU:H    | 4        | 0.15          |
| (1,3940) | 1:62:A:GLY:HA3  | 1:63:A:GLU:H    | 6        | 0.15          |
| (1,3940) | 1:62:A:GLY:HA3  | 1:63:A:GLU:H    | 8        | 0.15          |
| (1,3940) | 1:62:A:GLY:HA3  | 1:63:A:GLU:H    | 14       | 0.15          |
| (1,3935) | 1:63:A:GLU:HB3  | 1:65:A:ASN:H    | 7        | 0.15          |
| (1,3929) | 1:68:A:LYS:HD2  | 1:68:A:LYS:H    | 1        | 0.15          |
| (1,3929) | 1:68:A:LYS:HD2  | 1:68:A:LYS:H    | 13       | 0.15          |
| (1,3917) | 1:74:A:ALA:HA   | 1:75:A:LEU:H    | 1        | 0.15          |
| (1,3916) | 1:71:A:LEU:HA   | 1:74:A:ALA:H    | 2        | 0.15          |
| (1,3916) | 1:71:A:LEU:HA   | 1:74:A:ALA:H    | 11       | 0.15          |
| (1,3916) | 1:71:A:LEU:HA   | 1:74:A:ALA:H    | 13       | 0.15          |
| (1,3907) | 1:76:A:ARG:HD2  | 1:77:A:LEU:H    | 5        | 0.15          |
| (1,3907) | 1:76:A:ARG:HD2  | 1:77:A:LEU:H    | 14       | 0.15          |
| (1,3887) | 1:81:A:SER:HB2  | 1:82:A:TRP:H    | 2        | 0.15          |
| (1,3884) | 1:83:A:ARG:H    | 1:83:A:ARG:HB2  | 11       | 0.15          |
| (1,3879) | 1:127:A:GLN:H   | 1:127:A:GLN:HG2 | 9        | 0.15          |
| (1,3859) | 1:90:A:PRO:HB2  | 1:91:A:GLY:H    | 14       | 0.15          |
| (1,3830) | 1:101:A:PRO:HD3 | 1:100:A:ASN:H   | 13       | 0.15          |
| (1,3830) | 1:101:A:PRO:HD3 | 1:100:A:ASN:H   | 14       | 0.15          |
| (1,3797) | 1:44:A:GLU:HA   | 1:44:A:GLU:H    | 1        | 0.15          |
| (1,3797) | 1:44:A:GLU:HA   | 1:44:A:GLU:H    | 3        | 0.15          |
| (1,3797) | 1:44:A:GLU:HA   | 1:44:A:GLU:H    | 5        | 0.15          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3797) | 1:44:A:GLU:HA    | 1:44:A:GLU:H     | 7        | 0.15          |
| (1,3783) | 1:117:A:LEU:HB3  | 1:117:A:LEU:H    | 8        | 0.15          |
| (1,3768) | 1:130:A:GLU:H    | 1:130:A:GLU:HA   | 1        | 0.15          |
| (1,3768) | 1:130:A:GLU:H    | 1:130:A:GLU:HA   | 12       | 0.15          |
| (1,3768) | 1:130:A:GLU:H    | 1:130:A:GLU:HA   | 17       | 0.15          |
| (1,3767) | 1:129:A:ALA:HA   | 1:129:A:ALA:H    | 2        | 0.15          |
| (1,3766) | 1:128:A:ARG:HB3  | 1:129:A:ALA:H    | 6        | 0.15          |
| (1,3744) | 1:35:A:PHE:HD2   | 1:39:A:PHE:H     | 14       | 0.15          |
| (1,3731) | 1:66:A:LEU:HB3   | 1:66:A:LEU:H     | 5        | 0.15          |
| (1,3731) | 1:66:A:LEU:HB3   | 1:66:A:LEU:H     | 11       | 0.15          |
| (1,3599) | 1:92:A:ALA:HB3   | 1:113:A:ALA:HB1  | 5        | 0.15          |
| (1,3582) | 1:110:A:VAL:H    | 1:109:A:HIS:HA   | 6        | 0.15          |
| (1,3582) | 1:110:A:VAL:H    | 1:109:A:HIS:HA   | 7        | 0.15          |
| (1,3582) | 1:110:A:VAL:H    | 1:109:A:HIS:HA   | 14       | 0.15          |
| (1,3537) | 1:51:A:GLY:HA2   | 1:54:A:GLN:HB2   | 8        | 0.15          |
| (1,3537) | 1:51:A:GLY:HA2   | 1:54:A:GLN:HB2   | 9        | 0.15          |
| (1,3537) | 1:51:A:GLY:HA2   | 1:54:A:GLN:HB2   | 12       | 0.15          |
| (1,3523) | 1:56:A:LEU:HG    | 1:56:A:LEU:HB3   | 16       | 0.15          |
| (1,3523) | 1:56:A:LEU:HG    | 1:56:A:LEU:HB3   | 17       | 0.15          |
| (1,3520) | 1:100:A:ASN:HD22 | 1:98:A:ASP:HB3   | 16       | 0.15          |
| (1,3516) | 1:21:A:LEU:HG    | 1:65:A:ASN:HB3   | 9        | 0.15          |
| (1,3515) | 1:102:A:CYS:HB3  | 1:49:A:LYS:HA    | 2        | 0.15          |
| (1,3515) | 1:102:A:CYS:HB3  | 1:49:A:LYS:HA    | 3        | 0.15          |
| (1,3513) | 1:72:A:ARG:HG3   | 1:73:A:SER:HB3   | 6        | 0.15          |
| (1,3513) | 1:72:A:ARG:HG3   | 1:73:A:SER:HB3   | 8        | 0.15          |
| (1,3511) | 1:50:A:ILE:HG13  | 1:49:A:LYS:HA    | 4        | 0.15          |
| (1,3502) | 1:27:A:VAL:HG23  | 1:27:A:VAL:H     | 1        | 0.15          |
| (1,3502) | 1:27:A:VAL:HG21  | 1:27:A:VAL:H     | 2        | 0.15          |
| (1,3502) | 1:27:A:VAL:HG21  | 1:27:A:VAL:H     | 3        | 0.15          |
| (1,3502) | 1:27:A:VAL:HG21  | 1:27:A:VAL:H     | 10       | 0.15          |
| (1,3502) | 1:27:A:VAL:HG23  | 1:27:A:VAL:H     | 11       | 0.15          |
| (1,3497) | 1:27:A:VAL:HA    | 1:27:A:VAL:HG11  | 12       | 0.15          |
| (1,3465) | 1:88:A:VAL:HG23  | 1:85:A:LEU:HB3   | 17       | 0.15          |
| (1,3457) | 1:20:A:LYS:HE3   | 1:19:A:PRO:HA    | 4        | 0.15          |
| (1,3457) | 1:20:A:LYS:HE3   | 1:19:A:PRO:HA    | 6        | 0.15          |
| (1,3457) | 1:20:A:LYS:HE3   | 1:19:A:PRO:HA    | 11       | 0.15          |
| (1,3456) | 1:95:A:VAL:HG23  | 1:96:A:ASP:HA    | 12       | 0.15          |
| (1,3437) | 1:21:A:LEU:HB2   | 1:21:A:LEU:HD11  | 2        | 0.15          |
| (1,3422) | 1:77:A:LEU:HG    | 1:77:A:LEU:HD21  | 1        | 0.15          |
| (1,3415) | 1:117:A:LEU:HA   | 1:117:A:LEU:HD12 | 2        | 0.15          |
| (1,3398) | 1:117:A:LEU:HA   | 1:120:A:ALA:HB2  | 17       | 0.15          |
| (1,3378) | 1:67:A:SER:HB3   | 1:66:A:LEU:HA    | 5        | 0.15          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3370) | 1:24:A:SER:HA    | 1:27:A:VAL:HG11 | 3        | 0.15          |
| (1,3369) | 1:24:A:SER:HA    | 1:27:A:VAL:HG23 | 11       | 0.15          |
| (1,3369) | 1:24:A:SER:HA    | 1:27:A:VAL:HG23 | 16       | 0.15          |
| (1,3322) | 1:30:A:PHE:HD2   | 1:66:A:LEU:HD23 | 5        | 0.15          |
| (1,3322) | 1:30:A:PHE:HD2   | 1:66:A:LEU:HD21 | 11       | 0.15          |
| (1,3320) | 1:27:A:VAL:HA    | 1:66:A:LEU:HD21 | 15       | 0.15          |
| (1,3315) | 1:66:A:LEU:HD12  | 1:66:A:LEU:HA   | 5        | 0.15          |
| (1,3315) | 1:66:A:LEU:HD11  | 1:66:A:LEU:HA   | 6        | 0.15          |
| (1,3315) | 1:66:A:LEU:HD11  | 1:66:A:LEU:HA   | 9        | 0.15          |
| (1,3314) | 1:71:A:LEU:HD13  | 1:71:A:LEU:HG   | 12       | 0.15          |
| (1,3306) | 1:128:A:ARG:HG2  | 1:128:A:ARG:HD2 | 12       | 0.15          |
| (1,3306) | 1:128:A:ARG:HG2  | 1:128:A:ARG:HD2 | 15       | 0.15          |
| (1,3305) | 1:18:A:GLN:HB3   | 1:19:A:PRO:HD2  | 12       | 0.15          |
| (1,3299) | 1:20:A:LYS:H     | 1:20:A:LYS:HD3  | 6        | 0.15          |
| (1,3299) | 1:20:A:LYS:H     | 1:20:A:LYS:HD3  | 15       | 0.15          |
| (1,3282) | 1:44:A:GLU:HG2   | 1:45:A:ALA:HB3  | 6        | 0.15          |
| (1,3282) | 1:44:A:GLU:HG2   | 1:45:A:ALA:HB3  | 8        | 0.15          |
| (1,3275) | 1:119:A:GLU:HA   | 1:119:A:GLU:HG2 | 8        | 0.15          |
| (1,3275) | 1:119:A:GLU:HA   | 1:119:A:GLU:HG2 | 13       | 0.15          |
| (1,3270) | 1:42:A:GLU:HG2   | 1:41:A:ALA:HB1  | 17       | 0.15          |
| (1,3255) | 1:40:A:SER:HA    | 1:41:A:ALA:HB1  | 8        | 0.15          |
| (1,3255) | 1:40:A:SER:HA    | 1:41:A:ALA:HB1  | 17       | 0.15          |
| (1,3250) | 1:41:A:ALA:HA    | 1:41:A:ALA:HB2  | 10       | 0.15          |
| (1,3250) | 1:41:A:ALA:HA    | 1:41:A:ALA:HB2  | 16       | 0.15          |
| (1,3244) | 1:78:A:TYR:HA    | 1:28:A:ILE:HG12 | 2        | 0.15          |
| (1,3241) | 1:52:A:ILE:HG13  | 1:97:A:LEU:HD23 | 5        | 0.15          |
| (1,3221) | 1:37:A:HIS:HB2   | 1:99:A:GLY:HA2  | 3        | 0.15          |
| (1,3221) | 1:37:A:HIS:HB2   | 1:99:A:GLY:HA2  | 9        | 0.15          |
| (1,3210) | 1:128:A:ARG:HA   | 1:128:A:ARG:HB3 | 12       | 0.15          |
| (1,3208) | 1:124:A:VAL:HG11 | 1:124:A:VAL:HA  | 4        | 0.15          |
| (1,3208) | 1:124:A:VAL:HG13 | 1:124:A:VAL:HA  | 17       | 0.15          |
| (1,3200) | 1:116:A:GLN:HG3  | 1:113:A:ALA:HB3 | 11       | 0.15          |
| (1,3200) | 1:116:A:GLN:HG3  | 1:113:A:ALA:HB3 | 15       | 0.15          |
| (1,3197) | 1:87:A:GLY:HA3   | 1:113:A:ALA:HB1 | 4        | 0.15          |
| (1,3197) | 1:87:A:GLY:HA3   | 1:113:A:ALA:HB2 | 12       | 0.15          |
| (1,3197) | 1:87:A:GLY:HA3   | 1:113:A:ALA:HB1 | 17       | 0.15          |
| (1,3185) | 1:109:A:HIS:HB2  | 1:108:A:GLN:H   | 2        | 0.15          |
| (1,3185) | 1:109:A:HIS:HB2  | 1:108:A:GLN:H   | 7        | 0.15          |
| (1,3185) | 1:109:A:HIS:HB2  | 1:108:A:GLN:H   | 8        | 0.15          |
| (1,3185) | 1:109:A:HIS:HB2  | 1:108:A:GLN:H   | 12       | 0.15          |
| (1,3185) | 1:109:A:HIS:HB2  | 1:108:A:GLN:H   | 13       | 0.15          |
| (1,3169) | 1:53:A:PHE:HB3   | 1:75:A:LEU:HD21 | 11       | 0.15          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3165) | 1:126:A:ALA:HB2 | 1:125:A:GLN:HG3 | 1        | 0.15          |
| (1,3160) | 1:74:A:ALA:HB1  | 1:74:A:ALA:HA   | 1        | 0.15          |
| (1,3160) | 1:74:A:ALA:HB3  | 1:74:A:ALA:HA   | 11       | 0.15          |
| (1,3136) | 1:68:A:LYS:HB2  | 1:57:A:VAL:HG11 | 11       | 0.15          |
| (1,3134) | 1:15:A:MET:HB2  | 1:15:A:MET:HG2  | 3        | 0.15          |
| (1,3134) | 1:15:A:MET:HB2  | 1:15:A:MET:HG2  | 9        | 0.15          |
| (1,3134) | 1:15:A:MET:HB2  | 1:15:A:MET:HG2  | 14       | 0.15          |
| (1,3130) | 1:123:A:ARG:HG2 | 1:123:A:ARG:H   | 1        | 0.15          |
| (1,3130) | 1:123:A:ARG:HG2 | 1:123:A:ARG:H   | 7        | 0.15          |
| (1,3120) | 1:59:A:ARG:HB2  | 1:58:A:ASP:HB2  | 3        | 0.15          |
| (1,3120) | 1:59:A:ARG:HB2  | 1:58:A:ASP:HB2  | 6        | 0.15          |
| (1,3120) | 1:59:A:ARG:HB2  | 1:58:A:ASP:HB2  | 7        | 0.15          |
| (1,3120) | 1:59:A:ARG:HB2  | 1:58:A:ASP:HB2  | 11       | 0.15          |
| (1,3118) | 1:58:A:ASP:HA   | 1:58:A:ASP:HB2  | 3        | 0.15          |
| (1,3118) | 1:58:A:ASP:HA   | 1:58:A:ASP:HB2  | 5        | 0.15          |
| (1,3118) | 1:58:A:ASP:HA   | 1:58:A:ASP:HB2  | 6        | 0.15          |
| (1,3118) | 1:58:A:ASP:HA   | 1:58:A:ASP:HB2  | 8        | 0.15          |
| (1,3118) | 1:58:A:ASP:HA   | 1:58:A:ASP:HB2  | 10       | 0.15          |
| (1,3113) | 1:57:A:VAL:HG12 | 1:61:A:ALA:H    | 6        | 0.15          |
| (1,3087) | 1:56:A:LEU:HG   | 1:56:A:LEU:HA   | 3        | 0.15          |
| (1,3087) | 1:56:A:LEU:HG   | 1:56:A:LEU:HA   | 5        | 0.15          |
| (1,3087) | 1:56:A:LEU:HG   | 1:56:A:LEU:HA   | 9        | 0.15          |
| (1,3087) | 1:56:A:LEU:HG   | 1:56:A:LEU:HA   | 11       | 0.15          |
| (1,3087) | 1:56:A:LEU:HG   | 1:56:A:LEU:HA   | 16       | 0.15          |
| (1,3080) | 1:125:A:GLN:HB2 | 1:125:A:GLN:HA  | 1        | 0.15          |
| (1,3068) | 1:52:A:ILE:HG22 | 1:53:A:PHE:HB2  | 13       | 0.15          |
| (1,3068) | 1:52:A:ILE:HG23 | 1:53:A:PHE:HB2  | 15       | 0.15          |
| (1,3059) | 1:28:A:ILE:HB   | 1:28:A:ILE:HG23 | 3        | 0.15          |
| (1,3059) | 1:28:A:ILE:HB   | 1:28:A:ILE:HG22 | 9        | 0.15          |
| (1,3059) | 1:28:A:ILE:HB   | 1:28:A:ILE:HG23 | 10       | 0.15          |
| (1,3059) | 1:28:A:ILE:HB   | 1:28:A:ILE:HG23 | 16       | 0.15          |
| (1,3053) | 1:29:A:ALA:H    | 1:28:A:ILE:HG23 | 4        | 0.15          |
| (1,3053) | 1:29:A:ALA:H    | 1:28:A:ILE:HG23 | 6        | 0.15          |
| (1,3053) | 1:29:A:ALA:H    | 1:28:A:ILE:HG21 | 7        | 0.15          |
| (1,3053) | 1:29:A:ALA:H    | 1:28:A:ILE:HG23 | 8        | 0.15          |
| (1,3040) | 1:52:A:ILE:HA   | 1:52:A:ILE:HG12 | 2        | 0.15          |
| (1,3040) | 1:52:A:ILE:HA   | 1:52:A:ILE:HG12 | 5        | 0.15          |
| (1,3040) | 1:52:A:ILE:HA   | 1:52:A:ILE:HG12 | 8        | 0.15          |
| (1,3040) | 1:52:A:ILE:HA   | 1:52:A:ILE:HG12 | 13       | 0.15          |
| (1,3040) | 1:52:A:ILE:HA   | 1:52:A:ILE:HG12 | 14       | 0.15          |
| (1,3032) | 1:121:A:LYS:HG3 | 1:121:A:LYS:HE3 | 16       | 0.15          |
| (1,3022) | 1:64:A:MET:HE3  | 1:30:A:PHE:HA   | 16       | 0.15          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3019) | 1:64:A:MET:HE2   | 1:66:A:LEU:H    | 4        | 0.15          |
| (1,3019) | 1:64:A:MET:HE1   | 1:66:A:LEU:H    | 16       | 0.15          |
| (1,3000) | 1:57:A:VAL:HA    | 1:60:A:VAL:HB   | 7        | 0.15          |
| (1,3000) | 1:57:A:VAL:HA    | 1:60:A:VAL:HB   | 9        | 0.15          |
| (1,3000) | 1:57:A:VAL:HA    | 1:60:A:VAL:HB   | 12       | 0.15          |
| (1,2995) | 1:60:A:VAL:H     | 1:60:A:VAL:HB   | 3        | 0.15          |
| (1,2995) | 1:60:A:VAL:H     | 1:60:A:VAL:HB   | 5        | 0.15          |
| (1,2995) | 1:60:A:VAL:H     | 1:60:A:VAL:HB   | 7        | 0.15          |
| (1,2992) | 1:20:A:LYS:HB3   | 1:20:A:LYS:H    | 13       | 0.15          |
| (1,2960) | 1:77:A:LEU:HD12  | 1:25:A:LYS:HA   | 8        | 0.15          |
| (1,2960) | 1:77:A:LEU:HD13  | 1:25:A:LYS:HA   | 11       | 0.15          |
| (1,2950) | 1:75:A:LEU:HD12  | 1:75:A:LEU:H    | 8        | 0.15          |
| (1,2950) | 1:75:A:LEU:HD12  | 1:75:A:LEU:H    | 16       | 0.15          |
| (1,2946) | 1:88:A:VAL:HG12  | 1:84:A:TYR:HE1  | 1        | 0.15          |
| (1,2932) | 1:95:A:VAL:HG22  | 1:95:A:VAL:H    | 9        | 0.15          |
| (1,2930) | 1:31:A:LEU:HD23  | 1:60:A:VAL:HG12 | 12       | 0.15          |
| (1,2930) | 1:31:A:LEU:HD21  | 1:60:A:VAL:HG12 | 13       | 0.15          |
| (1,2899) | 1:28:A:ILE:HD13  | 1:75:A:LEU:H    | 17       | 0.15          |
| (1,2893) | 1:50:A:ILE:HB    | 1:50:A:ILE:HG21 | 3        | 0.15          |
| (1,2893) | 1:50:A:ILE:HB    | 1:50:A:ILE:HG21 | 11       | 0.15          |
| (1,2892) | 1:50:A:ILE:HG12  | 1:50:A:ILE:HG22 | 17       | 0.15          |
| (1,2875) | 1:122:A:ALA:HB3  | 1:122:A:ALA:H   | 11       | 0.15          |
| (1,2871) | 1:129:A:ALA:HB2  | 1:129:A:ALA:H   | 17       | 0.15          |
| (1,2855) | 1:78:A:TYR:HD2   | 1:28:A:ILE:HD11 | 1        | 0.15          |
| (1,2855) | 1:78:A:TYR:HD1   | 1:28:A:ILE:HD12 | 3        | 0.15          |
| (1,2855) | 1:78:A:TYR:HD1   | 1:28:A:ILE:HD11 | 7        | 0.15          |
| (1,2855) | 1:78:A:TYR:HD1   | 1:28:A:ILE:HD11 | 11       | 0.15          |
| (1,2855) | 1:78:A:TYR:HD1   | 1:28:A:ILE:HD13 | 17       | 0.15          |
| (1,2840) | 1:124:A:VAL:HG13 | 1:125:A:GLN:H   | 5        | 0.15          |
| (1,2840) | 1:124:A:VAL:HG12 | 1:125:A:GLN:H   | 6        | 0.15          |
| (1,2840) | 1:124:A:VAL:HG12 | 1:125:A:GLN:H   | 8        | 0.15          |
| (1,2840) | 1:124:A:VAL:HG11 | 1:125:A:GLN:H   | 16       | 0.15          |
| (1,2811) | 1:97:A:LEU:HD13  | 1:97:A:LEU:HB3  | 5        | 0.15          |
| (1,2791) | 1:84:A:TYR:HE1   | 1:84:A:TYR:HB3  | 2        | 0.15          |
| (1,2775) | 1:47:A:PRO:HB3   | 1:87:A:GLY:HA2  | 4        | 0.15          |
| (1,2775) | 1:47:A:PRO:HB3   | 1:87:A:GLY:HA2  | 17       | 0.15          |
| (1,2774) | 1:91:A:GLY:HA3   | 1:90:A:PRO:HB2  | 2        | 0.15          |
| (1,2774) | 1:91:A:GLY:HA3   | 1:90:A:PRO:HB2  | 11       | 0.15          |
| (1,2761) | 1:76:A:ARG:HA    | 1:76:A:ARG:HD2  | 4        | 0.15          |
| (1,2761) | 1:76:A:ARG:HA    | 1:76:A:ARG:HD2  | 6        | 0.15          |
| (1,2761) | 1:76:A:ARG:HA    | 1:76:A:ARG:HD2  | 9        | 0.15          |
| (1,2761) | 1:76:A:ARG:HA    | 1:76:A:ARG:HD2  | 16       | 0.15          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2761) | 1:76:A:ARG:HA    | 1:76:A:ARG:HD2  | 17       | 0.15          |
| (1,2754) | 1:60:A:VAL:HG13  | 1:59:A:ARG:HD3  | 5        | 0.15          |
| (1,2719) | 1:117:A:LEU:HD13 | 1:86:A:TYR:HB2  | 2        | 0.15          |
| (1,2719) | 1:117:A:LEU:HD12 | 1:86:A:TYR:HB2  | 5        | 0.15          |
| (1,2719) | 1:117:A:LEU:HD13 | 1:86:A:TYR:HB2  | 9        | 0.15          |
| (1,2719) | 1:117:A:LEU:HD11 | 1:86:A:TYR:HB2  | 10       | 0.15          |
| (1,2719) | 1:117:A:LEU:HD12 | 1:86:A:TYR:HB2  | 14       | 0.15          |
| (1,2712) | 1:39:A:PHE:HB3   | 1:35:A:PHE:HB3  | 6        | 0.15          |
| (1,2689) | 1:34:A:ARG:HB3   | 1:30:A:PHE:HD1  | 8        | 0.15          |
| (1,2672) | 1:31:A:LEU:HD13  | 1:35:A:PHE:HD2  | 10       | 0.15          |
| (1,2665) | 1:86:A:TYR:HE2   | 1:86:A:TYR:HB3  | 4        | 0.15          |
| (1,2648) | 1:56:A:LEU:HD13  | 1:52:A:ILE:HG12 | 2        | 0.15          |
| (1,2648) | 1:56:A:LEU:HD13  | 1:52:A:ILE:HG12 | 3        | 0.15          |
| (1,2648) | 1:56:A:LEU:HD13  | 1:52:A:ILE:HG12 | 9        | 0.15          |
| (1,2639) | 1:71:A:LEU:HD11  | 1:71:A:LEU:HB2  | 14       | 0.15          |
| (1,2637) | 1:71:A:LEU:HB3   | 1:71:A:LEU:HG   | 1        | 0.15          |
| (1,2637) | 1:71:A:LEU:HB3   | 1:71:A:LEU:HG   | 4        | 0.15          |
| (1,2637) | 1:71:A:LEU:HB3   | 1:71:A:LEU:HG   | 10       | 0.15          |
| (1,2637) | 1:71:A:LEU:HB3   | 1:71:A:LEU:HG   | 12       | 0.15          |
| (1,2637) | 1:71:A:LEU:HB3   | 1:71:A:LEU:HG   | 13       | 0.15          |
| (1,2629) | 1:53:A:PHE:HZ    | 1:71:A:LEU:HB2  | 6        | 0.15          |
| (1,2629) | 1:53:A:PHE:HZ    | 1:71:A:LEU:HB2  | 14       | 0.15          |
| (1,2629) | 1:53:A:PHE:HZ    | 1:71:A:LEU:HB2  | 16       | 0.15          |
| (1,2622) | 1:71:A:LEU:HD12  | 1:57:A:VAL:H    | 11       | 0.15          |
| (1,2621) | 1:105:A:LEU:HD11 | 1:92:A:ALA:H    | 6        | 0.15          |
| (1,2612) | 1:30:A:PHE:HD1   | 1:34:A:ARG:HG2  | 5        | 0.15          |
| (1,2612) | 1:30:A:PHE:HD1   | 1:34:A:ARG:HG2  | 6        | 0.15          |
| (1,2612) | 1:30:A:PHE:HD2   | 1:34:A:ARG:HG2  | 16       | 0.15          |
| (1,2579) | 1:59:A:ARG:HB2   | 1:60:A:VAL:HG13 | 2        | 0.15          |
| (1,2579) | 1:59:A:ARG:HB2   | 1:60:A:VAL:HG13 | 6        | 0.15          |
| (1,2579) | 1:59:A:ARG:HB2   | 1:60:A:VAL:HG11 | 8        | 0.15          |
| (1,2579) | 1:59:A:ARG:HB2   | 1:60:A:VAL:HG12 | 10       | 0.15          |
| (1,2579) | 1:59:A:ARG:HB2   | 1:60:A:VAL:HG11 | 12       | 0.15          |
| (1,2579) | 1:59:A:ARG:HB2   | 1:60:A:VAL:HG13 | 16       | 0.15          |
| (1,2579) | 1:59:A:ARG:HB2   | 1:60:A:VAL:HG11 | 17       | 0.15          |
| (1,2530) | 1:33:A:GLU:HA    | 1:34:A:ARG:H    | 1        | 0.15          |
| (1,2530) | 1:33:A:GLU:HA    | 1:34:A:ARG:H    | 3        | 0.15          |
| (1,2530) | 1:33:A:GLU:HA    | 1:34:A:ARG:H    | 10       | 0.15          |
| (1,2529) | 1:79:A:THR:HG22  | 1:75:A:LEU:HA   | 12       | 0.15          |
| (1,2514) | 1:120:A:ALA:H    | 1:120:A:ALA:HA  | 1        | 0.15          |
| (1,2514) | 1:120:A:ALA:H    | 1:120:A:ALA:HA  | 2        | 0.15          |
| (1,2514) | 1:120:A:ALA:H    | 1:120:A:ALA:HA  | 9        | 0.15          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2505) | 1:126:A:ALA:HA   | 1:126:A:ALA:H   | 11       | 0.15          |
| (1,2489) | 1:28:A:ILE:HA    | 1:28:A:ILE:HG22 | 3        | 0.15          |
| (1,2489) | 1:28:A:ILE:HA    | 1:28:A:ILE:HG22 | 5        | 0.15          |
| (1,2469) | 1:53:A:PHE:HZ    | 1:72:A:ARG:HG3  | 5        | 0.15          |
| (1,2469) | 1:53:A:PHE:HZ    | 1:72:A:ARG:HG3  | 13       | 0.15          |
| (1,2469) | 1:53:A:PHE:HZ    | 1:72:A:ARG:HG3  | 16       | 0.15          |
| (1,2417) | 1:129:A:ALA:HB3  | 1:127:A:GLN:HB3 | 15       | 0.15          |
| (1,2416) | 1:45:A:ALA:HB1   | 1:45:A:ALA:H    | 16       | 0.15          |
| (1,2409) | 1:49:A:LYS:H     | 1:52:A:ILE:HD11 | 11       | 0.15          |
| (1,2367) | 1:52:A:ILE:H     | 1:52:A:ILE:HD12 | 5        | 0.15          |
| (1,2351) | 1:110:A:VAL:HG21 | 1:109:A:HIS:HA  | 1        | 0.15          |
| (1,2351) | 1:110:A:VAL:HG21 | 1:109:A:HIS:HA  | 9        | 0.15          |
| (1,2351) | 1:110:A:VAL:HG22 | 1:109:A:HIS:HA  | 10       | 0.15          |
| (1,2351) | 1:110:A:VAL:HG22 | 1:109:A:HIS:HA  | 11       | 0.15          |
| (1,2351) | 1:110:A:VAL:HG22 | 1:109:A:HIS:HA  | 15       | 0.15          |
| (1,2351) | 1:110:A:VAL:HG21 | 1:109:A:HIS:HA  | 16       | 0.15          |
| (1,2306) | 1:38:A:CYS:H     | 1:97:A:LEU:HA   | 1        | 0.15          |
| (1,2299) | 1:55:A:ASP:HB3   | 1:96:A:ASP:HA   | 5        | 0.15          |
| (1,2295) | 1:121:A:LYS:HG2  | 1:121:A:LYS:HD3 | 2        | 0.15          |
| (1,2295) | 1:121:A:LYS:HG2  | 1:121:A:LYS:HD3 | 11       | 0.15          |
| (1,2283) | 1:33:A:GLU:HG2   | 1:33:A:GLU:HA   | 3        | 0.15          |
| (1,2283) | 1:33:A:GLU:HG2   | 1:33:A:GLU:HA   | 13       | 0.15          |
| (1,2283) | 1:33:A:GLU:HG2   | 1:33:A:GLU:HA   | 14       | 0.15          |
| (1,2197) | 1:39:A:PHE:HD2   | 1:56:A:LEU:HA   | 3        | 0.15          |
| (1,2197) | 1:39:A:PHE:HD2   | 1:56:A:LEU:HA   | 4        | 0.15          |
| (1,2197) | 1:39:A:PHE:HD1   | 1:56:A:LEU:HA   | 16       | 0.15          |
| (1,2185) | 1:53:A:PHE:H     | 1:97:A:LEU:HD23 | 10       | 0.15          |
| (1,2149) | 1:21:A:LEU:HD21  | 1:30:A:PHE:HD1  | 6        | 0.15          |
| (1,2149) | 1:21:A:LEU:HD23  | 1:30:A:PHE:HD2  | 13       | 0.15          |
| (1,2140) | 1:84:A:TYR:HB2   | 1:82:A:TRP:HA   | 12       | 0.15          |
| (1,2140) | 1:84:A:TYR:HB2   | 1:82:A:TRP:HA   | 15       | 0.15          |
| (1,2140) | 1:84:A:TYR:HB2   | 1:82:A:TRP:HA   | 16       | 0.15          |
| (1,2118) | 1:69:A:THR:HB    | 1:69:A:THR:HG23 | 1        | 0.15          |
| (1,2118) | 1:69:A:THR:HB    | 1:69:A:THR:HG23 | 7        | 0.15          |
| (1,2118) | 1:69:A:THR:HB    | 1:69:A:THR:HG23 | 10       | 0.15          |
| (1,2118) | 1:69:A:THR:HB    | 1:69:A:THR:HG23 | 14       | 0.15          |
| (1,2118) | 1:69:A:THR:HB    | 1:69:A:THR:HG23 | 17       | 0.15          |
| (1,2116) | 1:45:A:ALA:HB3   | 1:84:A:TYR:HA   | 1        | 0.15          |
| (1,2116) | 1:45:A:ALA:HB3   | 1:84:A:TYR:HA   | 7        | 0.15          |
| (1,2079) | 1:66:A:LEU:HD12  | 1:62:A:GLY:H    | 7        | 0.15          |
| (1,2079) | 1:66:A:LEU:HD11  | 1:62:A:GLY:H    | 15       | 0.15          |
| (1,2052) | 1:65:A:ASN:H     | 1:66:A:LEU:H    | 5        | 0.15          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2052) | 1:65:A:ASN:H     | 1:66:A:LEU:H     | 6        | 0.15          |
| (1,2052) | 1:65:A:ASN:H     | 1:66:A:LEU:H     | 8        | 0.15          |
| (1,2052) | 1:65:A:ASN:H     | 1:66:A:LEU:H     | 13       | 0.15          |
| (1,2045) | 1:77:A:LEU:H     | 1:78:A:TYR:H     | 4        | 0.15          |
| (1,2037) | 1:57:A:VAL:HG22  | 1:57:A:VAL:HG12  | 12       | 0.15          |
| (1,2035) | 1:52:A:ILE:HG13  | 1:97:A:LEU:HD22  | 1        | 0.15          |
| (1,2025) | 1:97:A:LEU:HD23  | 1:35:A:PHE:HD1   | 13       | 0.15          |
| (1,2005) | 1:95:A:VAL:HG21  | 1:48:A:LEU:HD13  | 4        | 0.15          |
| (1,1952) | 1:112:A:HIS:HA   | 1:115:A:LYS:HB3  | 12       | 0.15          |
| (1,1906) | 1:105:A:LEU:HB3  | 1:101:A:PRO:HB3  | 4        | 0.15          |
| (1,1906) | 1:105:A:LEU:HB3  | 1:101:A:PRO:HB3  | 7        | 0.15          |
| (1,1906) | 1:105:A:LEU:HB3  | 1:101:A:PRO:HB3  | 8        | 0.15          |
| (1,1906) | 1:105:A:LEU:HB3  | 1:101:A:PRO:HB3  | 10       | 0.15          |
| (1,1906) | 1:105:A:LEU:HB3  | 1:101:A:PRO:HB3  | 13       | 0.15          |
| (1,1886) | 1:102:A:CYS:HB3  | 1:49:A:LYS:HA    | 13       | 0.15          |
| (1,1881) | 1:113:A:ALA:HB2  | 1:88:A:VAL:HA    | 13       | 0.15          |
| (1,1877) | 1:27:A:VAL:HG21  | 1:27:A:VAL:H     | 6        | 0.15          |
| (1,1877) | 1:27:A:VAL:HG23  | 1:27:A:VAL:H     | 13       | 0.15          |
| (1,1876) | 1:27:A:VAL:HG22  | 1:31:A:LEU:HD11  | 4        | 0.15          |
| (1,1876) | 1:27:A:VAL:HG23  | 1:31:A:LEU:HD12  | 5        | 0.15          |
| (1,1872) | 1:56:A:LEU:HD21  | 1:55:A:ASP:HB3   | 15       | 0.15          |
| (1,1847) | 1:36:A:PRO:HB2   | 1:36:A:PRO:HD2   | 6        | 0.15          |
| (1,1818) | 1:118:A:GLU:HA   | 1:122:A:ALA:H    | 13       | 0.15          |
| (1,1801) | 1:117:A:LEU:HA   | 1:120:A:ALA:HB2  | 9        | 0.15          |
| (1,1793) | 1:88:A:VAL:HG22  | 1:84:A:TYR:HA    | 11       | 0.15          |
| (1,1776) | 1:88:A:VAL:HA    | 1:88:A:VAL:HG12  | 5        | 0.15          |
| (1,1775) | 1:88:A:VAL:HA    | 1:47:A:PRO:HB3   | 3        | 0.15          |
| (1,1775) | 1:88:A:VAL:HA    | 1:47:A:PRO:HB3   | 10       | 0.15          |
| (1,1773) | 1:24:A:SER:HA    | 1:27:A:VAL:HG23  | 13       | 0.15          |
| (1,1727) | 1:66:A:LEU:HD11  | 1:30:A:PHE:HD2   | 3        | 0.15          |
| (1,1727) | 1:66:A:LEU:HD12  | 1:30:A:PHE:HD2   | 11       | 0.15          |
| (1,1726) | 1:66:A:LEU:HD11  | 1:66:A:LEU:HA    | 8        | 0.15          |
| (1,1725) | 1:71:A:LEU:HD11  | 1:71:A:LEU:HG    | 7        | 0.15          |
| (1,1725) | 1:71:A:LEU:HD11  | 1:71:A:LEU:HG    | 8        | 0.15          |
| (1,1720) | 1:117:A:LEU:HG   | 1:117:A:LEU:HD12 | 17       | 0.15          |
| (1,1713) | 1:20:A:LYS:H     | 1:20:A:LYS:HD3   | 5        | 0.15          |
| (1,1709) | 1:72:A:ARG:HB3   | 1:53:A:PHE:HE1   | 4        | 0.15          |
| (1,1709) | 1:72:A:ARG:HB3   | 1:53:A:PHE:HE2   | 12       | 0.15          |
| (1,1709) | 1:72:A:ARG:HB3   | 1:53:A:PHE:HE1   | 15       | 0.15          |
| (1,1690) | 1:42:A:GLU:HG2   | 1:41:A:ALA:HB2   | 3        | 0.15          |
| (1,1690) | 1:42:A:GLU:HG2   | 1:41:A:ALA:HB1   | 16       | 0.15          |
| (1,1638) | 1:124:A:VAL:HG13 | 1:124:A:VAL:HA   | 2        | 0.15          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1638) | 1:124:A:VAL:HG12 | 1:124:A:VAL:HA  | 5        | 0.15          |
| (1,1636) | 1:124:A:VAL:HA   | 1:125:A:GLN:HG3 | 6        | 0.15          |
| (1,1629) | 1:116:A:GLN:HG3  | 1:113:A:ALA:HB2 | 13       | 0.15          |
| (1,1629) | 1:116:A:GLN:HG3  | 1:113:A:ALA:HB3 | 16       | 0.15          |
| (1,1613) | 1:124:A:VAL:HG22 | 1:121:A:LYS:HA  | 10       | 0.15          |
| (1,1588) | 1:74:A:ALA:HB2   | 1:74:A:ALA:HA   | 2        | 0.15          |
| (1,1588) | 1:74:A:ALA:HB3   | 1:74:A:ALA:HA   | 15       | 0.15          |
| (1,1580) | 1:97:A:LEU:HA    | 1:97:A:LEU:H    | 2        | 0.15          |
| (1,1580) | 1:97:A:LEU:HA    | 1:97:A:LEU:H    | 14       | 0.15          |
| (1,1553) | 1:57:A:VAL:HG12  | 1:61:A:ALA:H    | 16       | 0.15          |
| (1,1513) | 1:52:A:ILE:HG21  | 1:53:A:PHE:HB3  | 3        | 0.15          |
| (1,1513) | 1:52:A:ILE:HG21  | 1:53:A:PHE:HB3  | 9        | 0.15          |
| (1,1511) | 1:28:A:ILE:HA    | 1:28:A:ILE:HG22 | 3        | 0.15          |
| (1,1486) | 1:25:A:LYS:HG3   | 1:26:A:GLU:HA   | 4        | 0.15          |
| (1,1486) | 1:25:A:LYS:HG3   | 1:26:A:GLU:HA   | 6        | 0.15          |
| (1,1486) | 1:25:A:LYS:HG3   | 1:26:A:GLU:HA   | 11       | 0.15          |
| (1,1486) | 1:25:A:LYS:HG3   | 1:26:A:GLU:HA   | 15       | 0.15          |
| (1,1440) | 1:105:A:LEU:H    | 1:101:A:PRO:HD3 | 3        | 0.15          |
| (1,1440) | 1:105:A:LEU:H    | 1:101:A:PRO:HD3 | 7        | 0.15          |
| (1,1440) | 1:105:A:LEU:H    | 1:101:A:PRO:HD3 | 11       | 0.15          |
| (1,1439) | 1:103:A:GLY:HA3  | 1:101:A:PRO:HD3 | 1        | 0.15          |
| (1,1439) | 1:103:A:GLY:HA3  | 1:101:A:PRO:HD3 | 5        | 0.15          |
| (1,1439) | 1:103:A:GLY:HA3  | 1:101:A:PRO:HD3 | 6        | 0.15          |
| (1,1439) | 1:103:A:GLY:HA3  | 1:101:A:PRO:HD3 | 10       | 0.15          |
| (1,1439) | 1:103:A:GLY:HA3  | 1:101:A:PRO:HD3 | 13       | 0.15          |
| (1,1439) | 1:103:A:GLY:HA3  | 1:101:A:PRO:HD3 | 14       | 0.15          |
| (1,1439) | 1:103:A:GLY:HA3  | 1:101:A:PRO:HD3 | 15       | 0.15          |
| (1,1439) | 1:103:A:GLY:HA3  | 1:101:A:PRO:HD3 | 16       | 0.15          |
| (1,1414) | 1:74:A:ALA:HB3   | 1:75:A:LEU:HD11 | 9        | 0.15          |
| (1,1414) | 1:74:A:ALA:HB2   | 1:75:A:LEU:HD13 | 12       | 0.15          |
| (1,1412) | 1:39:A:PHE:HZ    | 1:75:A:LEU:HD13 | 8        | 0.15          |
| (1,1412) | 1:39:A:PHE:HZ    | 1:75:A:LEU:HD12 | 9        | 0.15          |
| (1,1412) | 1:39:A:PHE:HZ    | 1:75:A:LEU:HD12 | 14       | 0.15          |
| (1,1410) | 1:110:A:VAL:HG22 | 1:108:A:GLN:H   | 13       | 0.15          |
| (1,1409) | 1:57:A:VAL:HG22  | 1:57:A:VAL:HG12 | 12       | 0.15          |
| (1,1382) | 1:57:A:VAL:HG22  | 1:53:A:PHE:HE2  | 16       | 0.15          |
| (1,1371) | 1:28:A:ILE:HD11  | 1:75:A:LEU:H    | 2        | 0.15          |
| (1,1371) | 1:28:A:ILE:HD13  | 1:75:A:LEU:H    | 13       | 0.15          |
| (1,1371) | 1:28:A:ILE:HD13  | 1:75:A:LEU:H    | 14       | 0.15          |
| (1,1371) | 1:28:A:ILE:HD12  | 1:75:A:LEU:H    | 16       | 0.15          |
| (1,1365) | 1:32:A:ALA:HB2   | 1:28:A:ILE:HG23 | 8        | 0.15          |
| (1,1357) | 1:74:A:ALA:HB2   | 1:31:A:LEU:HD13 | 17       | 0.15          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1352) | 1:122:A:ALA:HB3 | 1:122:A:ALA:H    | 1        | 0.15          |
| (1,1352) | 1:122:A:ALA:HB1 | 1:122:A:ALA:H    | 5        | 0.15          |
| (1,1352) | 1:122:A:ALA:HB1 | 1:122:A:ALA:H    | 6        | 0.15          |
| (1,1352) | 1:122:A:ALA:HB1 | 1:122:A:ALA:H    | 14       | 0.15          |
| (1,1351) | 1:127:A:GLN:H   | 1:126:A:ALA:HB3  | 8        | 0.15          |
| (1,1342) | 1:48:A:LEU:HD11 | 1:84:A:TYR:HE1   | 4        | 0.15          |
| (1,1331) | 1:78:A:TYR:HE2  | 1:84:A:TYR:HD1   | 8        | 0.15          |
| (1,1325) | 1:53:A:PHE:HE2  | 1:75:A:LEU:HB3   | 6        | 0.15          |
| (1,1325) | 1:53:A:PHE:HE2  | 1:75:A:LEU:HB3   | 9        | 0.15          |
| (1,1315) | 1:95:A:VAL:HG22 | 1:97:A:LEU:HD21  | 12       | 0.15          |
| (1,1275) | 1:84:A:TYR:HE1  | 1:84:A:TYR:HB3   | 1        | 0.15          |
| (1,1275) | 1:84:A:TYR:HE2  | 1:84:A:TYR:HB3   | 4        | 0.15          |
| (1,1275) | 1:84:A:TYR:HE2  | 1:84:A:TYR:HB3   | 14       | 0.15          |
| (1,1240) | 1:78:A:TYR:HE2  | 1:79:A:THR:HB    | 4        | 0.15          |
| (1,1240) | 1:78:A:TYR:HE2  | 1:79:A:THR:HB    | 9        | 0.15          |
| (1,1240) | 1:78:A:TYR:HE1  | 1:79:A:THR:HB    | 11       | 0.15          |
| (1,1240) | 1:78:A:TYR:HE1  | 1:79:A:THR:HB    | 16       | 0.15          |
| (1,1240) | 1:78:A:TYR:HE1  | 1:79:A:THR:HB    | 17       | 0.15          |
| (1,1239) | 1:79:A:THR:H    | 1:78:A:TYR:HE2   | 1        | 0.15          |
| (1,1239) | 1:79:A:THR:H    | 1:78:A:TYR:HE1   | 3        | 0.15          |
| (1,1239) | 1:79:A:THR:H    | 1:78:A:TYR:HE2   | 5        | 0.15          |
| (1,1239) | 1:79:A:THR:H    | 1:78:A:TYR:HE1   | 14       | 0.15          |
| (1,1167) | 1:34:A:ARG:HB3  | 1:30:A:PHE:HD2   | 1        | 0.15          |
| (1,1167) | 1:34:A:ARG:HB3  | 1:30:A:PHE:HD1   | 4        | 0.15          |
| (1,1126) | 1:86:A:TYR:HE2  | 1:86:A:TYR:HB3   | 6        | 0.15          |
| (1,1111) | 1:75:A:LEU:HB3  | 1:75:A:LEU:H     | 11       | 0.15          |
| (1,1108) | 1:56:A:LEU:HD11 | 1:52:A:ILE:HG12  | 7        | 0.15          |
| (1,1108) | 1:56:A:LEU:HD12 | 1:52:A:ILE:HG12  | 12       | 0.15          |
| (1,1108) | 1:56:A:LEU:HD11 | 1:52:A:ILE:HG12  | 13       | 0.15          |
| (1,1108) | 1:56:A:LEU:HD13 | 1:52:A:ILE:HG12  | 14       | 0.15          |
| (1,1108) | 1:56:A:LEU:HD11 | 1:52:A:ILE:HG12  | 15       | 0.15          |
| (1,1053) | 1:93:A:THR:HG23 | 1:102:A:CYS:HA   | 1        | 0.15          |
| (1,1047) | 1:124:A:VAL:HA  | 1:124:A:VAL:HG21 | 3        | 0.15          |
| (1,1047) | 1:124:A:VAL:HA  | 1:124:A:VAL:HG22 | 9        | 0.15          |
| (1,1047) | 1:124:A:VAL:HA  | 1:124:A:VAL:HG21 | 17       | 0.15          |
| (1,1032) | 1:85:A:LEU:H    | 1:84:A:TYR:HE1   | 1        | 0.15          |
| (1,1032) | 1:85:A:LEU:H    | 1:84:A:TYR:HE1   | 2        | 0.15          |
| (1,1032) | 1:85:A:LEU:H    | 1:84:A:TYR:HE1   | 7        | 0.15          |
| (1,1032) | 1:85:A:LEU:H    | 1:84:A:TYR:HE1   | 15       | 0.15          |
| (1,1030) | 1:86:A:TYR:HE2  | 1:86:A:TYR:HB2   | 1        | 0.15          |
| (1,1013) | 1:11:A:SER:HA   | 1:12:A:GLN:H     | 15       | 0.15          |
| (1,983)  | 1:55:A:ASP:HB3  | 1:55:A:ASP:HA    | 8        | 0.15          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,852) | 1:65:A:ASN:HB3  | 1:65:A:ASN:HD21 | 6        | 0.15          |
| (1,830) | 1:129:A:ALA:HB1 | 1:127:A:GLN:HB3 | 1        | 0.15          |
| (1,827) | 1:45:A:ALA:HB1  | 1:45:A:ALA:H    | 10       | 0.15          |
| (1,822) | 1:49:A:LYS:H    | 1:52:A:ILE:HD12 | 17       | 0.15          |
| (1,815) | 1:50:A:ILE:HD11 | 1:50:A:ILE:HA   | 17       | 0.15          |
| (1,762) | 1:65:A:ASN:HA   | 1:66:A:LEU:H    | 7        | 0.15          |
| (1,762) | 1:65:A:ASN:HA   | 1:66:A:LEU:H    | 9        | 0.15          |
| (1,756) | 1:93:A:THR:HB   | 1:102:A:CYS:H   | 1        | 0.15          |
| (1,753) | 1:92:A:ALA:HB2  | 1:91:A:GLY:H    | 8        | 0.15          |
| (1,753) | 1:92:A:ALA:HB1  | 1:91:A:GLY:H    | 13       | 0.15          |
| (1,707) | 1:75:A:LEU:HB3  | 1:74:A:ALA:H    | 6        | 0.15          |
| (1,678) | 1:17:A:ASN:H    | 1:18:A:GLN:H    | 10       | 0.15          |
| (1,665) | 1:122:A:ALA:HB2 | 1:123:A:ARG:H   | 7        | 0.15          |
| (1,665) | 1:122:A:ALA:HB3 | 1:123:A:ARG:H   | 14       | 0.15          |
| (1,665) | 1:122:A:ALA:HB2 | 1:123:A:ARG:H   | 16       | 0.15          |
| (1,635) | 1:127:A:GLN:H   | 1:127:A:GLN:HB3 | 1        | 0.15          |
| (1,614) | 1:97:A:LEU:HD12 | 1:97:A:LEU:H    | 11       | 0.15          |
| (1,605) | 1:40:A:SER:HA   | 1:43:A:GLY:H    | 17       | 0.15          |
| (1,549) | 1:97:A:LEU:HD11 | 1:98:A:ASP:H    | 4        | 0.15          |
| (1,549) | 1:97:A:LEU:HD13 | 1:98:A:ASP:H    | 9        | 0.15          |
| (1,478) | 1:27:A:VAL:HG21 | 1:29:A:ALA:H    | 3        | 0.15          |
| (1,477) | 1:31:A:LEU:H    | 1:31:A:LEU:HD11 | 9        | 0.15          |
| (1,451) | 1:32:A:ALA:HB3  | 1:35:A:PHE:H    | 10       | 0.15          |
| (1,423) | 1:50:A:ILE:HG22 | 1:50:A:ILE:H    | 1        | 0.15          |
| (1,423) | 1:50:A:ILE:HG22 | 1:50:A:ILE:H    | 5        | 0.15          |
| (1,423) | 1:50:A:ILE:HG23 | 1:50:A:ILE:H    | 13       | 0.15          |
| (1,397) | 1:57:A:VAL:H    | 1:56:A:LEU:HB3  | 1        | 0.15          |
| (1,397) | 1:57:A:VAL:H    | 1:56:A:LEU:HB3  | 4        | 0.15          |
| (1,359) | 1:62:A:GLY:HA3  | 1:63:A:GLU:H    | 16       | 0.15          |
| (1,311) | 1:79:A:THR:H    | 1:77:A:LEU:HB2  | 3        | 0.15          |
| (1,311) | 1:79:A:THR:H    | 1:77:A:LEU:HB2  | 8        | 0.15          |
| (1,311) | 1:79:A:THR:H    | 1:77:A:LEU:HB2  | 10       | 0.15          |
| (1,308) | 1:79:A:THR:HG21 | 1:80:A:SER:H    | 6        | 0.15          |
| (1,308) | 1:79:A:THR:HG22 | 1:80:A:SER:H    | 12       | 0.15          |
| (1,241) | 1:95:A:VAL:HG12 | 1:96:A:ASP:H    | 15       | 0.15          |
| (1,134) | 1:123:A:ARG:H   | 1:121:A:LYS:H   | 3        | 0.15          |
| (1,134) | 1:123:A:ARG:H   | 1:121:A:LYS:H   | 6        | 0.15          |
| (1,134) | 1:123:A:ARG:H   | 1:121:A:LYS:H   | 12       | 0.15          |
| (1,134) | 1:123:A:ARG:H   | 1:121:A:LYS:H   | 13       | 0.15          |
| (1,134) | 1:123:A:ARG:H   | 1:121:A:LYS:H   | 17       | 0.15          |
| (1,128) | 1:35:A:PHE:HD2  | 1:39:A:PHE:H    | 9        | 0.15          |
| (1,128) | 1:35:A:PHE:HD1  | 1:39:A:PHE:H    | 12       | 0.15          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,101)  | 1:35:A:PHE:H    | 1:39:A:PHE:HE2  | 3        | 0.15          |
| (1,101)  | 1:35:A:PHE:H    | 1:39:A:PHE:HE2  | 4        | 0.15          |
| (1,101)  | 1:35:A:PHE:H    | 1:39:A:PHE:HE2  | 9        | 0.15          |
| (1,101)  | 1:35:A:PHE:H    | 1:39:A:PHE:HE1  | 13       | 0.15          |
| (1,101)  | 1:35:A:PHE:H    | 1:39:A:PHE:HE1  | 14       | 0.15          |
| (1,80)   | 1:30:A:PHE:HD2  | 1:30:A:PHE:H    | 3        | 0.15          |
| (1,80)   | 1:30:A:PHE:HD1  | 1:30:A:PHE:H    | 17       | 0.15          |
| (3,149)  | 1:82:A:TRP:HE1  | 1:82:A:TRP:HE3  | 1        | 0.14          |
| (3,149)  | 1:82:A:TRP:HE1  | 1:82:A:TRP:HE3  | 6        | 0.14          |
| (3,149)  | 1:82:A:TRP:HE1  | 1:82:A:TRP:HE3  | 14       | 0.14          |
| (3,137)  | 1:123:A:ARG:H   | 1:123:A:ARG:HA  | 1        | 0.14          |
| (3,137)  | 1:123:A:ARG:H   | 1:123:A:ARG:HA  | 5        | 0.14          |
| (3,137)  | 1:123:A:ARG:H   | 1:123:A:ARG:HA  | 6        | 0.14          |
| (3,137)  | 1:123:A:ARG:H   | 1:123:A:ARG:HA  | 7        | 0.14          |
| (3,137)  | 1:123:A:ARG:H   | 1:123:A:ARG:HA  | 8        | 0.14          |
| (3,137)  | 1:123:A:ARG:H   | 1:123:A:ARG:HA  | 9        | 0.14          |
| (3,137)  | 1:123:A:ARG:H   | 1:123:A:ARG:HA  | 10       | 0.14          |
| (3,137)  | 1:123:A:ARG:H   | 1:123:A:ARG:HA  | 11       | 0.14          |
| (3,137)  | 1:123:A:ARG:H   | 1:123:A:ARG:HA  | 12       | 0.14          |
| (3,137)  | 1:123:A:ARG:H   | 1:123:A:ARG:HA  | 16       | 0.14          |
| (3,137)  | 1:123:A:ARG:H   | 1:123:A:ARG:HA  | 17       | 0.14          |
| (3,122)  | 1:27:A:VAL:HG23 | 1:28:A:ILE:HD12 | 1        | 0.14          |
| (3,117)  | 1:48:A:LEU:HD23 | 1:39:A:PHE:HD1  | 11       | 0.14          |
| (3,109)  | 1:92:A:ALA:H    | 1:110:A:VAL:HB  | 7        | 0.14          |
| (3,106)  | 1:68:A:LYS:HD2  | 1:68:A:LYS:HA   | 1        | 0.14          |
| (3,106)  | 1:68:A:LYS:HD2  | 1:68:A:LYS:HA   | 8        | 0.14          |
| (3,105)  | 1:64:A:MET:H    | 1:66:A:LEU:HD21 | 5        | 0.14          |
| (3,105)  | 1:64:A:MET:H    | 1:66:A:LEU:HD22 | 11       | 0.14          |
| (3,94)   | 1:56:A:LEU:HB2  | 1:75:A:LEU:HD12 | 7        | 0.14          |
| (3,90)   | 1:115:A:LYS:HG3 | 1:116:A:GLN:HG3 | 1        | 0.14          |
| (3,90)   | 1:115:A:LYS:HG3 | 1:116:A:GLN:HG3 | 9        | 0.14          |
| (3,83)   | 1:114:A:ARG:HB2 | 1:113:A:ALA:HB1 | 17       | 0.14          |
| (3,81)   | 1:77:A:LEU:HA   | 1:77:A:LEU:HD11 | 2        | 0.14          |
| (3,81)   | 1:77:A:LEU:HA   | 1:77:A:LEU:HD13 | 8        | 0.14          |
| (3,64)   | 1:102:A:CYS:HB2 | 1:52:A:ILE:HG22 | 3        | 0.14          |
| (3,64)   | 1:55:A:ASP:HB2  | 1:52:A:ILE:HG22 | 17       | 0.14          |
| (3,48)   | 1:72:A:ARG:HD3  | 1:72:A:ARG:HB3  | 1        | 0.14          |
| (3,34)   | 1:97:A:LEU:HD23 | 1:31:A:LEU:HD12 | 6        | 0.14          |
| (3,34)   | 1:97:A:LEU:HD21 | 1:31:A:LEU:HD13 | 9        | 0.14          |
| (3,22)   | 1:48:A:LEU:HD11 | 1:97:A:LEU:H    | 8        | 0.14          |
| (1,4345) | 1:117:A:LEU:HA  | 1:121:A:LYS:H   | 2        | 0.14          |
| (1,4345) | 1:117:A:LEU:HA  | 1:121:A:LYS:H   | 15       | 0.14          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,4344) | 1:120:A:ALA:H   | 1:119:A:GLU:HG2 | 3        | 0.14          |
| (1,4344) | 1:120:A:ALA:H   | 1:119:A:GLU:HG2 | 11       | 0.14          |
| (1,4343) | 1:118:A:GLU:H   | 1:119:A:GLU:H   | 8        | 0.14          |
| (1,4343) | 1:118:A:GLU:H   | 1:119:A:GLU:H   | 10       | 0.14          |
| (1,4339) | 1:116:A:GLN:HG3 | 1:115:A:LYS:H   | 5        | 0.14          |
| (1,4326) | 1:65:A:ASN:HA   | 1:66:A:LEU:H    | 5        | 0.14          |
| (1,4323) | 1:62:A:GLY:H    | 1:68:A:LYS:HD2  | 8        | 0.14          |
| (1,4323) | 1:62:A:GLY:H    | 1:68:A:LYS:HD2  | 12       | 0.14          |
| (1,4320) | 1:62:A:GLY:H    | 1:66:A:LEU:H    | 2        | 0.14          |
| (1,4320) | 1:62:A:GLY:H    | 1:66:A:LEU:H    | 16       | 0.14          |
| (1,4317) | 1:93:A:THR:HB   | 1:102:A:CYS:H   | 3        | 0.14          |
| (1,4317) | 1:93:A:THR:HB   | 1:102:A:CYS:H   | 7        | 0.14          |
| (1,4317) | 1:93:A:THR:HB   | 1:102:A:CYS:H   | 10       | 0.14          |
| (1,4317) | 1:93:A:THR:HB   | 1:102:A:CYS:H   | 16       | 0.14          |
| (1,4316) | 1:95:A:VAL:H    | 1:94:A:ARG:HB3  | 2        | 0.14          |
| (1,4316) | 1:95:A:VAL:H    | 1:94:A:ARG:HB3  | 7        | 0.14          |
| (1,4316) | 1:95:A:VAL:H    | 1:94:A:ARG:HB3  | 8        | 0.14          |
| (1,4316) | 1:95:A:VAL:H    | 1:94:A:ARG:HB3  | 12       | 0.14          |
| (1,4316) | 1:95:A:VAL:H    | 1:94:A:ARG:HB3  | 13       | 0.14          |
| (1,4316) | 1:95:A:VAL:H    | 1:94:A:ARG:HB3  | 14       | 0.14          |
| (1,4301) | 1:97:A:LEU:HB2  | 1:97:A:LEU:H    | 3        | 0.14          |
| (1,4301) | 1:97:A:LEU:HB2  | 1:97:A:LEU:H    | 4        | 0.14          |
| (1,4295) | 1:116:A:GLN:HA  | 1:117:A:LEU:H   | 7        | 0.14          |
| (1,4295) | 1:116:A:GLN:HA  | 1:117:A:LEU:H   | 17       | 0.14          |
| (1,4271) | 1:78:A:TYR:HE1  | 1:75:A:LEU:H    | 3        | 0.14          |
| (1,4270) | 1:75:A:LEU:HB3  | 1:74:A:ALA:H    | 4        | 0.14          |
| (1,4270) | 1:75:A:LEU:HB3  | 1:74:A:ALA:H    | 15       | 0.14          |
| (1,4270) | 1:75:A:LEU:HB3  | 1:74:A:ALA:H    | 16       | 0.14          |
| (1,4228) | 1:123:A:ARG:HB3 | 1:124:A:VAL:H   | 2        | 0.14          |
| (1,4228) | 1:123:A:ARG:HB3 | 1:124:A:VAL:H   | 5        | 0.14          |
| (1,4228) | 1:123:A:ARG:HB3 | 1:124:A:VAL:H   | 6        | 0.14          |
| (1,4228) | 1:123:A:ARG:HB3 | 1:124:A:VAL:H   | 17       | 0.14          |
| (1,4225) | 1:122:A:ALA:HB1 | 1:123:A:ARG:H   | 4        | 0.14          |
| (1,4225) | 1:122:A:ALA:HB1 | 1:123:A:ARG:H   | 9        | 0.14          |
| (1,4212) | 1:115:A:LYS:HE3 | 1:115:A:LYS:H   | 5        | 0.14          |
| (1,4202) | 1:127:A:GLN:H   | 1:127:A:GLN:HB3 | 8        | 0.14          |
| (1,4202) | 1:127:A:GLN:H   | 1:127:A:GLN:HB3 | 10       | 0.14          |
| (1,4198) | 1:127:A:GLN:HA  | 1:127:A:GLN:H   | 6        | 0.14          |
| (1,4194) | 1:107:A:GLU:H   | 1:106:A:ASP:HA  | 1        | 0.14          |
| (1,4193) | 1:69:A:THR:HB   | 1:72:A:ARG:H    | 2        | 0.14          |
| (1,4193) | 1:69:A:THR:HB   | 1:72:A:ARG:H    | 8        | 0.14          |
| (1,4193) | 1:69:A:THR:HB   | 1:72:A:ARG:H    | 11       | 0.14          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,4170) | 1:49:A:LYS:HB2  | 1:49:A:LYS:H    | 8        | 0.14          |
| (1,4170) | 1:49:A:LYS:HB2  | 1:49:A:LYS:H    | 12       | 0.14          |
| (1,4170) | 1:49:A:LYS:HB2  | 1:49:A:LYS:H    | 13       | 0.14          |
| (1,4170) | 1:49:A:LYS:HB2  | 1:49:A:LYS:H    | 16       | 0.14          |
| (1,4148) | 1:25:A:LYS:HB2  | 1:26:A:GLU:H    | 4        | 0.14          |
| (1,4148) | 1:25:A:LYS:HB2  | 1:26:A:GLU:H    | 5        | 0.14          |
| (1,4148) | 1:25:A:LYS:HB2  | 1:26:A:GLU:H    | 6        | 0.14          |
| (1,4148) | 1:25:A:LYS:HB2  | 1:26:A:GLU:H    | 7        | 0.14          |
| (1,4148) | 1:25:A:LYS:HB2  | 1:26:A:GLU:H    | 8        | 0.14          |
| (1,4148) | 1:25:A:LYS:HB2  | 1:26:A:GLU:H    | 11       | 0.14          |
| (1,4148) | 1:25:A:LYS:HB2  | 1:26:A:GLU:H    | 12       | 0.14          |
| (1,4148) | 1:25:A:LYS:HB2  | 1:26:A:GLU:H    | 13       | 0.14          |
| (1,4148) | 1:25:A:LYS:HB2  | 1:26:A:GLU:H    | 15       | 0.14          |
| (1,4148) | 1:25:A:LYS:HB2  | 1:26:A:GLU:H    | 16       | 0.14          |
| (1,4143) | 1:37:A:HIS:HA   | 1:39:A:PHE:H    | 17       | 0.14          |
| (1,4133) | 1:82:A:TRP:HE1  | 1:82:A:TRP:HD1  | 2        | 0.14          |
| (1,4127) | 1:34:A:ARG:HE   | 1:30:A:PHE:HD1  | 2        | 0.14          |
| (1,4114) | 1:65:A:ASN:H    | 1:65:A:ASN:HD21 | 17       | 0.14          |
| (1,4113) | 1:22:A:ASN:H    | 1:22:A:ASN:HD22 | 5        | 0.14          |
| (1,4110) | 1:40:A:SER:HA   | 1:42:A:GLU:H    | 9        | 0.14          |
| (1,4110) | 1:40:A:SER:HA   | 1:42:A:GLU:H    | 14       | 0.14          |
| (1,4060) | 1:97:A:LEU:HD21 | 1:39:A:PHE:H    | 14       | 0.14          |
| (1,4040) | 1:25:A:LYS:HG3  | 1:25:A:LYS:H    | 5        | 0.14          |
| (1,4040) | 1:25:A:LYS:HG3  | 1:25:A:LYS:H    | 12       | 0.14          |
| (1,4037) | 1:27:A:VAL:HG22 | 1:29:A:ALA:H    | 13       | 0.14          |
| (1,4036) | 1:31:A:LEU:H    | 1:31:A:LEU:HD11 | 10       | 0.14          |
| (1,4019) | 1:33:A:GLU:HB3  | 1:34:A:ARG:H    | 4        | 0.14          |
| (1,4019) | 1:33:A:GLU:HB3  | 1:34:A:ARG:H    | 9        | 0.14          |
| (1,4019) | 1:33:A:GLU:HB3  | 1:34:A:ARG:H    | 13       | 0.14          |
| (1,4000) | 1:42:A:GLU:HB2  | 1:43:A:GLY:H    | 12       | 0.14          |
| (1,3979) | 1:50:A:ILE:HA   | 1:51:A:GLY:H    | 1        | 0.14          |
| (1,3961) | 1:57:A:VAL:H    | 1:56:A:LEU:HB3  | 11       | 0.14          |
| (1,3943) | 1:66:A:LEU:HD13 | 1:62:A:GLY:H    | 5        | 0.14          |
| (1,3940) | 1:62:A:GLY:HA3  | 1:63:A:GLU:H    | 3        | 0.14          |
| (1,3940) | 1:62:A:GLY:HA3  | 1:63:A:GLU:H    | 5        | 0.14          |
| (1,3940) | 1:62:A:GLY:HA3  | 1:63:A:GLU:H    | 10       | 0.14          |
| (1,3940) | 1:62:A:GLY:HA3  | 1:63:A:GLU:H    | 11       | 0.14          |
| (1,3940) | 1:62:A:GLY:HA3  | 1:63:A:GLU:H    | 17       | 0.14          |
| (1,3935) | 1:63:A:GLU:HB3  | 1:65:A:ASN:H    | 4        | 0.14          |
| (1,3935) | 1:63:A:GLU:HB3  | 1:65:A:ASN:H    | 5        | 0.14          |
| (1,3935) | 1:63:A:GLU:HB3  | 1:65:A:ASN:H    | 9        | 0.14          |
| (1,3935) | 1:63:A:GLU:HB3  | 1:65:A:ASN:H    | 10       | 0.14          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3935) | 1:63:A:GLU:HB3  | 1:65:A:ASN:H    | 14       | 0.14          |
| (1,3935) | 1:63:A:GLU:HB3  | 1:65:A:ASN:H    | 15       | 0.14          |
| (1,3935) | 1:63:A:GLU:HB3  | 1:65:A:ASN:H    | 17       | 0.14          |
| (1,3929) | 1:68:A:LYS:HD2  | 1:68:A:LYS:H    | 15       | 0.14          |
| (1,3916) | 1:71:A:LEU:HA   | 1:74:A:ALA:H    | 1        | 0.14          |
| (1,3916) | 1:71:A:LEU:HA   | 1:74:A:ALA:H    | 5        | 0.14          |
| (1,3916) | 1:71:A:LEU:HA   | 1:74:A:ALA:H    | 8        | 0.14          |
| (1,3916) | 1:71:A:LEU:HA   | 1:74:A:ALA:H    | 15       | 0.14          |
| (1,3884) | 1:83:A:ARG:H    | 1:83:A:ARG:HB2  | 9        | 0.14          |
| (1,3879) | 1:127:A:GLN:H   | 1:127:A:GLN:HG2 | 2        | 0.14          |
| (1,3879) | 1:127:A:GLN:H   | 1:127:A:GLN:HG2 | 8        | 0.14          |
| (1,3879) | 1:127:A:GLN:H   | 1:127:A:GLN:HG2 | 10       | 0.14          |
| (1,3832) | 1:100:A:ASN:HB3 | 1:100:A:ASN:H   | 11       | 0.14          |
| (1,3830) | 1:101:A:PRO:HD3 | 1:100:A:ASN:H   | 6        | 0.14          |
| (1,3830) | 1:101:A:PRO:HD3 | 1:100:A:ASN:H   | 7        | 0.14          |
| (1,3803) | 1:108:A:GLN:HB3 | 1:108:A:GLN:H   | 7        | 0.14          |
| (1,3797) | 1:44:A:GLU:HA   | 1:44:A:GLU:H    | 4        | 0.14          |
| (1,3797) | 1:44:A:GLU:HA   | 1:44:A:GLU:H    | 10       | 0.14          |
| (1,3797) | 1:44:A:GLU:HA   | 1:44:A:GLU:H    | 16       | 0.14          |
| (1,3786) | 1:27:A:VAL:HG11 | 1:21:A:LEU:H    | 1        | 0.14          |
| (1,3783) | 1:117:A:LEU:HB3 | 1:117:A:LEU:H   | 4        | 0.14          |
| (1,3783) | 1:117:A:LEU:HB3 | 1:117:A:LEU:H   | 13       | 0.14          |
| (1,3771) | 1:126:A:ALA:HB3 | 1:126:A:ALA:H   | 8        | 0.14          |
| (1,3771) | 1:126:A:ALA:HB3 | 1:126:A:ALA:H   | 10       | 0.14          |
| (1,3768) | 1:130:A:GLU:H   | 1:130:A:GLU:HA  | 9        | 0.14          |
| (1,3767) | 1:129:A:ALA:HA  | 1:129:A:ALA:H   | 10       | 0.14          |
| (1,3753) | 1:107:A:GLU:H   | 1:106:A:ASP:H   | 1        | 0.14          |
| (1,3753) | 1:107:A:GLU:H   | 1:106:A:ASP:H   | 5        | 0.14          |
| (1,3753) | 1:107:A:GLU:H   | 1:106:A:ASP:H   | 14       | 0.14          |
| (1,3744) | 1:35:A:PHE:HD2  | 1:39:A:PHE:H    | 1        | 0.14          |
| (1,3744) | 1:35:A:PHE:HD1  | 1:39:A:PHE:H    | 2        | 0.14          |
| (1,3744) | 1:35:A:PHE:HD2  | 1:39:A:PHE:H    | 5        | 0.14          |
| (1,3732) | 1:21:A:LEU:HD11 | 1:30:A:PHE:H    | 4        | 0.14          |
| (1,3708) | 1:62:A:GLY:H    | 1:62:A:GLY:HA3  | 11       | 0.14          |
| (1,3699) | 1:88:A:VAL:HA   | 1:89:A:LYS:H    | 5        | 0.14          |
| (1,3687) | 1:85:A:LEU:H    | 1:82:A:TRP:HD1  | 7        | 0.14          |
| (1,3673) | 1:49:A:LYS:H    | 1:50:A:ILE:H    | 3        | 0.14          |
| (1,3603) | 1:97:A:LEU:HA   | 1:97:A:LEU:HG   | 3        | 0.14          |
| (1,3603) | 1:97:A:LEU:HA   | 1:97:A:LEU:HG   | 4        | 0.14          |
| (1,3603) | 1:97:A:LEU:HA   | 1:97:A:LEU:HG   | 9        | 0.14          |
| (1,3591) | 1:93:A:THR:HB   | 1:88:A:VAL:HG11 | 16       | 0.14          |
| (1,3552) | 1:123:A:ARG:HG2 | 1:124:A:VAL:HA  | 17       | 0.14          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3539) | 1:63:A:GLU:HG3   | 1:63:A:GLU:H     | 7        | 0.14          |
| (1,3537) | 1:51:A:GLY:HA2   | 1:54:A:GLN:HB2   | 2        | 0.14          |
| (1,3537) | 1:51:A:GLY:HA2   | 1:54:A:GLN:HB2   | 4        | 0.14          |
| (1,3537) | 1:51:A:GLY:HA2   | 1:54:A:GLN:HB2   | 5        | 0.14          |
| (1,3537) | 1:51:A:GLY:HA2   | 1:54:A:GLN:HB2   | 17       | 0.14          |
| (1,3523) | 1:56:A:LEU:HG    | 1:56:A:LEU:HB3   | 2        | 0.14          |
| (1,3523) | 1:56:A:LEU:HG    | 1:56:A:LEU:HB3   | 13       | 0.14          |
| (1,3523) | 1:56:A:LEU:HG    | 1:56:A:LEU:HB3   | 15       | 0.14          |
| (1,3520) | 1:100:A:ASN:HD22 | 1:98:A:ASP:HB3   | 2        | 0.14          |
| (1,3520) | 1:100:A:ASN:HD22 | 1:98:A:ASP:HB3   | 6        | 0.14          |
| (1,3520) | 1:100:A:ASN:HD22 | 1:98:A:ASP:HB3   | 14       | 0.14          |
| (1,3520) | 1:100:A:ASN:HD22 | 1:98:A:ASP:HB3   | 17       | 0.14          |
| (1,3519) | 1:65:A:ASN:H     | 1:65:A:ASN:HB3   | 2        | 0.14          |
| (1,3513) | 1:72:A:ARG:HG3   | 1:73:A:SER:HB3   | 1        | 0.14          |
| (1,3513) | 1:72:A:ARG:HG3   | 1:73:A:SER:HB3   | 2        | 0.14          |
| (1,3513) | 1:72:A:ARG:HG3   | 1:73:A:SER:HB3   | 9        | 0.14          |
| (1,3513) | 1:72:A:ARG:HG3   | 1:73:A:SER:HB3   | 14       | 0.14          |
| (1,3511) | 1:50:A:ILE:HG13  | 1:49:A:LYS:HA    | 12       | 0.14          |
| (1,3510) | 1:64:A:MET:HE3   | 1:21:A:LEU:H     | 1        | 0.14          |
| (1,3502) | 1:27:A:VAL:HG23  | 1:27:A:VAL:H     | 4        | 0.14          |
| (1,3502) | 1:27:A:VAL:HG21  | 1:27:A:VAL:H     | 9        | 0.14          |
| (1,3502) | 1:27:A:VAL:HG22  | 1:27:A:VAL:H     | 12       | 0.14          |
| (1,3502) | 1:27:A:VAL:HG21  | 1:27:A:VAL:H     | 15       | 0.14          |
| (1,3502) | 1:27:A:VAL:HG21  | 1:27:A:VAL:H     | 17       | 0.14          |
| (1,3497) | 1:27:A:VAL:HA    | 1:27:A:VAL:HG12  | 2        | 0.14          |
| (1,3497) | 1:27:A:VAL:HA    | 1:27:A:VAL:HG13  | 15       | 0.14          |
| (1,3497) | 1:27:A:VAL:HA    | 1:27:A:VAL:HG11  | 16       | 0.14          |
| (1,3477) | 1:15:A:MET:HG3   | 1:15:A:MET:HB2   | 3        | 0.14          |
| (1,3476) | 1:107:A:GLU:HG2  | 1:108:A:GLN:H    | 5        | 0.14          |
| (1,3476) | 1:107:A:GLU:HG2  | 1:108:A:GLN:H    | 11       | 0.14          |
| (1,3456) | 1:95:A:VAL:HG23  | 1:96:A:ASP:HA    | 8        | 0.14          |
| (1,3437) | 1:21:A:LEU:HB2   | 1:21:A:LEU:HD12  | 6        | 0.14          |
| (1,3422) | 1:77:A:LEU:HG    | 1:77:A:LEU:HD21  | 14       | 0.14          |
| (1,3414) | 1:86:A:TYR:H     | 1:117:A:LEU:HD11 | 6        | 0.14          |
| (1,3414) | 1:86:A:TYR:H     | 1:117:A:LEU:HD11 | 10       | 0.14          |
| (1,3398) | 1:117:A:LEU:HA   | 1:120:A:ALA:HB3  | 3        | 0.14          |
| (1,3398) | 1:117:A:LEU:HA   | 1:120:A:ALA:HB3  | 7        | 0.14          |
| (1,3374) | 1:88:A:VAL:HA    | 1:88:A:VAL:HG13  | 11       | 0.14          |
| (1,3372) | 1:88:A:VAL:HA    | 1:47:A:PRO:HB3   | 12       | 0.14          |
| (1,3314) | 1:71:A:LEU:HD13  | 1:71:A:LEU:HG    | 16       | 0.14          |
| (1,3306) | 1:128:A:ARG:HG2  | 1:128:A:ARG:HD2  | 6        | 0.14          |
| (1,3306) | 1:128:A:ARG:HG2  | 1:128:A:ARG:HD2  | 8        | 0.14          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3306) | 1:128:A:ARG:HG2  | 1:128:A:ARG:HD2 | 9        | 0.14          |
| (1,3306) | 1:128:A:ARG:HG2  | 1:128:A:ARG:HD2 | 10       | 0.14          |
| (1,3306) | 1:128:A:ARG:HG2  | 1:128:A:ARG:HD2 | 13       | 0.14          |
| (1,3306) | 1:128:A:ARG:HG2  | 1:128:A:ARG:HD2 | 14       | 0.14          |
| (1,3306) | 1:128:A:ARG:HG2  | 1:128:A:ARG:HD2 | 17       | 0.14          |
| (1,3299) | 1:20:A:LYS:H     | 1:20:A:LYS:HD3  | 10       | 0.14          |
| (1,3299) | 1:20:A:LYS:H     | 1:20:A:LYS:HD3  | 14       | 0.14          |
| (1,3270) | 1:42:A:GLU:HG2   | 1:41:A:ALA:HB1  | 14       | 0.14          |
| (1,3263) | 1:121:A:LYS:HG2  | 1:122:A:ALA:H   | 8        | 0.14          |
| (1,3257) | 1:48:A:LEU:HD11  | 1:38:A:CYS:HA   | 3        | 0.14          |
| (1,3250) | 1:41:A:ALA:HA    | 1:41:A:ALA:HB1  | 7        | 0.14          |
| (1,3244) | 1:78:A:TYR:HA    | 1:28:A:ILE:HG12 | 11       | 0.14          |
| (1,3241) | 1:52:A:ILE:HG13  | 1:97:A:LEU:HD23 | 3        | 0.14          |
| (1,3241) | 1:52:A:ILE:HG13  | 1:97:A:LEU:HD23 | 14       | 0.14          |
| (1,3230) | 1:68:A:LYS:HB2   | 1:68:A:LYS:HA   | 1        | 0.14          |
| (1,3230) | 1:68:A:LYS:HB2   | 1:68:A:LYS:HA   | 7        | 0.14          |
| (1,3230) | 1:68:A:LYS:HB2   | 1:68:A:LYS:HA   | 8        | 0.14          |
| (1,3230) | 1:68:A:LYS:HB2   | 1:68:A:LYS:HA   | 10       | 0.14          |
| (1,3230) | 1:68:A:LYS:HB2   | 1:68:A:LYS:HA   | 15       | 0.14          |
| (1,3221) | 1:37:A:HIS:HB2   | 1:99:A:GLY:HA2  | 11       | 0.14          |
| (1,3210) | 1:128:A:ARG:HA   | 1:128:A:ARG:HB3 | 7        | 0.14          |
| (1,3210) | 1:128:A:ARG:HA   | 1:128:A:ARG:HB3 | 17       | 0.14          |
| (1,3208) | 1:124:A:VAL:HG11 | 1:124:A:VAL:HA  | 1        | 0.14          |
| (1,3208) | 1:124:A:VAL:HG11 | 1:124:A:VAL:HA  | 6        | 0.14          |
| (1,3208) | 1:124:A:VAL:HG11 | 1:124:A:VAL:HA  | 8        | 0.14          |
| (1,3208) | 1:124:A:VAL:HG13 | 1:124:A:VAL:HA  | 11       | 0.14          |
| (1,3208) | 1:124:A:VAL:HG13 | 1:124:A:VAL:HA  | 15       | 0.14          |
| (1,3208) | 1:124:A:VAL:HG13 | 1:124:A:VAL:HA  | 16       | 0.14          |
| (1,3205) | 1:124:A:VAL:HA   | 1:124:A:VAL:HB  | 4        | 0.14          |
| (1,3205) | 1:124:A:VAL:HA   | 1:124:A:VAL:HB  | 5        | 0.14          |
| (1,3205) | 1:124:A:VAL:HA   | 1:124:A:VAL:HB  | 6        | 0.14          |
| (1,3205) | 1:124:A:VAL:HA   | 1:124:A:VAL:HB  | 8        | 0.14          |
| (1,3205) | 1:124:A:VAL:HA   | 1:124:A:VAL:HB  | 10       | 0.14          |
| (1,3205) | 1:124:A:VAL:HA   | 1:124:A:VAL:HB  | 13       | 0.14          |
| (1,3205) | 1:124:A:VAL:HA   | 1:124:A:VAL:HB  | 14       | 0.14          |
| (1,3205) | 1:124:A:VAL:HA   | 1:124:A:VAL:HB  | 15       | 0.14          |
| (1,3205) | 1:124:A:VAL:HA   | 1:124:A:VAL:HB  | 16       | 0.14          |
| (1,3200) | 1:116:A:GLN:HG3  | 1:113:A:ALA:HB3 | 4        | 0.14          |
| (1,3197) | 1:87:A:GLY:HA3   | 1:113:A:ALA:HB3 | 13       | 0.14          |
| (1,3160) | 1:74:A:ALA:HB1   | 1:74:A:ALA:HA   | 8        | 0.14          |
| (1,3135) | 1:68:A:LYS:HD3   | 1:68:A:LYS:HB2  | 11       | 0.14          |
| (1,3134) | 1:15:A:MET:HB2   | 1:15:A:MET:HG2  | 1        | 0.14          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3134) | 1:15:A:MET:HB2  | 1:15:A:MET:HG2  | 5        | 0.14          |
| (1,3134) | 1:15:A:MET:HB2  | 1:15:A:MET:HG2  | 13       | 0.14          |
| (1,3130) | 1:123:A:ARG:HG2 | 1:123:A:ARG:H   | 5        | 0.14          |
| (1,3130) | 1:123:A:ARG:HG2 | 1:123:A:ARG:H   | 9        | 0.14          |
| (1,3130) | 1:123:A:ARG:HG2 | 1:123:A:ARG:H   | 10       | 0.14          |
| (1,3130) | 1:123:A:ARG:HG2 | 1:123:A:ARG:H   | 11       | 0.14          |
| (1,3127) | 1:76:A:ARG:HB2  | 1:77:A:LEU:H    | 11       | 0.14          |
| (1,3122) | 1:11:A:SER:HB2  | 1:11:A:SER:HA   | 16       | 0.14          |
| (1,3120) | 1:59:A:ARG:HB2  | 1:58:A:ASP:HB2  | 2        | 0.14          |
| (1,3120) | 1:59:A:ARG:HB2  | 1:58:A:ASP:HB2  | 4        | 0.14          |
| (1,3120) | 1:59:A:ARG:HB2  | 1:58:A:ASP:HB2  | 5        | 0.14          |
| (1,3120) | 1:59:A:ARG:HB2  | 1:58:A:ASP:HB2  | 8        | 0.14          |
| (1,3120) | 1:59:A:ARG:HB2  | 1:58:A:ASP:HB2  | 9        | 0.14          |
| (1,3120) | 1:59:A:ARG:HB2  | 1:58:A:ASP:HB2  | 10       | 0.14          |
| (1,3120) | 1:59:A:ARG:HB2  | 1:58:A:ASP:HB2  | 12       | 0.14          |
| (1,3120) | 1:59:A:ARG:HB2  | 1:58:A:ASP:HB2  | 13       | 0.14          |
| (1,3120) | 1:59:A:ARG:HB2  | 1:58:A:ASP:HB2  | 15       | 0.14          |
| (1,3120) | 1:59:A:ARG:HB2  | 1:58:A:ASP:HB2  | 17       | 0.14          |
| (1,3118) | 1:58:A:ASP:HA   | 1:58:A:ASP:HB2  | 4        | 0.14          |
| (1,3118) | 1:58:A:ASP:HA   | 1:58:A:ASP:HB2  | 9        | 0.14          |
| (1,3118) | 1:58:A:ASP:HA   | 1:58:A:ASP:HB2  | 12       | 0.14          |
| (1,3118) | 1:58:A:ASP:HA   | 1:58:A:ASP:HB2  | 13       | 0.14          |
| (1,3118) | 1:58:A:ASP:HA   | 1:58:A:ASP:HB2  | 16       | 0.14          |
| (1,3118) | 1:58:A:ASP:HA   | 1:58:A:ASP:HB2  | 17       | 0.14          |
| (1,3087) | 1:56:A:LEU:HG   | 1:56:A:LEU:HA   | 1        | 0.14          |
| (1,3087) | 1:56:A:LEU:HG   | 1:56:A:LEU:HA   | 2        | 0.14          |
| (1,3087) | 1:56:A:LEU:HG   | 1:56:A:LEU:HA   | 6        | 0.14          |
| (1,3087) | 1:56:A:LEU:HG   | 1:56:A:LEU:HA   | 13       | 0.14          |
| (1,3087) | 1:56:A:LEU:HG   | 1:56:A:LEU:HA   | 14       | 0.14          |
| (1,3068) | 1:52:A:ILE:HG22 | 1:53:A:PHE:HB2  | 12       | 0.14          |
| (1,3059) | 1:28:A:ILE:HB   | 1:28:A:ILE:HG23 | 6        | 0.14          |
| (1,3053) | 1:29:A:ALA:H    | 1:28:A:ILE:HG23 | 3        | 0.14          |
| (1,3040) | 1:52:A:ILE:HA   | 1:52:A:ILE:HG12 | 1        | 0.14          |
| (1,3040) | 1:52:A:ILE:HA   | 1:52:A:ILE:HG12 | 4        | 0.14          |
| (1,3040) | 1:52:A:ILE:HA   | 1:52:A:ILE:HG12 | 9        | 0.14          |
| (1,3021) | 1:64:A:MET:HE1  | 1:63:A:GLU:H    | 14       | 0.14          |
| (1,3000) | 1:57:A:VAL:HA   | 1:60:A:VAL:HB   | 1        | 0.14          |
| (1,3000) | 1:57:A:VAL:HA   | 1:60:A:VAL:HB   | 3        | 0.14          |
| (1,3000) | 1:57:A:VAL:HA   | 1:60:A:VAL:HB   | 5        | 0.14          |
| (1,3000) | 1:57:A:VAL:HA   | 1:60:A:VAL:HB   | 8        | 0.14          |
| (1,3000) | 1:57:A:VAL:HA   | 1:60:A:VAL:HB   | 10       | 0.14          |
| (1,3000) | 1:57:A:VAL:HA   | 1:60:A:VAL:HB   | 11       | 0.14          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3000) | 1:57:A:VAL:HA    | 1:60:A:VAL:HB   | 13       | 0.14          |
| (1,3000) | 1:57:A:VAL:HA    | 1:60:A:VAL:HB   | 15       | 0.14          |
| (1,3000) | 1:57:A:VAL:HA    | 1:60:A:VAL:HB   | 17       | 0.14          |
| (1,2995) | 1:60:A:VAL:H     | 1:60:A:VAL:HB   | 1        | 0.14          |
| (1,2992) | 1:20:A:LYS:HB3   | 1:20:A:LYS:H    | 14       | 0.14          |
| (1,2989) | 1:42:A:GLU:HA    | 1:42:A:GLU:HB2  | 17       | 0.14          |
| (1,2986) | 1:115:A:LYS:HB3  | 1:115:A:LYS:H   | 1        | 0.14          |
| (1,2961) | 1:56:A:LEU:HD22  | 1:52:A:ILE:HB   | 2        | 0.14          |
| (1,2950) | 1:75:A:LEU:HD11  | 1:75:A:LEU:H    | 3        | 0.14          |
| (1,2930) | 1:31:A:LEU:HD22  | 1:60:A:VAL:HG13 | 3        | 0.14          |
| (1,2893) | 1:50:A:ILE:HB    | 1:50:A:ILE:HG21 | 7        | 0.14          |
| (1,2893) | 1:50:A:ILE:HB    | 1:50:A:ILE:HG21 | 9        | 0.14          |
| (1,2891) | 1:32:A:ALA:HB3   | 1:28:A:ILE:HG21 | 12       | 0.14          |
| (1,2888) | 1:29:A:ALA:HA    | 1:32:A:ALA:HB2  | 12       | 0.14          |
| (1,2888) | 1:29:A:ALA:HA    | 1:32:A:ALA:HB1  | 17       | 0.14          |
| (1,2875) | 1:122:A:ALA:HB1  | 1:122:A:ALA:H   | 17       | 0.14          |
| (1,2871) | 1:129:A:ALA:HB2  | 1:129:A:ALA:H   | 5        | 0.14          |
| (1,2871) | 1:129:A:ALA:HB3  | 1:129:A:ALA:H   | 15       | 0.14          |
| (1,2855) | 1:78:A:TYR:HD1   | 1:28:A:ILE:HD11 | 2        | 0.14          |
| (1,2855) | 1:78:A:TYR:HD2   | 1:28:A:ILE:HD11 | 9        | 0.14          |
| (1,2846) | 1:53:A:PHE:HE2   | 1:75:A:LEU:HB3  | 12       | 0.14          |
| (1,2840) | 1:124:A:VAL:HG11 | 1:125:A:GLN:H   | 10       | 0.14          |
| (1,2836) | 1:95:A:VAL:HG22  | 1:97:A:LEU:HD22 | 8        | 0.14          |
| (1,2819) | 1:97:A:LEU:HD13  | 1:35:A:PHE:HE2  | 3        | 0.14          |
| (1,2804) | 1:66:A:LEU:HB3   | 1:60:A:VAL:HB   | 7        | 0.14          |
| (1,2804) | 1:66:A:LEU:HB3   | 1:60:A:VAL:HB   | 14       | 0.14          |
| (1,2775) | 1:47:A:PRO:HB3   | 1:87:A:GLY:HA2  | 8        | 0.14          |
| (1,2761) | 1:76:A:ARG:HA    | 1:76:A:ARG:HD2  | 12       | 0.14          |
| (1,2761) | 1:76:A:ARG:HA    | 1:76:A:ARG:HD2  | 15       | 0.14          |
| (1,2719) | 1:117:A:LEU:HD11 | 1:86:A:TYR:HB2  | 6        | 0.14          |
| (1,2672) | 1:31:A:LEU:HD13  | 1:35:A:PHE:HD2  | 5        | 0.14          |
| (1,2672) | 1:31:A:LEU:HD12  | 1:35:A:PHE:HD1  | 13       | 0.14          |
| (1,2672) | 1:31:A:LEU:HD12  | 1:35:A:PHE:HD2  | 14       | 0.14          |
| (1,2648) | 1:56:A:LEU:HD11  | 1:52:A:ILE:HG12 | 4        | 0.14          |
| (1,2648) | 1:56:A:LEU:HD13  | 1:52:A:ILE:HG12 | 5        | 0.14          |
| (1,2648) | 1:56:A:LEU:HD13  | 1:52:A:ILE:HG12 | 6        | 0.14          |
| (1,2648) | 1:56:A:LEU:HD13  | 1:52:A:ILE:HG12 | 8        | 0.14          |
| (1,2639) | 1:71:A:LEU:HD12  | 1:71:A:LEU:HB2  | 16       | 0.14          |
| (1,2637) | 1:71:A:LEU:HB3   | 1:71:A:LEU:HG   | 3        | 0.14          |
| (1,2637) | 1:71:A:LEU:HB3   | 1:71:A:LEU:HG   | 11       | 0.14          |
| (1,2637) | 1:71:A:LEU:HB3   | 1:71:A:LEU:HG   | 15       | 0.14          |
| (1,2621) | 1:105:A:LEU:HD13 | 1:92:A:ALA:H    | 14       | 0.14          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2619) | 1:48:A:LEU:HD22  | 1:84:A:TYR:HE2  | 2        | 0.14          |
| (1,2612) | 1:30:A:PHE:HD2   | 1:34:A:ARG:HG2  | 1        | 0.14          |
| (1,2612) | 1:30:A:PHE:HD2   | 1:34:A:ARG:HG2  | 7        | 0.14          |
| (1,2612) | 1:30:A:PHE:HD1   | 1:34:A:ARG:HG2  | 10       | 0.14          |
| (1,2612) | 1:30:A:PHE:HD2   | 1:34:A:ARG:HG2  | 12       | 0.14          |
| (1,2612) | 1:30:A:PHE:HD2   | 1:34:A:ARG:HG2  | 13       | 0.14          |
| (1,2597) | 1:21:A:LEU:HD23  | 1:27:A:VAL:HG12 | 4        | 0.14          |
| (1,2587) | 1:68:A:LYS:HB2   | 1:69:A:THR:HG22 | 10       | 0.14          |
| (1,2579) | 1:59:A:ARG:HB2   | 1:60:A:VAL:HG12 | 1        | 0.14          |
| (1,2579) | 1:59:A:ARG:HB2   | 1:60:A:VAL:HG11 | 13       | 0.14          |
| (1,2547) | 1:11:A:SER:HA    | 1:12:A:GLN:HG3  | 12       | 0.14          |
| (1,2547) | 1:11:A:SER:HA    | 1:12:A:GLN:HG3  | 17       | 0.14          |
| (1,2530) | 1:33:A:GLU:HA    | 1:34:A:ARG:H    | 11       | 0.14          |
| (1,2530) | 1:33:A:GLU:HA    | 1:34:A:ARG:H    | 13       | 0.14          |
| (1,2529) | 1:79:A:THR:HG23  | 1:75:A:LEU:HA   | 5        | 0.14          |
| (1,2529) | 1:79:A:THR:HG21  | 1:75:A:LEU:HA   | 7        | 0.14          |
| (1,2529) | 1:79:A:THR:HG21  | 1:75:A:LEU:HA   | 17       | 0.14          |
| (1,2514) | 1:120:A:ALA:H    | 1:120:A:ALA:HA  | 3        | 0.14          |
| (1,2514) | 1:120:A:ALA:H    | 1:120:A:ALA:HA  | 11       | 0.14          |
| (1,2514) | 1:120:A:ALA:H    | 1:120:A:ALA:HA  | 15       | 0.14          |
| (1,2469) | 1:53:A:PHE:HZ    | 1:72:A:ARG:HG3  | 4        | 0.14          |
| (1,2469) | 1:53:A:PHE:HZ    | 1:72:A:ARG:HG3  | 15       | 0.14          |
| (1,2435) | 1:33:A:GLU:HB3   | 1:13:A:ASP:HB2  | 10       | 0.14          |
| (1,2424) | 1:64:A:MET:HE1   | 1:30:A:PHE:HD1  | 10       | 0.14          |
| (1,2351) | 1:110:A:VAL:HG22 | 1:109:A:HIS:HA  | 2        | 0.14          |
| (1,2351) | 1:110:A:VAL:HG23 | 1:109:A:HIS:HA  | 7        | 0.14          |
| (1,2336) | 1:64:A:MET:HE3   | 1:31:A:LEU:HA   | 5        | 0.14          |
| (1,2295) | 1:121:A:LYS:HG2  | 1:121:A:LYS:HD3 | 1        | 0.14          |
| (1,2283) | 1:33:A:GLU:HG2   | 1:33:A:GLU:HA   | 4        | 0.14          |
| (1,2268) | 1:110:A:VAL:HG13 | 1:89:A:LYS:H    | 8        | 0.14          |
| (1,2253) | 1:44:A:GLU:HB3   | 1:44:A:GLU:H    | 17       | 0.14          |
| (1,2197) | 1:39:A:PHE:HD2   | 1:56:A:LEU:HA   | 6        | 0.14          |
| (1,2197) | 1:39:A:PHE:HD2   | 1:56:A:LEU:HA   | 7        | 0.14          |
| (1,2197) | 1:39:A:PHE:HD2   | 1:56:A:LEU:HA   | 9        | 0.14          |
| (1,2197) | 1:39:A:PHE:HD1   | 1:56:A:LEU:HA   | 13       | 0.14          |
| (1,2197) | 1:39:A:PHE:HD2   | 1:56:A:LEU:HA   | 17       | 0.14          |
| (1,2185) | 1:53:A:PHE:H     | 1:97:A:LEU:HD21 | 8        | 0.14          |
| (1,2185) | 1:53:A:PHE:H     | 1:97:A:LEU:HD23 | 12       | 0.14          |
| (1,2169) | 1:22:A:ASN:HB3   | 1:22:A:ASN:H    | 16       | 0.14          |
| (1,2140) | 1:84:A:TYR:HB2   | 1:82:A:TRP:HA   | 6        | 0.14          |
| (1,2140) | 1:84:A:TYR:HB2   | 1:82:A:TRP:HA   | 10       | 0.14          |
| (1,2140) | 1:84:A:TYR:HB2   | 1:82:A:TRP:HA   | 13       | 0.14          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2118) | 1:69:A:THR:HB   | 1:69:A:THR:HG22  | 2        | 0.14          |
| (1,2118) | 1:69:A:THR:HB   | 1:69:A:THR:HG21  | 3        | 0.14          |
| (1,2118) | 1:69:A:THR:HB   | 1:69:A:THR:HG21  | 4        | 0.14          |
| (1,2118) | 1:69:A:THR:HB   | 1:69:A:THR:HG22  | 5        | 0.14          |
| (1,2118) | 1:69:A:THR:HB   | 1:69:A:THR:HG22  | 6        | 0.14          |
| (1,2118) | 1:69:A:THR:HB   | 1:69:A:THR:HG22  | 11       | 0.14          |
| (1,2118) | 1:69:A:THR:HB   | 1:69:A:THR:HG23  | 12       | 0.14          |
| (1,2118) | 1:69:A:THR:HB   | 1:69:A:THR:HG22  | 13       | 0.14          |
| (1,2118) | 1:69:A:THR:HB   | 1:69:A:THR:HG23  | 16       | 0.14          |
| (1,2108) | 1:40:A:SER:H    | 1:41:A:ALA:H     | 17       | 0.14          |
| (1,2079) | 1:66:A:LEU:HD12 | 1:62:A:GLY:H     | 9        | 0.14          |
| (1,2079) | 1:66:A:LEU:HD13 | 1:62:A:GLY:H     | 10       | 0.14          |
| (1,2079) | 1:66:A:LEU:HD13 | 1:62:A:GLY:H     | 12       | 0.14          |
| (1,2079) | 1:66:A:LEU:HD11 | 1:62:A:GLY:H     | 13       | 0.14          |
| (1,2052) | 1:65:A:ASN:H    | 1:66:A:LEU:H     | 2        | 0.14          |
| (1,2052) | 1:65:A:ASN:H    | 1:66:A:LEU:H     | 11       | 0.14          |
| (1,2045) | 1:77:A:LEU:H    | 1:78:A:TYR:H     | 11       | 0.14          |
| (1,2045) | 1:77:A:LEU:H    | 1:78:A:TYR:H     | 15       | 0.14          |
| (1,2045) | 1:77:A:LEU:H    | 1:78:A:TYR:H     | 16       | 0.14          |
| (1,2035) | 1:52:A:ILE:HG13 | 1:97:A:LEU:HD22  | 16       | 0.14          |
| (1,2021) | 1:53:A:PHE:HE1  | 1:57:A:VAL:HG13  | 1        | 0.14          |
| (1,1955) | 1:92:A:ALA:HB3  | 1:113:A:ALA:HB1  | 15       | 0.14          |
| (1,1910) | 1:128:A:ARG:HB3 | 1:128:A:ARG:HD2  | 5        | 0.14          |
| (1,1906) | 1:105:A:LEU:HB3 | 1:101:A:PRO:HB3  | 11       | 0.14          |
| (1,1906) | 1:105:A:LEU:HB3 | 1:101:A:PRO:HB3  | 16       | 0.14          |
| (1,1906) | 1:105:A:LEU:HB3 | 1:101:A:PRO:HB3  | 17       | 0.14          |
| (1,1887) | 1:65:A:ASN:HB2  | 1:66:A:LEU:H     | 12       | 0.14          |
| (1,1885) | 1:83:A:ARG:HG3  | 1:84:A:TYR:H     | 3        | 0.14          |
| (1,1876) | 1:27:A:VAL:HG23 | 1:31:A:LEU:HD12  | 15       | 0.14          |
| (1,1847) | 1:36:A:PRO:HB2  | 1:36:A:PRO:HD2   | 14       | 0.14          |
| (1,1835) | 1:20:A:LYS:H    | 1:20:A:LYS:HG2   | 2        | 0.14          |
| (1,1812) | 1:117:A:LEU:HA  | 1:117:A:LEU:HD12 | 6        | 0.14          |
| (1,1796) | 1:53:A:PHE:HE1  | 1:68:A:LYS:HA    | 1        | 0.14          |
| (1,1796) | 1:53:A:PHE:HE1  | 1:68:A:LYS:HA    | 5        | 0.14          |
| (1,1796) | 1:53:A:PHE:HE2  | 1:68:A:LYS:HA    | 10       | 0.14          |
| (1,1796) | 1:53:A:PHE:HE2  | 1:68:A:LYS:HA    | 12       | 0.14          |
| (1,1796) | 1:53:A:PHE:HE2  | 1:68:A:LYS:HA    | 13       | 0.14          |
| (1,1793) | 1:88:A:VAL:HG23 | 1:84:A:TYR:HA    | 5        | 0.14          |
| (1,1787) | 1:93:A:THR:HB   | 1:49:A:LYS:HB3   | 4        | 0.14          |
| (1,1775) | 1:88:A:VAL:HA   | 1:47:A:PRO:HB3   | 2        | 0.14          |
| (1,1775) | 1:88:A:VAL:HA   | 1:47:A:PRO:HB3   | 8        | 0.14          |
| (1,1773) | 1:24:A:SER:HA   | 1:27:A:VAL:HG21  | 3        | 0.14          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1773) | 1:24:A:SER:HA    | 1:27:A:VAL:HG21  | 10       | 0.14          |
| (1,1756) | 1:79:A:THR:HG22  | 1:84:A:TYR:HE2   | 1        | 0.14          |
| (1,1726) | 1:66:A:LEU:HD13  | 1:66:A:LEU:HA    | 11       | 0.14          |
| (1,1725) | 1:71:A:LEU:HD13  | 1:71:A:LEU:HG    | 9        | 0.14          |
| (1,1720) | 1:117:A:LEU:HG   | 1:117:A:LEU:HD13 | 3        | 0.14          |
| (1,1718) | 1:18:A:GLN:HB3   | 1:19:A:PRO:HD2   | 3        | 0.14          |
| (1,1718) | 1:18:A:GLN:HB3   | 1:19:A:PRO:HD2   | 13       | 0.14          |
| (1,1713) | 1:20:A:LYS:H     | 1:20:A:LYS:HD3   | 16       | 0.14          |
| (1,1709) | 1:72:A:ARG:HB3   | 1:53:A:PHE:HE2   | 9        | 0.14          |
| (1,1690) | 1:42:A:GLU:HG2   | 1:41:A:ALA:HB2   | 5        | 0.14          |
| (1,1690) | 1:42:A:GLU:HG2   | 1:41:A:ALA:HB1   | 8        | 0.14          |
| (1,1683) | 1:48:A:LEU:HD12  | 1:38:A:CYS:HA    | 5        | 0.14          |
| (1,1668) | 1:52:A:ILE:HG13  | 1:48:A:LEU:HD12  | 10       | 0.14          |
| (1,1640) | 1:33:A:GLU:HG3   | 1:33:A:GLU:H     | 17       | 0.14          |
| (1,1638) | 1:124:A:VAL:HG12 | 1:124:A:VAL:HA   | 13       | 0.14          |
| (1,1636) | 1:124:A:VAL:HA   | 1:125:A:GLN:HG3  | 3        | 0.14          |
| (1,1636) | 1:124:A:VAL:HA   | 1:125:A:GLN:HG3  | 12       | 0.14          |
| (1,1599) | 1:53:A:PHE:HB3   | 1:75:A:LEU:HD23  | 3        | 0.14          |
| (1,1599) | 1:53:A:PHE:HB3   | 1:75:A:LEU:HD23  | 9        | 0.14          |
| (1,1599) | 1:53:A:PHE:HB3   | 1:75:A:LEU:HD23  | 14       | 0.14          |
| (1,1591) | 1:120:A:ALA:HB1  | 1:120:A:ALA:H    | 4        | 0.14          |
| (1,1591) | 1:120:A:ALA:HB1  | 1:120:A:ALA:H    | 6        | 0.14          |
| (1,1553) | 1:57:A:VAL:HG12  | 1:61:A:ALA:H     | 13       | 0.14          |
| (1,1513) | 1:52:A:ILE:HG23  | 1:53:A:PHE:HB3   | 1        | 0.14          |
| (1,1486) | 1:25:A:LYS:HG3   | 1:26:A:GLU:HA    | 13       | 0.14          |
| (1,1486) | 1:25:A:LYS:HG3   | 1:26:A:GLU:HA    | 16       | 0.14          |
| (1,1464) | 1:102:A:CYS:HB3  | 1:103:A:GLY:H    | 6        | 0.14          |
| (1,1464) | 1:102:A:CYS:HB3  | 1:103:A:GLY:H    | 13       | 0.14          |
| (1,1441) | 1:42:A:GLU:HB2   | 1:43:A:GLY:H     | 12       | 0.14          |
| (1,1439) | 1:103:A:GLY:HA3  | 1:101:A:PRO:HD3  | 2        | 0.14          |
| (1,1439) | 1:103:A:GLY:HA3  | 1:101:A:PRO:HD3  | 3        | 0.14          |
| (1,1439) | 1:103:A:GLY:HA3  | 1:101:A:PRO:HD3  | 4        | 0.14          |
| (1,1439) | 1:103:A:GLY:HA3  | 1:101:A:PRO:HD3  | 8        | 0.14          |
| (1,1439) | 1:103:A:GLY:HA3  | 1:101:A:PRO:HD3  | 9        | 0.14          |
| (1,1439) | 1:103:A:GLY:HA3  | 1:101:A:PRO:HD3  | 11       | 0.14          |
| (1,1439) | 1:103:A:GLY:HA3  | 1:101:A:PRO:HD3  | 12       | 0.14          |
| (1,1439) | 1:103:A:GLY:HA3  | 1:101:A:PRO:HD3  | 17       | 0.14          |
| (1,1414) | 1:74:A:ALA:HB3   | 1:75:A:LEU:HD12  | 13       | 0.14          |
| (1,1412) | 1:39:A:PHE:HZ    | 1:75:A:LEU:HD12  | 1        | 0.14          |
| (1,1412) | 1:39:A:PHE:HZ    | 1:75:A:LEU:HD11  | 5        | 0.14          |
| (1,1412) | 1:39:A:PHE:HZ    | 1:75:A:LEU:HD12  | 6        | 0.14          |
| (1,1412) | 1:39:A:PHE:HZ    | 1:75:A:LEU:HD11  | 10       | 0.14          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1410) | 1:110:A:VAL:HG22 | 1:108:A:GLN:H   | 2        | 0.14          |
| (1,1410) | 1:110:A:VAL:HG23 | 1:108:A:GLN:H   | 8        | 0.14          |
| (1,1410) | 1:110:A:VAL:HG22 | 1:108:A:GLN:H   | 10       | 0.14          |
| (1,1405) | 1:102:A:CYS:H    | 1:95:A:VAL:HG11 | 4        | 0.14          |
| (1,1399) | 1:95:A:VAL:HG21  | 1:95:A:VAL:H    | 12       | 0.14          |
| (1,1397) | 1:31:A:LEU:HD21  | 1:60:A:VAL:HG12 | 4        | 0.14          |
| (1,1397) | 1:31:A:LEU:HD22  | 1:60:A:VAL:HG12 | 9        | 0.14          |
| (1,1382) | 1:57:A:VAL:HG22  | 1:53:A:PHE:HE2  | 2        | 0.14          |
| (1,1382) | 1:57:A:VAL:HG21  | 1:53:A:PHE:HE1  | 9        | 0.14          |
| (1,1352) | 1:122:A:ALA:HB3  | 1:122:A:ALA:H   | 3        | 0.14          |
| (1,1352) | 1:122:A:ALA:HB3  | 1:122:A:ALA:H   | 7        | 0.14          |
| (1,1352) | 1:122:A:ALA:HB1  | 1:122:A:ALA:H   | 10       | 0.14          |
| (1,1352) | 1:122:A:ALA:HB1  | 1:122:A:ALA:H   | 15       | 0.14          |
| (1,1352) | 1:122:A:ALA:HB3  | 1:122:A:ALA:H   | 16       | 0.14          |
| (1,1350) | 1:129:A:ALA:HB2  | 1:129:A:ALA:H   | 4        | 0.14          |
| (1,1350) | 1:129:A:ALA:HB3  | 1:129:A:ALA:H   | 8        | 0.14          |
| (1,1350) | 1:129:A:ALA:HB2  | 1:129:A:ALA:H   | 12       | 0.14          |
| (1,1331) | 1:78:A:TYR:HE2   | 1:84:A:TYR:HD2  | 1        | 0.14          |
| (1,1325) | 1:53:A:PHE:HE1   | 1:75:A:LEU:HB3  | 14       | 0.14          |
| (1,1275) | 1:84:A:TYR:HE2   | 1:84:A:TYR:HB3  | 8        | 0.14          |
| (1,1275) | 1:84:A:TYR:HE2   | 1:84:A:TYR:HB3  | 10       | 0.14          |
| (1,1275) | 1:84:A:TYR:HE2   | 1:84:A:TYR:HB3  | 13       | 0.14          |
| (1,1275) | 1:84:A:TYR:HE1   | 1:84:A:TYR:HB3  | 17       | 0.14          |
| (1,1240) | 1:78:A:TYR:HE1   | 1:79:A:THR:HB   | 2        | 0.14          |
| (1,1240) | 1:78:A:TYR:HE2   | 1:79:A:THR:HB   | 5        | 0.14          |
| (1,1240) | 1:78:A:TYR:HE2   | 1:79:A:THR:HB   | 6        | 0.14          |
| (1,1240) | 1:78:A:TYR:HE1   | 1:79:A:THR:HB   | 7        | 0.14          |
| (1,1239) | 1:79:A:THR:H     | 1:78:A:TYR:HE1  | 7        | 0.14          |
| (1,1239) | 1:79:A:THR:H     | 1:78:A:TYR:HE2  | 8        | 0.14          |
| (1,1239) | 1:79:A:THR:H     | 1:78:A:TYR:HE2  | 9        | 0.14          |
| (1,1239) | 1:79:A:THR:H     | 1:78:A:TYR:HE2  | 13       | 0.14          |
| (1,1239) | 1:79:A:THR:H     | 1:78:A:TYR:HE1  | 15       | 0.14          |
| (1,1239) | 1:79:A:THR:H     | 1:78:A:TYR:HE1  | 17       | 0.14          |
| (1,1214) | 1:17:A:ASN:HB3   | 1:17:A:ASN:H    | 3        | 0.14          |
| (1,1206) | 1:117:A:LEU:HD11 | 1:86:A:TYR:HB2  | 7        | 0.14          |
| (1,1206) | 1:117:A:LEU:HD13 | 1:86:A:TYR:HB2  | 12       | 0.14          |
| (1,1206) | 1:117:A:LEU:HD11 | 1:86:A:TYR:HB2  | 15       | 0.14          |
| (1,1126) | 1:86:A:TYR:HE1   | 1:86:A:TYR:HB3  | 5        | 0.14          |
| (1,1126) | 1:86:A:TYR:HE2   | 1:86:A:TYR:HB3  | 10       | 0.14          |
| (1,1073) | 1:97:A:LEU:HD12  | 1:97:A:LEU:H    | 11       | 0.14          |
| (1,1053) | 1:93:A:THR:HG23  | 1:102:A:CYS:HA  | 4        | 0.14          |
| (1,1053) | 1:93:A:THR:HG21  | 1:102:A:CYS:HA  | 9        | 0.14          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1049) | 1:59:A:ARG:HB2  | 1:60:A:VAL:HG12 | 3        | 0.14          |
| (1,1049) | 1:59:A:ARG:HB2  | 1:60:A:VAL:HG12 | 11       | 0.14          |
| (1,1032) | 1:85:A:LEU:H    | 1:84:A:TYR:HE1  | 3        | 0.14          |
| (1,1032) | 1:85:A:LEU:H    | 1:84:A:TYR:HE2  | 9        | 0.14          |
| (1,1032) | 1:85:A:LEU:H    | 1:84:A:TYR:HE2  | 11       | 0.14          |
| (1,1013) | 1:11:A:SER:HA   | 1:12:A:GLN:H    | 3        | 0.14          |
| (1,1009) | 1:37:A:HIS:HD2  | 1:38:A:CYS:HA   | 15       | 0.14          |
| (1,1004) | 1:82:A:TRP:HA   | 1:86:A:TYR:HD1  | 2        | 0.14          |
| (1,983)  | 1:55:A:ASP:HB3  | 1:55:A:ASP:HA   | 7        | 0.14          |
| (1,983)  | 1:55:A:ASP:HB3  | 1:55:A:ASP:HA   | 10       | 0.14          |
| (1,983)  | 1:55:A:ASP:HB3  | 1:55:A:ASP:HA   | 12       | 0.14          |
| (1,980)  | 1:132:A:GLN:HG2 | 1:132:A:GLN:HA  | 15       | 0.14          |
| (1,959)  | 1:30:A:PHE:HD2  | 1:31:A:LEU:HA   | 2        | 0.14          |
| (1,959)  | 1:30:A:PHE:HD1  | 1:31:A:LEU:HA   | 16       | 0.14          |
| (1,872)  | 1:56:A:LEU:HB3  | 1:56:A:LEU:HA   | 3        | 0.14          |
| (1,872)  | 1:56:A:LEU:HB3  | 1:56:A:LEU:HA   | 5        | 0.14          |
| (1,830)  | 1:129:A:ALA:HB1 | 1:127:A:GLN:HB3 | 2        | 0.14          |
| (1,830)  | 1:129:A:ALA:HB1 | 1:127:A:GLN:HB3 | 3        | 0.14          |
| (1,830)  | 1:129:A:ALA:HB3 | 1:127:A:GLN:HB3 | 10       | 0.14          |
| (1,827)  | 1:45:A:ALA:HB2  | 1:45:A:ALA:H    | 17       | 0.14          |
| (1,762)  | 1:65:A:ASN:HA   | 1:66:A:LEU:H    | 4        | 0.14          |
| (1,761)  | 1:62:A:GLY:HA3  | 1:66:A:LEU:H    | 11       | 0.14          |
| (1,756)  | 1:93:A:THR:HB   | 1:102:A:CYS:H   | 2        | 0.14          |
| (1,756)  | 1:93:A:THR:HB   | 1:102:A:CYS:H   | 6        | 0.14          |
| (1,756)  | 1:93:A:THR:HB   | 1:102:A:CYS:H   | 17       | 0.14          |
| (1,707)  | 1:75:A:LEU:HB3  | 1:74:A:ALA:H    | 9        | 0.14          |
| (1,707)  | 1:75:A:LEU:HB3  | 1:74:A:ALA:H    | 14       | 0.14          |
| (1,665)  | 1:122:A:ALA:HB3 | 1:123:A:ARG:H   | 5        | 0.14          |
| (1,635)  | 1:127:A:GLN:H   | 1:127:A:GLN:HB3 | 2        | 0.14          |
| (1,618)  | 1:95:A:VAL:H    | 1:48:A:LEU:HD11 | 6        | 0.14          |
| (1,552)  | 1:65:A:ASN:H    | 1:65:A:ASN:HD21 | 10       | 0.14          |
| (1,512)  | 1:13:A:ASP:HB2  | 1:13:A:ASP:H    | 4        | 0.14          |
| (1,478)  | 1:27:A:VAL:HG21 | 1:29:A:ALA:H    | 10       | 0.14          |
| (1,477)  | 1:31:A:LEU:H    | 1:31:A:LEU:HD11 | 2        | 0.14          |
| (1,477)  | 1:31:A:LEU:H    | 1:31:A:LEU:HD11 | 11       | 0.14          |
| (1,477)  | 1:31:A:LEU:H    | 1:31:A:LEU:HD13 | 12       | 0.14          |
| (1,477)  | 1:31:A:LEU:H    | 1:31:A:LEU:HD13 | 13       | 0.14          |
| (1,435)  | 1:42:A:GLU:HB2  | 1:43:A:GLY:H    | 12       | 0.14          |
| (1,423)  | 1:50:A:ILE:HG22 | 1:50:A:ILE:H    | 14       | 0.14          |
| (1,397)  | 1:57:A:VAL:H    | 1:56:A:LEU:HB3  | 3        | 0.14          |
| (1,397)  | 1:57:A:VAL:H    | 1:56:A:LEU:HB3  | 5        | 0.14          |
| (1,397)  | 1:57:A:VAL:H    | 1:56:A:LEU:HB3  | 7        | 0.14          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,397) | 1:57:A:VAL:H     | 1:56:A:LEU:HB3  | 9        | 0.14          |
| (1,361) | 1:66:A:LEU:HD12  | 1:63:A:GLU:H    | 1        | 0.14          |
| (1,359) | 1:62:A:GLY:HA3   | 1:63:A:GLU:H    | 7        | 0.14          |
| (1,319) | 1:76:A:ARG:HD2   | 1:77:A:LEU:H    | 8        | 0.14          |
| (1,311) | 1:79:A:THR:H     | 1:77:A:LEU:HB2  | 5        | 0.14          |
| (1,311) | 1:79:A:THR:H     | 1:77:A:LEU:HB2  | 6        | 0.14          |
| (1,311) | 1:79:A:THR:H     | 1:77:A:LEU:HB2  | 7        | 0.14          |
| (1,311) | 1:79:A:THR:H     | 1:77:A:LEU:HB2  | 9        | 0.14          |
| (1,311) | 1:79:A:THR:H     | 1:77:A:LEU:HB2  | 12       | 0.14          |
| (1,311) | 1:79:A:THR:H     | 1:77:A:LEU:HB2  | 13       | 0.14          |
| (1,311) | 1:79:A:THR:H     | 1:77:A:LEU:HB2  | 15       | 0.14          |
| (1,311) | 1:79:A:THR:H     | 1:77:A:LEU:HB2  | 16       | 0.14          |
| (1,311) | 1:79:A:THR:H     | 1:77:A:LEU:HB2  | 17       | 0.14          |
| (1,297) | 1:81:A:SER:HB2   | 1:82:A:TRP:H    | 11       | 0.14          |
| (1,241) | 1:95:A:VAL:HG12  | 1:96:A:ASP:H    | 13       | 0.14          |
| (1,234) | 1:95:A:VAL:HG21  | 1:99:A:GLY:H    | 16       | 0.14          |
| (1,184) | 1:43:A:GLY:HA3   | 1:44:A:GLU:H    | 15       | 0.14          |
| (1,155) | 1:130:A:GLU:HG3  | 1:130:A:GLU:H   | 14       | 0.14          |
| (1,152) | 1:128:A:ARG:HB3  | 1:129:A:ALA:H   | 13       | 0.14          |
| (1,101) | 1:35:A:PHE:H     | 1:39:A:PHE:HE2  | 7        | 0.14          |
| (1,101) | 1:35:A:PHE:H     | 1:39:A:PHE:HE1  | 10       | 0.14          |
| (1,101) | 1:35:A:PHE:H     | 1:39:A:PHE:HE1  | 12       | 0.14          |
| (1,101) | 1:35:A:PHE:H     | 1:39:A:PHE:HE1  | 15       | 0.14          |
| (1,101) | 1:35:A:PHE:H     | 1:39:A:PHE:HE2  | 17       | 0.14          |
| (1,80)  | 1:30:A:PHE:HD1   | 1:30:A:PHE:H    | 1        | 0.14          |
| (1,80)  | 1:30:A:PHE:HD2   | 1:30:A:PHE:H    | 11       | 0.14          |
| (1,80)  | 1:30:A:PHE:HD1   | 1:30:A:PHE:H    | 12       | 0.14          |
| (1,80)  | 1:30:A:PHE:HD1   | 1:30:A:PHE:H    | 14       | 0.14          |
| (3,137) | 1:123:A:ARG:H    | 1:123:A:ARG:HA  | 2        | 0.13          |
| (3,137) | 1:123:A:ARG:H    | 1:123:A:ARG:HA  | 3        | 0.13          |
| (3,137) | 1:123:A:ARG:H    | 1:123:A:ARG:HA  | 13       | 0.13          |
| (3,137) | 1:123:A:ARG:H    | 1:123:A:ARG:HA  | 14       | 0.13          |
| (3,122) | 1:27:A:VAL:HG23  | 1:28:A:ILE:HD13 | 4        | 0.13          |
| (3,117) | 1:48:A:LEU:HD21  | 1:39:A:PHE:HD1  | 2        | 0.13          |
| (3,94)  | 1:56:A:LEU:HB2   | 1:75:A:LEU:HD12 | 12       | 0.13          |
| (3,92)  | 1:88:A:VAL:HG21  | 1:87:A:GLY:HA2  | 4        | 0.13          |
| (3,90)  | 1:115:A:LYS:HG3  | 1:116:A:GLN:HG3 | 4        | 0.13          |
| (3,90)  | 1:115:A:LYS:HG3  | 1:116:A:GLN:HG3 | 6        | 0.13          |
| (3,90)  | 1:115:A:LYS:HG3  | 1:116:A:GLN:HG3 | 14       | 0.13          |
| (3,87)  | 1:117:A:LEU:HD12 | 1:121:A:LYS:H   | 8        | 0.13          |
| (3,54)  | 1:71:A:LEU:HB3   | 1:75:A:LEU:HD11 | 9        | 0.13          |
| (3,48)  | 1:72:A:ARG:HD3   | 1:72:A:ARG:HB3  | 2        | 0.13          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,48)   | 1:72:A:ARG:HD3  | 1:72:A:ARG:HB3  | 5        | 0.13          |
| (3,48)   | 1:72:A:ARG:HD3  | 1:72:A:ARG:HB3  | 8        | 0.13          |
| (3,48)   | 1:72:A:ARG:HD3  | 1:72:A:ARG:HB3  | 14       | 0.13          |
| (1,4345) | 1:117:A:LEU:HA  | 1:121:A:LYS:H   | 6        | 0.13          |
| (1,4345) | 1:117:A:LEU:HA  | 1:121:A:LYS:H   | 11       | 0.13          |
| (1,4344) | 1:120:A:ALA:H   | 1:119:A:GLU:HG2 | 4        | 0.13          |
| (1,4343) | 1:118:A:GLU:H   | 1:119:A:GLU:H   | 5        | 0.13          |
| (1,4343) | 1:118:A:GLU:H   | 1:119:A:GLU:H   | 7        | 0.13          |
| (1,4343) | 1:118:A:GLU:H   | 1:119:A:GLU:H   | 11       | 0.13          |
| (1,4339) | 1:116:A:GLN:HG3 | 1:115:A:LYS:H   | 2        | 0.13          |
| (1,4339) | 1:116:A:GLN:HG3 | 1:115:A:LYS:H   | 10       | 0.13          |
| (1,4339) | 1:116:A:GLN:HG3 | 1:115:A:LYS:H   | 13       | 0.13          |
| (1,4339) | 1:116:A:GLN:HG3 | 1:115:A:LYS:H   | 14       | 0.13          |
| (1,4326) | 1:65:A:ASN:HA   | 1:66:A:LEU:H    | 11       | 0.13          |
| (1,4325) | 1:62:A:GLY:HA3  | 1:66:A:LEU:H    | 3        | 0.13          |
| (1,4323) | 1:62:A:GLY:H    | 1:68:A:LYS:HD2  | 10       | 0.13          |
| (1,4323) | 1:62:A:GLY:H    | 1:68:A:LYS:HD2  | 15       | 0.13          |
| (1,4320) | 1:62:A:GLY:H    | 1:66:A:LEU:H    | 7        | 0.13          |
| (1,4316) | 1:95:A:VAL:H    | 1:94:A:ARG:HB3  | 16       | 0.13          |
| (1,4295) | 1:116:A:GLN:HA  | 1:117:A:LEU:H   | 2        | 0.13          |
| (1,4293) | 1:130:A:GLU:H   | 1:132:A:GLN:HB2 | 15       | 0.13          |
| (1,4283) | 1:120:A:ALA:H   | 1:85:A:LEU:HD21 | 8        | 0.13          |
| (1,4273) | 1:73:A:SER:HA   | 1:75:A:LEU:H    | 2        | 0.13          |
| (1,4273) | 1:73:A:SER:HA   | 1:75:A:LEU:H    | 8        | 0.13          |
| (1,4271) | 1:78:A:TYR:HE2  | 1:75:A:LEU:H    | 6        | 0.13          |
| (1,4271) | 1:78:A:TYR:HE1  | 1:75:A:LEU:H    | 12       | 0.13          |
| (1,4270) | 1:75:A:LEU:HB3  | 1:74:A:ALA:H    | 3        | 0.13          |
| (1,4270) | 1:75:A:LEU:HB3  | 1:74:A:ALA:H    | 5        | 0.13          |
| (1,4270) | 1:75:A:LEU:HB3  | 1:74:A:ALA:H    | 12       | 0.13          |
| (1,4270) | 1:75:A:LEU:HB3  | 1:74:A:ALA:H    | 13       | 0.13          |
| (1,4270) | 1:75:A:LEU:HB3  | 1:74:A:ALA:H    | 17       | 0.13          |
| (1,4228) | 1:123:A:ARG:HB3 | 1:124:A:VAL:H   | 1        | 0.13          |
| (1,4228) | 1:123:A:ARG:HB3 | 1:124:A:VAL:H   | 3        | 0.13          |
| (1,4228) | 1:123:A:ARG:HB3 | 1:124:A:VAL:H   | 4        | 0.13          |
| (1,4228) | 1:123:A:ARG:HB3 | 1:124:A:VAL:H   | 8        | 0.13          |
| (1,4228) | 1:123:A:ARG:HB3 | 1:124:A:VAL:H   | 9        | 0.13          |
| (1,4228) | 1:123:A:ARG:HB3 | 1:124:A:VAL:H   | 10       | 0.13          |
| (1,4228) | 1:123:A:ARG:HB3 | 1:124:A:VAL:H   | 11       | 0.13          |
| (1,4228) | 1:123:A:ARG:HB3 | 1:124:A:VAL:H   | 12       | 0.13          |
| (1,4228) | 1:123:A:ARG:HB3 | 1:124:A:VAL:H   | 13       | 0.13          |
| (1,4228) | 1:123:A:ARG:HB3 | 1:124:A:VAL:H   | 15       | 0.13          |
| (1,4228) | 1:123:A:ARG:HB3 | 1:124:A:VAL:H   | 16       | 0.13          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,4223) | 1:123:A:ARG:H   | 1:125:A:GLN:HG3 | 7        | 0.13          |
| (1,4223) | 1:123:A:ARG:H   | 1:125:A:GLN:HG3 | 13       | 0.13          |
| (1,4223) | 1:123:A:ARG:H   | 1:125:A:GLN:HG3 | 14       | 0.13          |
| (1,4223) | 1:123:A:ARG:H   | 1:125:A:GLN:HG3 | 15       | 0.13          |
| (1,4198) | 1:127:A:GLN:HA  | 1:127:A:GLN:H   | 9        | 0.13          |
| (1,4198) | 1:127:A:GLN:HA  | 1:127:A:GLN:H   | 14       | 0.13          |
| (1,4194) | 1:107:A:GLU:H   | 1:106:A:ASP:HA  | 3        | 0.13          |
| (1,4194) | 1:107:A:GLU:H   | 1:106:A:ASP:HA  | 8        | 0.13          |
| (1,4194) | 1:107:A:GLU:H   | 1:106:A:ASP:HA  | 9        | 0.13          |
| (1,4194) | 1:107:A:GLU:H   | 1:106:A:ASP:HA  | 14       | 0.13          |
| (1,4193) | 1:69:A:THR:HB   | 1:72:A:ARG:H    | 1        | 0.13          |
| (1,4150) | 1:17:A:ASN:HB3  | 1:18:A:GLN:H    | 8        | 0.13          |
| (1,4143) | 1:37:A:HIS:HA   | 1:39:A:PHE:H    | 10       | 0.13          |
| (1,4143) | 1:37:A:HIS:HA   | 1:39:A:PHE:H    | 13       | 0.13          |
| (1,4127) | 1:34:A:ARG:HE   | 1:30:A:PHE:HD2  | 7        | 0.13          |
| (1,4127) | 1:34:A:ARG:HE   | 1:30:A:PHE:HD1  | 11       | 0.13          |
| (1,4106) | 1:99:A:GLY:HA3  | 1:98:A:ASP:H    | 8        | 0.13          |
| (1,4106) | 1:99:A:GLY:HA3  | 1:98:A:ASP:H    | 10       | 0.13          |
| (1,4106) | 1:99:A:GLY:HA3  | 1:98:A:ASP:H    | 12       | 0.13          |
| (1,4060) | 1:97:A:LEU:HD22 | 1:39:A:PHE:H    | 13       | 0.13          |
| (1,4037) | 1:27:A:VAL:HG23 | 1:29:A:ALA:H    | 5        | 0.13          |
| (1,4037) | 1:27:A:VAL:HG23 | 1:29:A:ALA:H    | 6        | 0.13          |
| (1,4019) | 1:33:A:GLU:HB3  | 1:34:A:ARG:H    | 6        | 0.13          |
| (1,4019) | 1:33:A:GLU:HB3  | 1:34:A:ARG:H    | 8        | 0.13          |
| (1,4016) | 1:15:A:MET:HA   | 1:15:A:MET:H    | 15       | 0.13          |
| (1,3987) | 1:50:A:ILE:HG21 | 1:50:A:ILE:H    | 6        | 0.13          |
| (1,3979) | 1:50:A:ILE:HA   | 1:51:A:GLY:H    | 3        | 0.13          |
| (1,3940) | 1:62:A:GLY:HA3  | 1:63:A:GLU:H    | 12       | 0.13          |
| (1,3929) | 1:68:A:LYS:HD2  | 1:68:A:LYS:H    | 2        | 0.13          |
| (1,3929) | 1:68:A:LYS:HD2  | 1:68:A:LYS:H    | 7        | 0.13          |
| (1,3929) | 1:68:A:LYS:HD2  | 1:68:A:LYS:H    | 10       | 0.13          |
| (1,3916) | 1:71:A:LEU:HA   | 1:74:A:ALA:H    | 4        | 0.13          |
| (1,3916) | 1:71:A:LEU:HA   | 1:74:A:ALA:H    | 7        | 0.13          |
| (1,3907) | 1:76:A:ARG:HD2  | 1:77:A:LEU:H    | 15       | 0.13          |
| (1,3892) | 1:45:A:ALA:HB2  | 1:81:A:SER:H    | 9        | 0.13          |
| (1,3887) | 1:81:A:SER:HB2  | 1:82:A:TRP:H    | 5        | 0.13          |
| (1,3887) | 1:81:A:SER:HB2  | 1:82:A:TRP:H    | 7        | 0.13          |
| (1,3887) | 1:81:A:SER:HB2  | 1:82:A:TRP:H    | 8        | 0.13          |
| (1,3887) | 1:81:A:SER:HB2  | 1:82:A:TRP:H    | 9        | 0.13          |
| (1,3887) | 1:81:A:SER:HB2  | 1:82:A:TRP:H    | 14       | 0.13          |
| (1,3879) | 1:127:A:GLN:H   | 1:127:A:GLN:HG2 | 1        | 0.13          |
| (1,3859) | 1:90:A:PRO:HB2  | 1:91:A:GLY:H    | 1        | 0.13          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3859) | 1:90:A:PRO:HB2  | 1:91:A:GLY:H    | 5        | 0.13          |
| (1,3859) | 1:90:A:PRO:HB2  | 1:91:A:GLY:H    | 11       | 0.13          |
| (1,3830) | 1:101:A:PRO:HD3 | 1:100:A:ASN:H   | 3        | 0.13          |
| (1,3830) | 1:101:A:PRO:HD3 | 1:100:A:ASN:H   | 4        | 0.13          |
| (1,3830) | 1:101:A:PRO:HD3 | 1:100:A:ASN:H   | 9        | 0.13          |
| (1,3830) | 1:101:A:PRO:HD3 | 1:100:A:ASN:H   | 11       | 0.13          |
| (1,3830) | 1:101:A:PRO:HD3 | 1:100:A:ASN:H   | 15       | 0.13          |
| (1,3824) | 1:102:A:CYS:H   | 1:100:A:ASN:HB3 | 13       | 0.13          |
| (1,3824) | 1:102:A:CYS:H   | 1:100:A:ASN:HB3 | 17       | 0.13          |
| (1,3820) | 1:101:A:PRO:HB3 | 1:103:A:GLY:H   | 10       | 0.13          |
| (1,3820) | 1:101:A:PRO:HB3 | 1:103:A:GLY:H   | 13       | 0.13          |
| (1,3820) | 1:101:A:PRO:HB3 | 1:103:A:GLY:H   | 16       | 0.13          |
| (1,3798) | 1:43:A:GLY:HA3  | 1:44:A:GLU:H    | 9        | 0.13          |
| (1,3783) | 1:117:A:LEU:HB3 | 1:117:A:LEU:H   | 6        | 0.13          |
| (1,3768) | 1:130:A:GLU:H   | 1:130:A:GLU:HA  | 3        | 0.13          |
| (1,3766) | 1:128:A:ARG:HB3 | 1:129:A:ALA:H   | 7        | 0.13          |
| (1,3757) | 1:116:A:GLN:H   | 1:117:A:LEU:H   | 4        | 0.13          |
| (1,3757) | 1:116:A:GLN:H   | 1:117:A:LEU:H   | 8        | 0.13          |
| (1,3757) | 1:116:A:GLN:H   | 1:117:A:LEU:H   | 12       | 0.13          |
| (1,3757) | 1:116:A:GLN:H   | 1:117:A:LEU:H   | 14       | 0.13          |
| (1,3753) | 1:107:A:GLU:H   | 1:106:A:ASP:H   | 3        | 0.13          |
| (1,3753) | 1:107:A:GLU:H   | 1:106:A:ASP:H   | 6        | 0.13          |
| (1,3753) | 1:107:A:GLU:H   | 1:106:A:ASP:H   | 7        | 0.13          |
| (1,3753) | 1:107:A:GLU:H   | 1:106:A:ASP:H   | 8        | 0.13          |
| (1,3753) | 1:107:A:GLU:H   | 1:106:A:ASP:H   | 9        | 0.13          |
| (1,3753) | 1:107:A:GLU:H   | 1:106:A:ASP:H   | 11       | 0.13          |
| (1,3753) | 1:107:A:GLU:H   | 1:106:A:ASP:H   | 12       | 0.13          |
| (1,3753) | 1:107:A:GLU:H   | 1:106:A:ASP:H   | 13       | 0.13          |
| (1,3753) | 1:107:A:GLU:H   | 1:106:A:ASP:H   | 15       | 0.13          |
| (1,3753) | 1:107:A:GLU:H   | 1:106:A:ASP:H   | 16       | 0.13          |
| (1,3753) | 1:107:A:GLU:H   | 1:106:A:ASP:H   | 17       | 0.13          |
| (1,3732) | 1:21:A:LEU:HD13 | 1:30:A:PHE:H    | 9        | 0.13          |
| (1,3687) | 1:85:A:LEU:H    | 1:82:A:TRP:HD1  | 3        | 0.13          |
| (1,3685) | 1:81:A:SER:H    | 1:84:A:TYR:H    | 11       | 0.13          |
| (1,3623) | 1:40:A:SER:H    | 1:78:A:TYR:HD2  | 11       | 0.13          |
| (1,3605) | 1:38:A:CYS:HB3  | 1:97:A:LEU:HA   | 11       | 0.13          |
| (1,3603) | 1:97:A:LEU:HA   | 1:97:A:LEU:HG   | 15       | 0.13          |
| (1,3600) | 1:113:A:ALA:HB3 | 1:92:A:ALA:HA   | 13       | 0.13          |
| (1,3600) | 1:113:A:ALA:HB1 | 1:92:A:ALA:HA   | 17       | 0.13          |
| (1,3599) | 1:92:A:ALA:HB1  | 1:113:A:ALA:HB1 | 11       | 0.13          |
| (1,3596) | 1:112:A:HIS:HA  | 1:115:A:LYS:HB3 | 14       | 0.13          |
| (1,3579) | 1:33:A:GLU:HB3  | 1:30:A:PHE:HA   | 12       | 0.13          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3568) | 1:105:A:LEU:HB3  | 1:109:A:HIS:HB2  | 7        | 0.13          |
| (1,3568) | 1:105:A:LEU:HB3  | 1:109:A:HIS:HB2  | 9        | 0.13          |
| (1,3568) | 1:105:A:LEU:HB3  | 1:109:A:HIS:HB2  | 14       | 0.13          |
| (1,3552) | 1:123:A:ARG:HG2  | 1:124:A:VAL:HA   | 10       | 0.13          |
| (1,3537) | 1:51:A:GLY:HA2   | 1:54:A:GLN:HB2   | 10       | 0.13          |
| (1,3531) | 1:65:A:ASN:H     | 1:65:A:ASN:HA    | 3        | 0.13          |
| (1,3523) | 1:56:A:LEU:HG    | 1:56:A:LEU:HB3   | 8        | 0.13          |
| (1,3523) | 1:56:A:LEU:HG    | 1:56:A:LEU:HB3   | 10       | 0.13          |
| (1,3520) | 1:100:A:ASN:HD22 | 1:98:A:ASP:HB3   | 1        | 0.13          |
| (1,3519) | 1:65:A:ASN:H     | 1:65:A:ASN:HB3   | 8        | 0.13          |
| (1,3516) | 1:21:A:LEU:HG    | 1:65:A:ASN:HB3   | 14       | 0.13          |
| (1,3510) | 1:64:A:MET:HE3   | 1:21:A:LEU:H     | 15       | 0.13          |
| (1,3508) | 1:113:A:ALA:HB3  | 1:88:A:VAL:HA    | 6        | 0.13          |
| (1,3502) | 1:27:A:VAL:HG21  | 1:27:A:VAL:H     | 5        | 0.13          |
| (1,3502) | 1:27:A:VAL:HG23  | 1:27:A:VAL:H     | 14       | 0.13          |
| (1,3502) | 1:27:A:VAL:HG23  | 1:27:A:VAL:H     | 16       | 0.13          |
| (1,3501) | 1:27:A:VAL:HG21  | 1:28:A:ILE:HA    | 12       | 0.13          |
| (1,3501) | 1:27:A:VAL:HG23  | 1:28:A:ILE:HA    | 15       | 0.13          |
| (1,3477) | 1:15:A:MET:HG3   | 1:15:A:MET:HB2   | 4        | 0.13          |
| (1,3456) | 1:95:A:VAL:HG22  | 1:96:A:ASP:HA    | 6        | 0.13          |
| (1,3437) | 1:21:A:LEU:HB2   | 1:21:A:LEU:HD11  | 12       | 0.13          |
| (1,3424) | 1:118:A:GLU:HA   | 1:122:A:ALA:H    | 8        | 0.13          |
| (1,3422) | 1:77:A:LEU:HG    | 1:77:A:LEU:HD22  | 2        | 0.13          |
| (1,3414) | 1:86:A:TYR:H     | 1:117:A:LEU:HD11 | 13       | 0.13          |
| (1,3372) | 1:88:A:VAL:HA    | 1:47:A:PRO:HB3   | 6        | 0.13          |
| (1,3372) | 1:88:A:VAL:HA    | 1:47:A:PRO:HB3   | 7        | 0.13          |
| (1,3372) | 1:88:A:VAL:HA    | 1:47:A:PRO:HB3   | 14       | 0.13          |
| (1,3372) | 1:88:A:VAL:HA    | 1:47:A:PRO:HB3   | 15       | 0.13          |
| (1,3372) | 1:88:A:VAL:HA    | 1:47:A:PRO:HB3   | 16       | 0.13          |
| (1,3344) | 1:113:A:ALA:HB2  | 1:89:A:LYS:H     | 3        | 0.13          |
| (1,3344) | 1:113:A:ALA:HB3  | 1:89:A:LYS:H     | 4        | 0.13          |
| (1,3344) | 1:113:A:ALA:HB3  | 1:89:A:LYS:H     | 15       | 0.13          |
| (1,3316) | 1:66:A:LEU:HD11  | 1:30:A:PHE:HD2   | 5        | 0.13          |
| (1,3315) | 1:66:A:LEU:HD12  | 1:66:A:LEU:HA    | 2        | 0.13          |
| (1,3315) | 1:66:A:LEU:HD12  | 1:66:A:LEU:HA    | 4        | 0.13          |
| (1,3315) | 1:66:A:LEU:HD11  | 1:66:A:LEU:HA    | 7        | 0.13          |
| (1,3315) | 1:66:A:LEU:HD12  | 1:66:A:LEU:HA    | 10       | 0.13          |
| (1,3315) | 1:66:A:LEU:HD13  | 1:66:A:LEU:HA    | 17       | 0.13          |
| (1,3306) | 1:128:A:ARG:HG2  | 1:128:A:ARG:HD2  | 2        | 0.13          |
| (1,3306) | 1:128:A:ARG:HG2  | 1:128:A:ARG:HD2  | 3        | 0.13          |
| (1,3306) | 1:128:A:ARG:HG2  | 1:128:A:ARG:HD2  | 11       | 0.13          |
| (1,3291) | 1:72:A:ARG:HB3   | 1:53:A:PHE:HE2   | 17       | 0.13          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3275) | 1:119:A:GLU:HA   | 1:119:A:GLU:HG2 | 7        | 0.13          |
| (1,3275) | 1:119:A:GLU:HA   | 1:119:A:GLU:HG2 | 16       | 0.13          |
| (1,3273) | 1:42:A:GLU:HG2   | 1:43:A:GLY:H    | 7        | 0.13          |
| (1,3269) | 1:33:A:GLU:HB3   | 1:17:A:ASN:HB2  | 5        | 0.13          |
| (1,3269) | 1:33:A:GLU:HB3   | 1:17:A:ASN:HB2  | 8        | 0.13          |
| (1,3263) | 1:121:A:LYS:HG2  | 1:122:A:ALA:H   | 11       | 0.13          |
| (1,3263) | 1:121:A:LYS:HG2  | 1:122:A:ALA:H   | 13       | 0.13          |
| (1,3263) | 1:121:A:LYS:HG2  | 1:122:A:ALA:H   | 16       | 0.13          |
| (1,3255) | 1:40:A:SER:HA    | 1:41:A:ALA:HB1  | 6        | 0.13          |
| (1,3244) | 1:78:A:TYR:HA    | 1:28:A:ILE:HG12 | 1        | 0.13          |
| (1,3244) | 1:78:A:TYR:HA    | 1:28:A:ILE:HG12 | 6        | 0.13          |
| (1,3244) | 1:78:A:TYR:HA    | 1:28:A:ILE:HG12 | 9        | 0.13          |
| (1,3244) | 1:78:A:TYR:HA    | 1:28:A:ILE:HG12 | 14       | 0.13          |
| (1,3241) | 1:52:A:ILE:HG13  | 1:97:A:LEU:HD23 | 7        | 0.13          |
| (1,3230) | 1:68:A:LYS:HB2   | 1:68:A:LYS:HA   | 2        | 0.13          |
| (1,3230) | 1:68:A:LYS:HB2   | 1:68:A:LYS:HA   | 12       | 0.13          |
| (1,3230) | 1:68:A:LYS:HB2   | 1:68:A:LYS:HA   | 13       | 0.13          |
| (1,3221) | 1:37:A:HIS:HB2   | 1:99:A:GLY:HA2  | 7        | 0.13          |
| (1,3210) | 1:128:A:ARG:HA   | 1:128:A:ARG:HB3 | 3        | 0.13          |
| (1,3210) | 1:128:A:ARG:HA   | 1:128:A:ARG:HB3 | 9        | 0.13          |
| (1,3210) | 1:128:A:ARG:HA   | 1:128:A:ARG:HB3 | 16       | 0.13          |
| (1,3208) | 1:124:A:VAL:HG12 | 1:124:A:VAL:HA  | 3        | 0.13          |
| (1,3208) | 1:124:A:VAL:HG12 | 1:124:A:VAL:HA  | 5        | 0.13          |
| (1,3208) | 1:124:A:VAL:HG12 | 1:124:A:VAL:HA  | 7        | 0.13          |
| (1,3208) | 1:124:A:VAL:HG12 | 1:124:A:VAL:HA  | 9        | 0.13          |
| (1,3208) | 1:124:A:VAL:HG13 | 1:124:A:VAL:HA  | 10       | 0.13          |
| (1,3208) | 1:124:A:VAL:HG12 | 1:124:A:VAL:HA  | 12       | 0.13          |
| (1,3208) | 1:124:A:VAL:HG13 | 1:124:A:VAL:HA  | 14       | 0.13          |
| (1,3205) | 1:124:A:VAL:HA   | 1:124:A:VAL:HB  | 1        | 0.13          |
| (1,3205) | 1:124:A:VAL:HA   | 1:124:A:VAL:HB  | 3        | 0.13          |
| (1,3205) | 1:124:A:VAL:HA   | 1:124:A:VAL:HB  | 7        | 0.13          |
| (1,3205) | 1:124:A:VAL:HA   | 1:124:A:VAL:HB  | 9        | 0.13          |
| (1,3205) | 1:124:A:VAL:HA   | 1:124:A:VAL:HB  | 11       | 0.13          |
| (1,3205) | 1:124:A:VAL:HA   | 1:124:A:VAL:HB  | 12       | 0.13          |
| (1,3205) | 1:124:A:VAL:HA   | 1:124:A:VAL:HB  | 17       | 0.13          |
| (1,3200) | 1:116:A:GLN:HG3  | 1:113:A:ALA:HB2 | 10       | 0.13          |
| (1,3197) | 1:87:A:GLY:HA3   | 1:113:A:ALA:HB3 | 8        | 0.13          |
| (1,3197) | 1:87:A:GLY:HA3   | 1:113:A:ALA:HB3 | 10       | 0.13          |
| (1,3185) | 1:109:A:HIS:HB2  | 1:108:A:GLN:H   | 11       | 0.13          |
| (1,3185) | 1:109:A:HIS:HB2  | 1:108:A:GLN:H   | 15       | 0.13          |
| (1,3183) | 1:124:A:VAL:HG22 | 1:121:A:LYS:HA  | 12       | 0.13          |
| (1,3183) | 1:124:A:VAL:HG21 | 1:121:A:LYS:HA  | 16       | 0.13          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3172) | 1:25:A:LYS:HE3  | 1:25:A:LYS:HA   | 10       | 0.13          |
| (1,3163) | 1:61:A:ALA:HB3  | 1:61:A:ALA:H    | 5        | 0.13          |
| (1,3151) | 1:97:A:LEU:HA   | 1:97:A:LEU:H    | 5        | 0.13          |
| (1,3151) | 1:97:A:LEU:HA   | 1:97:A:LEU:H    | 7        | 0.13          |
| (1,3151) | 1:97:A:LEU:HA   | 1:97:A:LEU:H    | 16       | 0.13          |
| (1,3134) | 1:15:A:MET:HB2  | 1:15:A:MET:HG2  | 2        | 0.13          |
| (1,3134) | 1:15:A:MET:HB2  | 1:15:A:MET:HG2  | 4        | 0.13          |
| (1,3134) | 1:15:A:MET:HB2  | 1:15:A:MET:HG2  | 6        | 0.13          |
| (1,3134) | 1:15:A:MET:HB2  | 1:15:A:MET:HG2  | 7        | 0.13          |
| (1,3134) | 1:15:A:MET:HB2  | 1:15:A:MET:HG2  | 11       | 0.13          |
| (1,3134) | 1:15:A:MET:HB2  | 1:15:A:MET:HG2  | 17       | 0.13          |
| (1,3130) | 1:123:A:ARG:HG2 | 1:123:A:ARG:H   | 3        | 0.13          |
| (1,3130) | 1:123:A:ARG:HG2 | 1:123:A:ARG:H   | 4        | 0.13          |
| (1,3130) | 1:123:A:ARG:HG2 | 1:123:A:ARG:H   | 6        | 0.13          |
| (1,3130) | 1:123:A:ARG:HG2 | 1:123:A:ARG:H   | 15       | 0.13          |
| (1,3130) | 1:123:A:ARG:HG2 | 1:123:A:ARG:H   | 17       | 0.13          |
| (1,3120) | 1:59:A:ARG:HB2  | 1:58:A:ASP:HB2  | 1        | 0.13          |
| (1,3120) | 1:59:A:ARG:HB2  | 1:58:A:ASP:HB2  | 14       | 0.13          |
| (1,3120) | 1:59:A:ARG:HB2  | 1:58:A:ASP:HB2  | 16       | 0.13          |
| (1,3118) | 1:58:A:ASP:HA   | 1:58:A:ASP:HB2  | 2        | 0.13          |
| (1,3118) | 1:58:A:ASP:HA   | 1:58:A:ASP:HB2  | 11       | 0.13          |
| (1,3118) | 1:58:A:ASP:HA   | 1:58:A:ASP:HB2  | 14       | 0.13          |
| (1,3118) | 1:58:A:ASP:HA   | 1:58:A:ASP:HB2  | 15       | 0.13          |
| (1,3108) | 1:102:A:CYS:H   | 1:101:A:PRO:HB3 | 9        | 0.13          |
| (1,3087) | 1:56:A:LEU:HG   | 1:56:A:LEU:HA   | 15       | 0.13          |
| (1,3087) | 1:56:A:LEU:HG   | 1:56:A:LEU:HA   | 17       | 0.13          |
| (1,3080) | 1:125:A:GLN:HB2 | 1:125:A:GLN:HA  | 17       | 0.13          |
| (1,3068) | 1:52:A:ILE:HG22 | 1:53:A:PHE:HB2  | 16       | 0.13          |
| (1,3059) | 1:28:A:ILE:HB   | 1:28:A:ILE:HG21 | 12       | 0.13          |
| (1,3040) | 1:52:A:ILE:HA   | 1:52:A:ILE:HG12 | 3        | 0.13          |
| (1,3040) | 1:52:A:ILE:HA   | 1:52:A:ILE:HG12 | 7        | 0.13          |
| (1,3035) | 1:25:A:LYS:H    | 1:25:A:LYS:HG2  | 6        | 0.13          |
| (1,3021) | 1:64:A:MET:HE3  | 1:63:A:GLU:H    | 12       | 0.13          |
| (1,2995) | 1:60:A:VAL:H    | 1:60:A:VAL:HB   | 11       | 0.13          |
| (1,2986) | 1:115:A:LYS:HB3 | 1:115:A:LYS:H   | 5        | 0.13          |
| (1,2986) | 1:115:A:LYS:HB3 | 1:115:A:LYS:H   | 13       | 0.13          |
| (1,2979) | 1:53:A:PHE:HZ   | 1:68:A:LYS:HB2  | 11       | 0.13          |
| (1,2978) | 1:105:A:LEU:H   | 1:101:A:PRO:HD3 | 12       | 0.13          |
| (1,2961) | 1:56:A:LEU:HD22 | 1:52:A:ILE:HB   | 14       | 0.13          |
| (1,2950) | 1:75:A:LEU:HD13 | 1:75:A:LEU:H    | 7        | 0.13          |
| (1,2950) | 1:75:A:LEU:HD12 | 1:75:A:LEU:H    | 13       | 0.13          |
| (1,2949) | 1:39:A:PHE:HZ   | 1:75:A:LEU:HD12 | 2        | 0.13          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2949) | 1:39:A:PHE:HZ    | 1:75:A:LEU:HD13 | 4        | 0.13          |
| (1,2949) | 1:39:A:PHE:HZ    | 1:75:A:LEU:HD13 | 17       | 0.13          |
| (1,2943) | 1:110:A:VAL:HG21 | 1:108:A:GLN:H   | 5        | 0.13          |
| (1,2937) | 1:95:A:VAL:HG23  | 1:95:A:VAL:HG12 | 9        | 0.13          |
| (1,2932) | 1:95:A:VAL:HG21  | 1:95:A:VAL:H    | 4        | 0.13          |
| (1,2915) | 1:38:A:CYS:HB2   | 1:39:A:PHE:HE2  | 11       | 0.13          |
| (1,2899) | 1:28:A:ILE:HD12  | 1:75:A:LEU:H    | 3        | 0.13          |
| (1,2899) | 1:28:A:ILE:HD12  | 1:75:A:LEU:H    | 4        | 0.13          |
| (1,2893) | 1:50:A:ILE:HB    | 1:50:A:ILE:HG23 | 16       | 0.13          |
| (1,2888) | 1:29:A:ALA:HA    | 1:32:A:ALA:HB2  | 14       | 0.13          |
| (1,2875) | 1:122:A:ALA:HB3  | 1:122:A:ALA:H   | 1        | 0.13          |
| (1,2875) | 1:122:A:ALA:HB1  | 1:122:A:ALA:H   | 5        | 0.13          |
| (1,2875) | 1:122:A:ALA:HB1  | 1:122:A:ALA:H   | 6        | 0.13          |
| (1,2875) | 1:122:A:ALA:HB3  | 1:122:A:ALA:H   | 13       | 0.13          |
| (1,2875) | 1:122:A:ALA:HB1  | 1:122:A:ALA:H   | 14       | 0.13          |
| (1,2874) | 1:127:A:GLN:H    | 1:126:A:ALA:HB3 | 8        | 0.13          |
| (1,2859) | 1:86:A:TYR:HE1   | 1:85:A:LEU:H    | 8        | 0.13          |
| (1,2846) | 1:53:A:PHE:HE2   | 1:75:A:LEU:HB3  | 10       | 0.13          |
| (1,2823) | 1:97:A:LEU:HD23  | 1:97:A:LEU:HA   | 1        | 0.13          |
| (1,2811) | 1:97:A:LEU:HD12  | 1:97:A:LEU:HB3  | 2        | 0.13          |
| (1,2811) | 1:97:A:LEU:HD13  | 1:97:A:LEU:HB3  | 14       | 0.13          |
| (1,2786) | 1:82:A:TRP:HH2   | 1:82:A:TRP:HE1  | 5        | 0.13          |
| (1,2786) | 1:82:A:TRP:HH2   | 1:82:A:TRP:HE1  | 6        | 0.13          |
| (1,2786) | 1:82:A:TRP:HH2   | 1:82:A:TRP:HE1  | 13       | 0.13          |
| (1,2786) | 1:82:A:TRP:HH2   | 1:82:A:TRP:HE1  | 16       | 0.13          |
| (1,2786) | 1:82:A:TRP:HH2   | 1:82:A:TRP:HE1  | 17       | 0.13          |
| (1,2775) | 1:47:A:PRO:HB3   | 1:87:A:GLY:HA2  | 2        | 0.13          |
| (1,2775) | 1:47:A:PRO:HB3   | 1:87:A:GLY:HA2  | 6        | 0.13          |
| (1,2775) | 1:47:A:PRO:HB3   | 1:87:A:GLY:HA2  | 10       | 0.13          |
| (1,2775) | 1:47:A:PRO:HB3   | 1:87:A:GLY:HA2  | 11       | 0.13          |
| (1,2775) | 1:47:A:PRO:HB3   | 1:87:A:GLY:HA2  | 14       | 0.13          |
| (1,2774) | 1:91:A:GLY:HA3   | 1:90:A:PRO:HB2  | 5        | 0.13          |
| (1,2774) | 1:91:A:GLY:HA3   | 1:90:A:PRO:HB2  | 14       | 0.13          |
| (1,2765) | 1:79:A:THR:H     | 1:78:A:TYR:HE1  | 2        | 0.13          |
| (1,2719) | 1:117:A:LEU:HD13 | 1:86:A:TYR:HB2  | 1        | 0.13          |
| (1,2689) | 1:34:A:ARG:HB3   | 1:30:A:PHE:HD1  | 5        | 0.13          |
| (1,2689) | 1:34:A:ARG:HB3   | 1:30:A:PHE:HD1  | 6        | 0.13          |
| (1,2689) | 1:34:A:ARG:HB3   | 1:30:A:PHE:HD2  | 13       | 0.13          |
| (1,2672) | 1:31:A:LEU:HD12  | 1:35:A:PHE:HD2  | 4        | 0.13          |
| (1,2672) | 1:31:A:LEU:HD11  | 1:35:A:PHE:HD1  | 16       | 0.13          |
| (1,2665) | 1:86:A:TYR:HE2   | 1:86:A:TYR:HB3  | 8        | 0.13          |
| (1,2648) | 1:56:A:LEU:HD11  | 1:52:A:ILE:HG12 | 7        | 0.13          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2648) | 1:56:A:LEU:HD13  | 1:52:A:ILE:HG12 | 14       | 0.13          |
| (1,2648) | 1:56:A:LEU:HD12  | 1:52:A:ILE:HG12 | 16       | 0.13          |
| (1,2648) | 1:56:A:LEU:HD12  | 1:52:A:ILE:HG12 | 17       | 0.13          |
| (1,2637) | 1:71:A:LEU:HB3   | 1:71:A:LEU:HG   | 5        | 0.13          |
| (1,2629) | 1:53:A:PHE:HZ    | 1:71:A:LEU:HB2  | 17       | 0.13          |
| (1,2621) | 1:105:A:LEU:HD11 | 1:92:A:ALA:H    | 5        | 0.13          |
| (1,2619) | 1:48:A:LEU:HD22  | 1:84:A:TYR:HE2  | 17       | 0.13          |
| (1,2612) | 1:30:A:PHE:HD1   | 1:34:A:ARG:HG2  | 2        | 0.13          |
| (1,2612) | 1:30:A:PHE:HD2   | 1:34:A:ARG:HG2  | 14       | 0.13          |
| (1,2612) | 1:30:A:PHE:HD1   | 1:34:A:ARG:HG2  | 15       | 0.13          |
| (1,2612) | 1:30:A:PHE:HD2   | 1:34:A:ARG:HG2  | 17       | 0.13          |
| (1,2579) | 1:59:A:ARG:HB2   | 1:60:A:VAL:HG11 | 4        | 0.13          |
| (1,2579) | 1:59:A:ARG:HB2   | 1:60:A:VAL:HG11 | 9        | 0.13          |
| (1,2579) | 1:59:A:ARG:HB2   | 1:60:A:VAL:HG13 | 15       | 0.13          |
| (1,2561) | 1:85:A:LEU:H     | 1:84:A:TYR:HE2  | 4        | 0.13          |
| (1,2529) | 1:79:A:THR:HG21  | 1:75:A:LEU:HA   | 6        | 0.13          |
| (1,2529) | 1:79:A:THR:HG22  | 1:75:A:LEU:HA   | 13       | 0.13          |
| (1,2480) | 1:71:A:LEU:HB2   | 1:27:A:VAL:HG13 | 4        | 0.13          |
| (1,2480) | 1:71:A:LEU:HB2   | 1:27:A:VAL:HG11 | 17       | 0.13          |
| (1,2469) | 1:53:A:PHE:HZ    | 1:72:A:ARG:HG3  | 17       | 0.13          |
| (1,2438) | 1:13:A:ASP:HB3   | 1:14:A:PRO:HD3  | 8        | 0.13          |
| (1,2436) | 1:13:A:ASP:HB3   | 1:33:A:GLU:HB3  | 10       | 0.13          |
| (1,2416) | 1:45:A:ALA:HB1   | 1:45:A:ALA:H    | 11       | 0.13          |
| (1,2415) | 1:45:A:ALA:HB2   | 1:84:A:TYR:HD2  | 2        | 0.13          |
| (1,2351) | 1:110:A:VAL:HG21 | 1:109:A:HIS:HA  | 5        | 0.13          |
| (1,2306) | 1:38:A:CYS:H     | 1:97:A:LEU:HA   | 4        | 0.13          |
| (1,2306) | 1:38:A:CYS:H     | 1:97:A:LEU:HA   | 7        | 0.13          |
| (1,2299) | 1:55:A:ASP:HB3   | 1:96:A:ASP:HA   | 3        | 0.13          |
| (1,2295) | 1:121:A:LYS:HG2  | 1:121:A:LYS:HD3 | 9        | 0.13          |
| (1,2283) | 1:33:A:GLU:HG2   | 1:33:A:GLU:HA   | 7        | 0.13          |
| (1,2283) | 1:33:A:GLU:HG2   | 1:33:A:GLU:HA   | 9        | 0.13          |
| (1,2283) | 1:33:A:GLU:HG2   | 1:33:A:GLU:HA   | 16       | 0.13          |
| (1,2236) | 1:54:A:GLN:HB2   | 1:54:A:GLN:HG2  | 16       | 0.13          |
| (1,2197) | 1:39:A:PHE:HD2   | 1:56:A:LEU:HA   | 2        | 0.13          |
| (1,2197) | 1:39:A:PHE:HD1   | 1:56:A:LEU:HA   | 5        | 0.13          |
| (1,2197) | 1:39:A:PHE:HD1   | 1:56:A:LEU:HA   | 14       | 0.13          |
| (1,2185) | 1:53:A:PHE:H     | 1:97:A:LEU:HD23 | 5        | 0.13          |
| (1,2185) | 1:53:A:PHE:H     | 1:97:A:LEU:HD23 | 7        | 0.13          |
| (1,2185) | 1:53:A:PHE:H     | 1:97:A:LEU:HD21 | 9        | 0.13          |
| (1,2185) | 1:53:A:PHE:H     | 1:97:A:LEU:HD21 | 13       | 0.13          |
| (1,2160) | 1:82:A:TRP:HZ3   | 1:82:A:TRP:HB2  | 7        | 0.13          |
| (1,2160) | 1:82:A:TRP:HZ3   | 1:82:A:TRP:HB2  | 12       | 0.13          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2160) | 1:82:A:TRP:HZ3  | 1:82:A:TRP:HB2  | 17       | 0.13          |
| (1,2140) | 1:84:A:TYR:HB2  | 1:82:A:TRP:HA   | 2        | 0.13          |
| (1,2140) | 1:84:A:TYR:HB2  | 1:82:A:TRP:HA   | 7        | 0.13          |
| (1,2140) | 1:84:A:TYR:HB2  | 1:82:A:TRP:HA   | 8        | 0.13          |
| (1,2140) | 1:84:A:TYR:HB2  | 1:82:A:TRP:HA   | 14       | 0.13          |
| (1,2118) | 1:69:A:THR:HB   | 1:69:A:THR:HG21 | 8        | 0.13          |
| (1,2118) | 1:69:A:THR:HB   | 1:69:A:THR:HG22 | 9        | 0.13          |
| (1,2118) | 1:69:A:THR:HB   | 1:69:A:THR:HG22 | 15       | 0.13          |
| (1,2116) | 1:45:A:ALA:HB3  | 1:84:A:TYR:HA   | 3        | 0.13          |
| (1,2116) | 1:45:A:ALA:HB3  | 1:84:A:TYR:HA   | 9        | 0.13          |
| (1,2116) | 1:45:A:ALA:HB1  | 1:84:A:TYR:HA   | 15       | 0.13          |
| (1,2079) | 1:66:A:LEU:HD12 | 1:62:A:GLY:H    | 6        | 0.13          |
| (1,2079) | 1:66:A:LEU:HD11 | 1:62:A:GLY:H    | 16       | 0.13          |
| (1,2079) | 1:66:A:LEU:HD11 | 1:62:A:GLY:H    | 17       | 0.13          |
| (1,2052) | 1:65:A:ASN:H    | 1:66:A:LEU:H    | 3        | 0.13          |
| (1,2047) | 1:60:A:VAL:H    | 1:61:A:ALA:H    | 4        | 0.13          |
| (1,2047) | 1:60:A:VAL:H    | 1:61:A:ALA:H    | 8        | 0.13          |
| (1,2045) | 1:77:A:LEU:H    | 1:78:A:TYR:H    | 9        | 0.13          |
| (1,2045) | 1:77:A:LEU:H    | 1:78:A:TYR:H    | 17       | 0.13          |
| (1,2042) | 1:15:A:MET:H    | 1:16:A:GLU:H    | 12       | 0.13          |
| (1,2037) | 1:57:A:VAL:HG22 | 1:57:A:VAL:HG13 | 14       | 0.13          |
| (1,2021) | 1:53:A:PHE:HE2  | 1:57:A:VAL:HG12 | 7        | 0.13          |
| (1,2021) | 1:53:A:PHE:HE1  | 1:57:A:VAL:HG13 | 16       | 0.13          |
| (1,1997) | 1:107:A:GLU:HG2 | 1:107:A:GLU:H   | 1        | 0.13          |
| (1,1954) | 1:116:A:GLN:H   | 1:113:A:ALA:HA  | 12       | 0.13          |
| (1,1939) | 1:33:A:GLU:HB3  | 1:30:A:PHE:HA   | 8        | 0.13          |
| (1,1939) | 1:33:A:GLU:HB3  | 1:30:A:PHE:HA   | 17       | 0.13          |
| (1,1906) | 1:105:A:LEU:HB3 | 1:101:A:PRO:HB3 | 3        | 0.13          |
| (1,1906) | 1:105:A:LEU:HB3 | 1:101:A:PRO:HB3 | 5        | 0.13          |
| (1,1906) | 1:105:A:LEU:HB3 | 1:101:A:PRO:HB3 | 9        | 0.13          |
| (1,1906) | 1:105:A:LEU:HB3 | 1:101:A:PRO:HB3 | 12       | 0.13          |
| (1,1906) | 1:105:A:LEU:HB3 | 1:101:A:PRO:HB3 | 14       | 0.13          |
| (1,1886) | 1:102:A:CYS:HB3 | 1:49:A:LYS:HA   | 10       | 0.13          |
| (1,1886) | 1:102:A:CYS:HB3 | 1:49:A:LYS:HA   | 15       | 0.13          |
| (1,1885) | 1:83:A:ARG:HG3  | 1:84:A:TYR:H    | 13       | 0.13          |
| (1,1876) | 1:27:A:VAL:HG23 | 1:31:A:LEU:HD11 | 3        | 0.13          |
| (1,1845) | 1:95:A:VAL:HG22 | 1:96:A:ASP:HA   | 13       | 0.13          |
| (1,1845) | 1:95:A:VAL:HG22 | 1:96:A:ASP:HA   | 15       | 0.13          |
| (1,1845) | 1:95:A:VAL:HG21 | 1:96:A:ASP:HA   | 17       | 0.13          |
| (1,1819) | 1:112:A:HIS:HA  | 1:112:A:HIS:H   | 1        | 0.13          |
| (1,1819) | 1:112:A:HIS:HA  | 1:112:A:HIS:H   | 3        | 0.13          |
| (1,1819) | 1:112:A:HIS:HA  | 1:112:A:HIS:H   | 15       | 0.13          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1812) | 1:117:A:LEU:HA  | 1:117:A:LEU:HD11 | 1        | 0.13          |
| (1,1812) | 1:117:A:LEU:HA  | 1:117:A:LEU:HD12 | 4        | 0.13          |
| (1,1812) | 1:117:A:LEU:HA  | 1:117:A:LEU:HD13 | 5        | 0.13          |
| (1,1812) | 1:117:A:LEU:HA  | 1:117:A:LEU:HD12 | 8        | 0.13          |
| (1,1812) | 1:117:A:LEU:HA  | 1:117:A:LEU:HD12 | 10       | 0.13          |
| (1,1812) | 1:117:A:LEU:HA  | 1:117:A:LEU:HD12 | 13       | 0.13          |
| (1,1812) | 1:117:A:LEU:HA  | 1:117:A:LEU:HD13 | 14       | 0.13          |
| (1,1812) | 1:117:A:LEU:HA  | 1:117:A:LEU:HD12 | 16       | 0.13          |
| (1,1796) | 1:53:A:PHE:HE2  | 1:68:A:LYS:HA    | 3        | 0.13          |
| (1,1796) | 1:53:A:PHE:HE2  | 1:68:A:LYS:HA    | 4        | 0.13          |
| (1,1796) | 1:53:A:PHE:HE2  | 1:68:A:LYS:HA    | 7        | 0.13          |
| (1,1796) | 1:53:A:PHE:HE2  | 1:68:A:LYS:HA    | 9        | 0.13          |
| (1,1796) | 1:53:A:PHE:HE1  | 1:68:A:LYS:HA    | 16       | 0.13          |
| (1,1796) | 1:53:A:PHE:HE2  | 1:68:A:LYS:HA    | 17       | 0.13          |
| (1,1787) | 1:93:A:THR:HB   | 1:49:A:LYS:HB3   | 2        | 0.13          |
| (1,1775) | 1:88:A:VAL:HA   | 1:47:A:PRO:HB3   | 1        | 0.13          |
| (1,1775) | 1:88:A:VAL:HA   | 1:47:A:PRO:HB3   | 4        | 0.13          |
| (1,1775) | 1:88:A:VAL:HA   | 1:47:A:PRO:HB3   | 5        | 0.13          |
| (1,1773) | 1:24:A:SER:HA   | 1:27:A:VAL:HG21  | 6        | 0.13          |
| (1,1756) | 1:79:A:THR:HG22 | 1:84:A:TYR:HE1   | 11       | 0.13          |
| (1,1756) | 1:79:A:THR:HG21 | 1:84:A:TYR:HE2   | 16       | 0.13          |
| (1,1727) | 1:66:A:LEU:HD13 | 1:30:A:PHE:HD1   | 1        | 0.13          |
| (1,1726) | 1:66:A:LEU:HD11 | 1:66:A:LEU:HA    | 1        | 0.13          |
| (1,1726) | 1:66:A:LEU:HD13 | 1:66:A:LEU:HA    | 13       | 0.13          |
| (1,1726) | 1:66:A:LEU:HD13 | 1:66:A:LEU:HA    | 15       | 0.13          |
| (1,1725) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HG    | 2        | 0.13          |
| (1,1725) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HG    | 13       | 0.13          |
| (1,1718) | 1:18:A:GLN:HB3  | 1:19:A:PRO:HD2   | 6        | 0.13          |
| (1,1718) | 1:18:A:GLN:HB3  | 1:19:A:PRO:HD2   | 11       | 0.13          |
| (1,1718) | 1:18:A:GLN:HB3  | 1:19:A:PRO:HD2   | 14       | 0.13          |
| (1,1718) | 1:18:A:GLN:HB3  | 1:19:A:PRO:HD2   | 15       | 0.13          |
| (1,1718) | 1:18:A:GLN:HB3  | 1:19:A:PRO:HD2   | 17       | 0.13          |
| (1,1713) | 1:20:A:LYS:H    | 1:20:A:LYS:HD3   | 8        | 0.13          |
| (1,1709) | 1:72:A:ARG:HB3  | 1:53:A:PHE:HE2   | 6        | 0.13          |
| (1,1709) | 1:72:A:ARG:HB3  | 1:53:A:PHE:HE1   | 10       | 0.13          |
| (1,1709) | 1:72:A:ARG:HB3  | 1:53:A:PHE:HE1   | 16       | 0.13          |
| (1,1707) | 1:70:A:GLN:HG3  | 1:70:A:GLN:HB3   | 1        | 0.13          |
| (1,1707) | 1:70:A:GLN:HG3  | 1:70:A:GLN:HB3   | 2        | 0.13          |
| (1,1707) | 1:70:A:GLN:HG3  | 1:70:A:GLN:HB3   | 3        | 0.13          |
| (1,1707) | 1:70:A:GLN:HG3  | 1:70:A:GLN:HB3   | 4        | 0.13          |
| (1,1707) | 1:70:A:GLN:HG3  | 1:70:A:GLN:HB3   | 6        | 0.13          |
| (1,1707) | 1:70:A:GLN:HG3  | 1:70:A:GLN:HB3   | 7        | 0.13          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1707) | 1:70:A:GLN:HG3  | 1:70:A:GLN:HB3  | 8        | 0.13          |
| (1,1707) | 1:70:A:GLN:HG3  | 1:70:A:GLN:HB3  | 9        | 0.13          |
| (1,1707) | 1:70:A:GLN:HG3  | 1:70:A:GLN:HB3  | 10       | 0.13          |
| (1,1707) | 1:70:A:GLN:HG3  | 1:70:A:GLN:HB3  | 11       | 0.13          |
| (1,1707) | 1:70:A:GLN:HG3  | 1:70:A:GLN:HB3  | 12       | 0.13          |
| (1,1707) | 1:70:A:GLN:HG3  | 1:70:A:GLN:HB3  | 13       | 0.13          |
| (1,1707) | 1:70:A:GLN:HG3  | 1:70:A:GLN:HB3  | 15       | 0.13          |
| (1,1707) | 1:70:A:GLN:HG3  | 1:70:A:GLN:HB3  | 16       | 0.13          |
| (1,1707) | 1:70:A:GLN:HG3  | 1:70:A:GLN:HB3  | 17       | 0.13          |
| (1,1636) | 1:124:A:VAL:HA  | 1:125:A:GLN:HG3 | 5        | 0.13          |
| (1,1636) | 1:124:A:VAL:HA  | 1:125:A:GLN:HG3 | 7        | 0.13          |
| (1,1636) | 1:124:A:VAL:HA  | 1:125:A:GLN:HG3 | 11       | 0.13          |
| (1,1636) | 1:124:A:VAL:HA  | 1:125:A:GLN:HG3 | 16       | 0.13          |
| (1,1629) | 1:116:A:GLN:HG3 | 1:113:A:ALA:HB2 | 3        | 0.13          |
| (1,1599) | 1:53:A:PHE:HB3  | 1:75:A:LEU:HD23 | 5        | 0.13          |
| (1,1599) | 1:53:A:PHE:HB3  | 1:75:A:LEU:HD22 | 7        | 0.13          |
| (1,1599) | 1:53:A:PHE:HB3  | 1:75:A:LEU:HD22 | 17       | 0.13          |
| (1,1591) | 1:120:A:ALA:HB3 | 1:120:A:ALA:H   | 9        | 0.13          |
| (1,1591) | 1:120:A:ALA:HB1 | 1:120:A:ALA:H   | 14       | 0.13          |
| (1,1591) | 1:120:A:ALA:HB3 | 1:120:A:ALA:H   | 17       | 0.13          |
| (1,1589) | 1:120:A:ALA:HB3 | 1:121:A:LYS:H   | 2        | 0.13          |
| (1,1567) | 1:68:A:LYS:HB2  | 1:68:A:LYS:HA   | 4        | 0.13          |
| (1,1567) | 1:68:A:LYS:HB2  | 1:68:A:LYS:HA   | 6        | 0.13          |
| (1,1567) | 1:68:A:LYS:HB2  | 1:68:A:LYS:HA   | 9        | 0.13          |
| (1,1567) | 1:68:A:LYS:HB2  | 1:68:A:LYS:HA   | 14       | 0.13          |
| (1,1546) | 1:56:A:LEU:HD13 | 1:52:A:ILE:HG13 | 6        | 0.13          |
| (1,1546) | 1:56:A:LEU:HD12 | 1:52:A:ILE:HG13 | 10       | 0.13          |
| (1,1546) | 1:56:A:LEU:HD12 | 1:52:A:ILE:HG13 | 16       | 0.13          |
| (1,1546) | 1:56:A:LEU:HD12 | 1:52:A:ILE:HG13 | 17       | 0.13          |
| (1,1526) | 1:54:A:GLN:HB3  | 1:54:A:GLN:HA   | 1        | 0.13          |
| (1,1526) | 1:54:A:GLN:HB3  | 1:54:A:GLN:HA   | 5        | 0.13          |
| (1,1526) | 1:54:A:GLN:HB3  | 1:54:A:GLN:HA   | 8        | 0.13          |
| (1,1526) | 1:54:A:GLN:HB3  | 1:54:A:GLN:HA   | 10       | 0.13          |
| (1,1526) | 1:54:A:GLN:HB3  | 1:54:A:GLN:HA   | 11       | 0.13          |
| (1,1526) | 1:54:A:GLN:HB3  | 1:54:A:GLN:HA   | 15       | 0.13          |
| (1,1510) | 1:52:A:ILE:HG23 | 1:50:A:ILE:H    | 16       | 0.13          |
| (1,1464) | 1:102:A:CYS:HB3 | 1:103:A:GLY:H   | 5        | 0.13          |
| (1,1464) | 1:102:A:CYS:HB3 | 1:103:A:GLY:H   | 14       | 0.13          |
| (1,1454) | 1:60:A:VAL:HB   | 1:61:A:ALA:H    | 11       | 0.13          |
| (1,1414) | 1:74:A:ALA:HB2  | 1:75:A:LEU:HD12 | 4        | 0.13          |
| (1,1414) | 1:74:A:ALA:HB2  | 1:75:A:LEU:HD13 | 7        | 0.13          |
| (1,1414) | 1:74:A:ALA:HB2  | 1:75:A:LEU:HD12 | 16       | 0.13          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1412) | 1:39:A:PHE:HZ    | 1:75:A:LEU:HD12  | 3        | 0.13          |
| (1,1412) | 1:39:A:PHE:HZ    | 1:75:A:LEU:HD13  | 13       | 0.13          |
| (1,1412) | 1:39:A:PHE:HZ    | 1:75:A:LEU:HD13  | 15       | 0.13          |
| (1,1410) | 1:110:A:VAL:HG21 | 1:108:A:GLN:H    | 4        | 0.13          |
| (1,1410) | 1:110:A:VAL:HG23 | 1:108:A:GLN:H    | 6        | 0.13          |
| (1,1410) | 1:110:A:VAL:HG21 | 1:108:A:GLN:H    | 17       | 0.13          |
| (1,1400) | 1:95:A:VAL:HG21  | 1:99:A:GLY:H     | 11       | 0.13          |
| (1,1399) | 1:95:A:VAL:HG23  | 1:95:A:VAL:H     | 10       | 0.13          |
| (1,1397) | 1:31:A:LEU:HD21  | 1:60:A:VAL:HG11  | 5        | 0.13          |
| (1,1382) | 1:57:A:VAL:HG21  | 1:53:A:PHE:HE1   | 4        | 0.13          |
| (1,1382) | 1:57:A:VAL:HG22  | 1:53:A:PHE:HE2   | 14       | 0.13          |
| (1,1371) | 1:28:A:ILE:HD11  | 1:75:A:LEU:H     | 15       | 0.13          |
| (1,1366) | 1:50:A:ILE:HG12  | 1:50:A:ILE:HG22  | 4        | 0.13          |
| (1,1358) | 1:32:A:ALA:HB1   | 1:33:A:GLU:H     | 13       | 0.13          |
| (1,1357) | 1:74:A:ALA:HB2   | 1:31:A:LEU:HD11  | 4        | 0.13          |
| (1,1352) | 1:122:A:ALA:HB2  | 1:122:A:ALA:H    | 8        | 0.13          |
| (1,1350) | 1:129:A:ALA:HB2  | 1:129:A:ALA:H    | 16       | 0.13          |
| (1,1327) | 1:73:A:SER:HB2   | 1:73:A:SER:H     | 2        | 0.13          |
| (1,1327) | 1:73:A:SER:HB2   | 1:73:A:SER:H     | 6        | 0.13          |
| (1,1327) | 1:73:A:SER:HB2   | 1:73:A:SER:H     | 9        | 0.13          |
| (1,1325) | 1:53:A:PHE:HE2   | 1:75:A:LEU:HB3   | 11       | 0.13          |
| (1,1303) | 1:97:A:LEU:HD13  | 1:35:A:PHE:HE2   | 1        | 0.13          |
| (1,1284) | 1:48:A:LEU:HB2   | 1:48:A:LEU:HD23  | 4        | 0.13          |
| (1,1275) | 1:84:A:TYR:HE1   | 1:84:A:TYR:HB3   | 16       | 0.13          |
| (1,1273) | 1:45:A:ALA:HB3   | 1:84:A:TYR:HB3   | 4        | 0.13          |
| (1,1240) | 1:78:A:TYR:HE2   | 1:79:A:THR:HB    | 1        | 0.13          |
| (1,1240) | 1:78:A:TYR:HE1   | 1:79:A:THR:HB    | 3        | 0.13          |
| (1,1240) | 1:78:A:TYR:HE2   | 1:79:A:THR:HB    | 13       | 0.13          |
| (1,1239) | 1:79:A:THR:H     | 1:78:A:TYR:HE2   | 4        | 0.13          |
| (1,1239) | 1:79:A:THR:H     | 1:78:A:TYR:HE1   | 10       | 0.13          |
| (1,1126) | 1:86:A:TYR:HE2   | 1:86:A:TYR:HB3   | 14       | 0.13          |
| (1,1108) | 1:56:A:LEU:HD12  | 1:52:A:ILE:HG12  | 10       | 0.13          |
| (1,1052) | 1:69:A:THR:HG22  | 1:69:A:THR:HA    | 2        | 0.13          |
| (1,1049) | 1:59:A:ARG:HB2   | 1:60:A:VAL:HG13  | 5        | 0.13          |
| (1,1047) | 1:124:A:VAL:HA   | 1:124:A:VAL:HG23 | 13       | 0.13          |
| (1,1047) | 1:124:A:VAL:HA   | 1:124:A:VAL:HG21 | 14       | 0.13          |
| (1,1032) | 1:85:A:LEU:H     | 1:84:A:TYR:HE2   | 5        | 0.13          |
| (1,872)  | 1:56:A:LEU:HB3   | 1:56:A:LEU:HA    | 4        | 0.13          |
| (1,872)  | 1:56:A:LEU:HB3   | 1:56:A:LEU:HA    | 7        | 0.13          |
| (1,872)  | 1:56:A:LEU:HB3   | 1:56:A:LEU:HA    | 8        | 0.13          |
| (1,872)  | 1:56:A:LEU:HB3   | 1:56:A:LEU:HA    | 9        | 0.13          |
| (1,872)  | 1:56:A:LEU:HB3   | 1:56:A:LEU:HA    | 11       | 0.13          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,872) | 1:56:A:LEU:HB3   | 1:56:A:LEU:HA   | 13       | 0.13          |
| (1,872) | 1:56:A:LEU:HB3   | 1:56:A:LEU:HA   | 15       | 0.13          |
| (1,856) | 1:13:A:ASP:HB3   | 1:14:A:PRO:HD3  | 16       | 0.13          |
| (1,847) | 1:49:A:LYS:HB2   | 1:102:A:CYS:HB3 | 15       | 0.13          |
| (1,830) | 1:129:A:ALA:HB2  | 1:127:A:GLN:HB3 | 11       | 0.13          |
| (1,830) | 1:129:A:ALA:HB1  | 1:127:A:GLN:HB3 | 13       | 0.13          |
| (1,818) | 1:28:A:ILE:HD11  | 1:78:A:TYR:HB3  | 11       | 0.13          |
| (1,773) | 1:116:A:GLN:HG3  | 1:115:A:LYS:H   | 12       | 0.13          |
| (1,767) | 1:104:A:GLU:HG2  | 1:104:A:GLU:H   | 7        | 0.13          |
| (1,761) | 1:62:A:GLY:HA3   | 1:66:A:LEU:H    | 5        | 0.13          |
| (1,756) | 1:93:A:THR:HB    | 1:102:A:CYS:H   | 4        | 0.13          |
| (1,756) | 1:93:A:THR:HB    | 1:102:A:CYS:H   | 5        | 0.13          |
| (1,755) | 1:95:A:VAL:H     | 1:94:A:ARG:HB3  | 11       | 0.13          |
| (1,755) | 1:95:A:VAL:H     | 1:94:A:ARG:HB3  | 17       | 0.13          |
| (1,714) | 1:12:A:GLN:HA    | 1:13:A:ASP:H    | 10       | 0.13          |
| (1,665) | 1:122:A:ALA:HB2  | 1:123:A:ARG:H   | 3        | 0.13          |
| (1,665) | 1:122:A:ALA:HB3  | 1:123:A:ARG:H   | 10       | 0.13          |
| (1,618) | 1:95:A:VAL:H     | 1:48:A:LEU:HD11 | 9        | 0.13          |
| (1,614) | 1:97:A:LEU:HD11  | 1:97:A:LEU:H    | 4        | 0.13          |
| (1,609) | 1:49:A:LYS:HB2   | 1:49:A:LYS:H    | 15       | 0.13          |
| (1,593) | 1:17:A:ASN:HA    | 1:18:A:GLN:H    | 10       | 0.13          |
| (1,549) | 1:97:A:LEU:HD11  | 1:98:A:ASP:H    | 1        | 0.13          |
| (1,527) | 1:65:A:ASN:HB3   | 1:65:A:ASN:HD21 | 6        | 0.13          |
| (1,512) | 1:13:A:ASP:HB2   | 1:13:A:ASP:H    | 1        | 0.13          |
| (1,451) | 1:32:A:ALA:HB2   | 1:35:A:PHE:H    | 5        | 0.13          |
| (1,451) | 1:32:A:ALA:HB2   | 1:35:A:PHE:H    | 7        | 0.13          |
| (1,451) | 1:32:A:ALA:HB2   | 1:35:A:PHE:H    | 16       | 0.13          |
| (1,359) | 1:62:A:GLY:HA3   | 1:63:A:GLU:H    | 9        | 0.13          |
| (1,359) | 1:62:A:GLY:HA3   | 1:63:A:GLU:H    | 15       | 0.13          |
| (1,351) | 1:63:A:GLU:HB3   | 1:65:A:ASN:H    | 16       | 0.13          |
| (1,348) | 1:65:A:ASN:HB2   | 1:65:A:ASN:H    | 3        | 0.13          |
| (1,319) | 1:76:A:ARG:HD2   | 1:77:A:LEU:H    | 1        | 0.13          |
| (1,319) | 1:76:A:ARG:HD2   | 1:77:A:LEU:H    | 2        | 0.13          |
| (1,311) | 1:79:A:THR:H     | 1:77:A:LEU:HB2  | 4        | 0.13          |
| (1,311) | 1:79:A:THR:H     | 1:77:A:LEU:HB2  | 11       | 0.13          |
| (1,287) | 1:127:A:GLN:H    | 1:127:A:GLN:HG2 | 11       | 0.13          |
| (1,287) | 1:127:A:GLN:H    | 1:127:A:GLN:HG2 | 14       | 0.13          |
| (1,263) | 1:110:A:VAL:HG21 | 1:91:A:GLY:H    | 6        | 0.13          |
| (1,156) | 1:126:A:ALA:HB1  | 1:126:A:ALA:H   | 4        | 0.13          |
| (1,153) | 1:129:A:ALA:HA   | 1:129:A:ALA:H   | 1        | 0.13          |
| (1,153) | 1:129:A:ALA:HA   | 1:129:A:ALA:H   | 2        | 0.13          |
| (1,128) | 1:35:A:PHE:HD2   | 1:39:A:PHE:H    | 3        | 0.13          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,128)  | 1:35:A:PHE:HD2  | 1:39:A:PHE:H    | 17       | 0.13          |
| (1,101)  | 1:35:A:PHE:H    | 1:39:A:PHE:HE1  | 5        | 0.13          |
| (1,101)  | 1:35:A:PHE:H    | 1:39:A:PHE:HE2  | 6        | 0.13          |
| (1,101)  | 1:35:A:PHE:H    | 1:39:A:PHE:HE1  | 8        | 0.13          |
| (1,101)  | 1:35:A:PHE:H    | 1:39:A:PHE:HE2  | 11       | 0.13          |
| (1,80)   | 1:30:A:PHE:HD2  | 1:30:A:PHE:H    | 2        | 0.13          |
| (1,80)   | 1:30:A:PHE:HD2  | 1:30:A:PHE:H    | 10       | 0.13          |
| (1,80)   | 1:30:A:PHE:HD1  | 1:30:A:PHE:H    | 16       | 0.13          |
| (3,149)  | 1:82:A:TRP:HE1  | 1:86:A:TYR:HD1  | 4        | 0.12          |
| (3,149)  | 1:82:A:TRP:HE1  | 1:86:A:TYR:HD2  | 5        | 0.12          |
| (3,143)  | 1:25:A:LYS:H    | 1:77:A:LEU:HD23 | 2        | 0.12          |
| (3,123)  | 1:50:A:ILE:HD13 | 1:79:A:THR:HA   | 17       | 0.12          |
| (3,92)   | 1:88:A:VAL:HG23 | 1:87:A:GLY:HA2  | 8        | 0.12          |
| (3,90)   | 1:115:A:LYS:HG3 | 1:116:A:GLN:HG3 | 3        | 0.12          |
| (3,90)   | 1:115:A:LYS:HG3 | 1:116:A:GLN:HG3 | 8        | 0.12          |
| (3,90)   | 1:115:A:LYS:HG3 | 1:116:A:GLN:HG3 | 16       | 0.12          |
| (3,54)   | 1:71:A:LEU:HB3  | 1:75:A:LEU:HD12 | 8        | 0.12          |
| (3,48)   | 1:72:A:ARG:HD3  | 1:72:A:ARG:HB3  | 9        | 0.12          |
| (3,48)   | 1:72:A:ARG:HD3  | 1:72:A:ARG:HB3  | 11       | 0.12          |
| (3,48)   | 1:72:A:ARG:HD3  | 1:72:A:ARG:HB3  | 12       | 0.12          |
| (3,34)   | 1:97:A:LEU:HD21 | 1:31:A:LEU:HD11 | 8        | 0.12          |
| (3,29)   | 1:48:A:LEU:HD23 | 1:39:A:PHE:HD2  | 16       | 0.12          |
| (1,4344) | 1:120:A:ALA:H   | 1:119:A:GLU:HG2 | 15       | 0.12          |
| (1,4344) | 1:120:A:ALA:H   | 1:119:A:GLU:HG2 | 17       | 0.12          |
| (1,4343) | 1:118:A:GLU:H   | 1:119:A:GLU:H   | 13       | 0.12          |
| (1,4343) | 1:118:A:GLU:H   | 1:119:A:GLU:H   | 14       | 0.12          |
| (1,4343) | 1:118:A:GLU:H   | 1:119:A:GLU:H   | 17       | 0.12          |
| (1,4339) | 1:116:A:GLN:HG3 | 1:115:A:LYS:H   | 6        | 0.12          |
| (1,4339) | 1:116:A:GLN:HG3 | 1:115:A:LYS:H   | 17       | 0.12          |
| (1,4331) | 1:104:A:GLU:HG2 | 1:104:A:GLU:H   | 4        | 0.12          |
| (1,4331) | 1:104:A:GLU:HG2 | 1:104:A:GLU:H   | 8        | 0.12          |
| (1,4331) | 1:104:A:GLU:HG2 | 1:104:A:GLU:H   | 10       | 0.12          |
| (1,4331) | 1:104:A:GLU:HG2 | 1:104:A:GLU:H   | 12       | 0.12          |
| (1,4331) | 1:104:A:GLU:HG2 | 1:104:A:GLU:H   | 16       | 0.12          |
| (1,4331) | 1:104:A:GLU:HG2 | 1:104:A:GLU:H   | 17       | 0.12          |
| (1,4326) | 1:65:A:ASN:HA   | 1:66:A:LEU:H    | 1        | 0.12          |
| (1,4323) | 1:62:A:GLY:H    | 1:68:A:LYS:HD2  | 1        | 0.12          |
| (1,4323) | 1:62:A:GLY:H    | 1:68:A:LYS:HD2  | 13       | 0.12          |
| (1,4320) | 1:62:A:GLY:H    | 1:66:A:LEU:H    | 4        | 0.12          |
| (1,4320) | 1:62:A:GLY:H    | 1:66:A:LEU:H    | 9        | 0.12          |
| (1,4316) | 1:95:A:VAL:H    | 1:94:A:ARG:HB3  | 6        | 0.12          |
| (1,4302) | 1:94:A:ARG:H    | 1:94:A:ARG:HB3  | 1        | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,4302) | 1:94:A:ARG:H    | 1:94:A:ARG:HB3  | 3        | 0.12          |
| (1,4302) | 1:94:A:ARG:H    | 1:94:A:ARG:HB3  | 9        | 0.12          |
| (1,4301) | 1:97:A:LEU:HB2  | 1:97:A:LEU:H    | 13       | 0.12          |
| (1,4295) | 1:116:A:GLN:HA  | 1:117:A:LEU:H   | 3        | 0.12          |
| (1,4295) | 1:116:A:GLN:HA  | 1:117:A:LEU:H   | 11       | 0.12          |
| (1,4295) | 1:116:A:GLN:HA  | 1:117:A:LEU:H   | 12       | 0.12          |
| (1,4295) | 1:116:A:GLN:HA  | 1:117:A:LEU:H   | 15       | 0.12          |
| (1,4273) | 1:73:A:SER:HA   | 1:75:A:LEU:H    | 15       | 0.12          |
| (1,4271) | 1:78:A:TYR:HE2  | 1:75:A:LEU:H    | 1        | 0.12          |
| (1,4271) | 1:78:A:TYR:HE1  | 1:75:A:LEU:H    | 16       | 0.12          |
| (1,4270) | 1:75:A:LEU:HB3  | 1:74:A:ALA:H    | 7        | 0.12          |
| (1,4270) | 1:75:A:LEU:HB3  | 1:74:A:ALA:H    | 10       | 0.12          |
| (1,4268) | 1:73:A:SER:HA   | 1:73:A:SER:H    | 11       | 0.12          |
| (1,4258) | 1:52:A:ILE:HG12 | 1:56:A:LEU:H    | 1        | 0.12          |
| (1,4258) | 1:52:A:ILE:HG12 | 1:56:A:LEU:H    | 2        | 0.12          |
| (1,4258) | 1:52:A:ILE:HG12 | 1:56:A:LEU:H    | 3        | 0.12          |
| (1,4258) | 1:52:A:ILE:HG12 | 1:56:A:LEU:H    | 9        | 0.12          |
| (1,4258) | 1:52:A:ILE:HG12 | 1:56:A:LEU:H    | 11       | 0.12          |
| (1,4258) | 1:52:A:ILE:HG12 | 1:56:A:LEU:H    | 16       | 0.12          |
| (1,4238) | 1:97:A:LEU:H    | 1:96:A:ASP:H    | 5        | 0.12          |
| (1,4238) | 1:97:A:LEU:H    | 1:96:A:ASP:H    | 7        | 0.12          |
| (1,4228) | 1:123:A:ARG:HB3 | 1:124:A:VAL:H   | 7        | 0.12          |
| (1,4228) | 1:123:A:ARG:HB3 | 1:124:A:VAL:H   | 14       | 0.12          |
| (1,4223) | 1:123:A:ARG:H   | 1:125:A:GLN:HG3 | 1        | 0.12          |
| (1,4223) | 1:123:A:ARG:H   | 1:125:A:GLN:HG3 | 4        | 0.12          |
| (1,4223) | 1:123:A:ARG:H   | 1:125:A:GLN:HG3 | 8        | 0.12          |
| (1,4223) | 1:123:A:ARG:H   | 1:125:A:GLN:HG3 | 9        | 0.12          |
| (1,4212) | 1:115:A:LYS:HE3 | 1:115:A:LYS:H   | 8        | 0.12          |
| (1,4203) | 1:106:A:ASP:HB2 | 1:109:A:HIS:H   | 2        | 0.12          |
| (1,4203) | 1:106:A:ASP:HB2 | 1:109:A:HIS:H   | 3        | 0.12          |
| (1,4203) | 1:106:A:ASP:HB2 | 1:109:A:HIS:H   | 4        | 0.12          |
| (1,4203) | 1:106:A:ASP:HB2 | 1:109:A:HIS:H   | 5        | 0.12          |
| (1,4203) | 1:106:A:ASP:HB2 | 1:109:A:HIS:H   | 6        | 0.12          |
| (1,4203) | 1:106:A:ASP:HB2 | 1:109:A:HIS:H   | 7        | 0.12          |
| (1,4203) | 1:106:A:ASP:HB2 | 1:109:A:HIS:H   | 8        | 0.12          |
| (1,4203) | 1:106:A:ASP:HB2 | 1:109:A:HIS:H   | 9        | 0.12          |
| (1,4203) | 1:106:A:ASP:HB2 | 1:109:A:HIS:H   | 11       | 0.12          |
| (1,4203) | 1:106:A:ASP:HB2 | 1:109:A:HIS:H   | 12       | 0.12          |
| (1,4203) | 1:106:A:ASP:HB2 | 1:109:A:HIS:H   | 14       | 0.12          |
| (1,4203) | 1:106:A:ASP:HB2 | 1:109:A:HIS:H   | 15       | 0.12          |
| (1,4203) | 1:106:A:ASP:HB2 | 1:109:A:HIS:H   | 16       | 0.12          |
| (1,4198) | 1:127:A:GLN:HA  | 1:127:A:GLN:H   | 1        | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,4198) | 1:127:A:GLN:HA  | 1:127:A:GLN:H   | 8        | 0.12          |
| (1,4194) | 1:107:A:GLU:H   | 1:106:A:ASP:HA  | 2        | 0.12          |
| (1,4194) | 1:107:A:GLU:H   | 1:106:A:ASP:HA  | 4        | 0.12          |
| (1,4194) | 1:107:A:GLU:H   | 1:106:A:ASP:HA  | 6        | 0.12          |
| (1,4194) | 1:107:A:GLU:H   | 1:106:A:ASP:HA  | 7        | 0.12          |
| (1,4194) | 1:107:A:GLU:H   | 1:106:A:ASP:HA  | 11       | 0.12          |
| (1,4194) | 1:107:A:GLU:H   | 1:106:A:ASP:HA  | 13       | 0.12          |
| (1,4194) | 1:107:A:GLU:H   | 1:106:A:ASP:HA  | 16       | 0.12          |
| (1,4194) | 1:107:A:GLU:H   | 1:106:A:ASP:HA  | 17       | 0.12          |
| (1,4165) | 1:40:A:SER:HA   | 1:43:A:GLY:H    | 10       | 0.12          |
| (1,4151) | 1:18:A:GLN:HG2  | 1:18:A:GLN:H    | 7        | 0.12          |
| (1,4150) | 1:17:A:ASN:HB3  | 1:18:A:GLN:H    | 3        | 0.12          |
| (1,4150) | 1:17:A:ASN:HB3  | 1:18:A:GLN:H    | 11       | 0.12          |
| (1,4148) | 1:25:A:LYS:HB2  | 1:26:A:GLU:H    | 1        | 0.12          |
| (1,4148) | 1:25:A:LYS:HB2  | 1:26:A:GLU:H    | 2        | 0.12          |
| (1,4128) | 1:34:A:ARG:HE   | 1:34:A:ARG:HA   | 7        | 0.12          |
| (1,4128) | 1:34:A:ARG:HE   | 1:34:A:ARG:HA   | 11       | 0.12          |
| (1,4127) | 1:34:A:ARG:HE   | 1:30:A:PHE:HD2  | 1        | 0.12          |
| (1,4119) | 1:66:A:LEU:HB2  | 1:70:A:GLN:HE22 | 13       | 0.12          |
| (1,4113) | 1:22:A:ASN:H    | 1:22:A:ASN:HD22 | 8        | 0.12          |
| (1,4110) | 1:40:A:SER:HA   | 1:42:A:GLU:H    | 15       | 0.12          |
| (1,4106) | 1:99:A:GLY:HA3  | 1:98:A:ASP:H    | 4        | 0.12          |
| (1,4106) | 1:99:A:GLY:HA3  | 1:98:A:ASP:H    | 9        | 0.12          |
| (1,4106) | 1:99:A:GLY:HA3  | 1:98:A:ASP:H    | 13       | 0.12          |
| (1,4090) | 1:65:A:ASN:HD22 | 1:21:A:LEU:HG   | 13       | 0.12          |
| (1,4060) | 1:97:A:LEU:HD21 | 1:39:A:PHE:H    | 2        | 0.12          |
| (1,4060) | 1:97:A:LEU:HD21 | 1:39:A:PHE:H    | 12       | 0.12          |
| (1,4050) | 1:20:A:LYS:H    | 1:20:A:LYS:HE2  | 12       | 0.12          |
| (1,4041) | 1:21:A:LEU:HA   | 1:23:A:SER:H    | 1        | 0.12          |
| (1,4041) | 1:21:A:LEU:HA   | 1:23:A:SER:H    | 5        | 0.12          |
| (1,4041) | 1:21:A:LEU:HA   | 1:23:A:SER:H    | 12       | 0.12          |
| (1,4036) | 1:31:A:LEU:H    | 1:31:A:LEU:HD12 | 16       | 0.12          |
| (1,4036) | 1:31:A:LEU:H    | 1:31:A:LEU:HD12 | 17       | 0.12          |
| (1,3994) | 1:45:A:ALA:H    | 1:83:A:ARG:HB2  | 13       | 0.12          |
| (1,3987) | 1:50:A:ILE:HG21 | 1:50:A:ILE:H    | 3        | 0.12          |
| (1,3940) | 1:62:A:GLY:HA3  | 1:63:A:GLU:H    | 1        | 0.12          |
| (1,3935) | 1:63:A:GLU:HB3  | 1:65:A:ASN:H    | 11       | 0.12          |
| (1,3934) | 1:65:A:ASN:H    | 1:64:A:MET:HG2  | 11       | 0.12          |
| (1,3931) | 1:67:A:SER:H    | 1:66:A:LEU:H    | 17       | 0.12          |
| (1,3929) | 1:68:A:LYS:HD2  | 1:68:A:LYS:H    | 8        | 0.12          |
| (1,3929) | 1:68:A:LYS:HD2  | 1:68:A:LYS:H    | 12       | 0.12          |
| (1,3907) | 1:76:A:ARG:HD2  | 1:77:A:LEU:H    | 3        | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3907) | 1:76:A:ARG:HD2  | 1:77:A:LEU:H    | 4        | 0.12          |
| (1,3907) | 1:76:A:ARG:HD2  | 1:77:A:LEU:H    | 6        | 0.12          |
| (1,3907) | 1:76:A:ARG:HD2  | 1:77:A:LEU:H    | 7        | 0.12          |
| (1,3907) | 1:76:A:ARG:HD2  | 1:77:A:LEU:H    | 9        | 0.12          |
| (1,3907) | 1:76:A:ARG:HD2  | 1:77:A:LEU:H    | 10       | 0.12          |
| (1,3907) | 1:76:A:ARG:HD2  | 1:77:A:LEU:H    | 12       | 0.12          |
| (1,3907) | 1:76:A:ARG:HD2  | 1:77:A:LEU:H    | 16       | 0.12          |
| (1,3907) | 1:76:A:ARG:HD2  | 1:77:A:LEU:H    | 17       | 0.12          |
| (1,3887) | 1:81:A:SER:HB2  | 1:82:A:TRP:H    | 10       | 0.12          |
| (1,3884) | 1:83:A:ARG:H    | 1:83:A:ARG:HB2  | 2        | 0.12          |
| (1,3884) | 1:83:A:ARG:H    | 1:83:A:ARG:HB2  | 10       | 0.12          |
| (1,3884) | 1:83:A:ARG:H    | 1:83:A:ARG:HB2  | 14       | 0.12          |
| (1,3880) | 1:83:A:ARG:HB3  | 1:84:A:TYR:H    | 11       | 0.12          |
| (1,3845) | 1:95:A:VAL:HG11 | 1:96:A:ASP:H    | 12       | 0.12          |
| (1,3824) | 1:102:A:CYS:H   | 1:100:A:ASN:HB3 | 1        | 0.12          |
| (1,3824) | 1:102:A:CYS:H   | 1:100:A:ASN:HB3 | 2        | 0.12          |
| (1,3824) | 1:102:A:CYS:H   | 1:100:A:ASN:HB3 | 5        | 0.12          |
| (1,3824) | 1:102:A:CYS:H   | 1:100:A:ASN:HB3 | 11       | 0.12          |
| (1,3824) | 1:102:A:CYS:H   | 1:100:A:ASN:HB3 | 15       | 0.12          |
| (1,3820) | 1:101:A:PRO:HB3 | 1:103:A:GLY:H   | 1        | 0.12          |
| (1,3820) | 1:101:A:PRO:HB3 | 1:103:A:GLY:H   | 2        | 0.12          |
| (1,3820) | 1:101:A:PRO:HB3 | 1:103:A:GLY:H   | 5        | 0.12          |
| (1,3820) | 1:101:A:PRO:HB3 | 1:103:A:GLY:H   | 6        | 0.12          |
| (1,3820) | 1:101:A:PRO:HB3 | 1:103:A:GLY:H   | 7        | 0.12          |
| (1,3820) | 1:101:A:PRO:HB3 | 1:103:A:GLY:H   | 8        | 0.12          |
| (1,3820) | 1:101:A:PRO:HB3 | 1:103:A:GLY:H   | 12       | 0.12          |
| (1,3820) | 1:101:A:PRO:HB3 | 1:103:A:GLY:H   | 14       | 0.12          |
| (1,3820) | 1:101:A:PRO:HB3 | 1:103:A:GLY:H   | 15       | 0.12          |
| (1,3820) | 1:101:A:PRO:HB3 | 1:103:A:GLY:H   | 17       | 0.12          |
| (1,3801) | 1:108:A:GLN:HA  | 1:108:A:GLN:H   | 1        | 0.12          |
| (1,3801) | 1:108:A:GLN:HA  | 1:108:A:GLN:H   | 2        | 0.12          |
| (1,3801) | 1:108:A:GLN:HA  | 1:108:A:GLN:H   | 5        | 0.12          |
| (1,3801) | 1:108:A:GLN:HA  | 1:108:A:GLN:H   | 13       | 0.12          |
| (1,3801) | 1:108:A:GLN:HA  | 1:108:A:GLN:H   | 14       | 0.12          |
| (1,3801) | 1:108:A:GLN:HA  | 1:108:A:GLN:H   | 15       | 0.12          |
| (1,3797) | 1:44:A:GLU:HA   | 1:44:A:GLU:H    | 2        | 0.12          |
| (1,3797) | 1:44:A:GLU:HA   | 1:44:A:GLU:H    | 6        | 0.12          |
| (1,3797) | 1:44:A:GLU:HA   | 1:44:A:GLU:H    | 8        | 0.12          |
| (1,3797) | 1:44:A:GLU:HA   | 1:44:A:GLU:H    | 11       | 0.12          |
| (1,3797) | 1:44:A:GLU:HA   | 1:44:A:GLU:H    | 13       | 0.12          |
| (1,3783) | 1:117:A:LEU:HB3 | 1:117:A:LEU:H   | 1        | 0.12          |
| (1,3783) | 1:117:A:LEU:HB3 | 1:117:A:LEU:H   | 5        | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3783) | 1:117:A:LEU:HB3 | 1:117:A:LEU:H   | 10       | 0.12          |
| (1,3768) | 1:130:A:GLU:H   | 1:130:A:GLU:HA  | 10       | 0.12          |
| (1,3768) | 1:130:A:GLU:H   | 1:130:A:GLU:HA  | 16       | 0.12          |
| (1,3767) | 1:129:A:ALA:HA  | 1:129:A:ALA:H   | 3        | 0.12          |
| (1,3757) | 1:116:A:GLN:H   | 1:117:A:LEU:H   | 1        | 0.12          |
| (1,3757) | 1:116:A:GLN:H   | 1:117:A:LEU:H   | 3        | 0.12          |
| (1,3757) | 1:116:A:GLN:H   | 1:117:A:LEU:H   | 11       | 0.12          |
| (1,3757) | 1:116:A:GLN:H   | 1:117:A:LEU:H   | 15       | 0.12          |
| (1,3753) | 1:107:A:GLU:H   | 1:106:A:ASP:H   | 2        | 0.12          |
| (1,3753) | 1:107:A:GLU:H   | 1:106:A:ASP:H   | 4        | 0.12          |
| (1,3736) | 1:41:A:ALA:HA   | 1:29:A:ALA:H    | 4        | 0.12          |
| (1,3736) | 1:41:A:ALA:HA   | 1:29:A:ALA:H    | 7        | 0.12          |
| (1,3731) | 1:66:A:LEU:HB3  | 1:66:A:LEU:H    | 3        | 0.12          |
| (1,3708) | 1:62:A:GLY:H    | 1:62:A:GLY:HA3  | 5        | 0.12          |
| (1,3687) | 1:85:A:LEU:H    | 1:82:A:TRP:HD1  | 15       | 0.12          |
| (1,3687) | 1:85:A:LEU:H    | 1:82:A:TRP:HD1  | 17       | 0.12          |
| (1,3667) | 1:37:A:HIS:H    | 1:37:A:HIS:HD2  | 2        | 0.12          |
| (1,3667) | 1:37:A:HIS:H    | 1:37:A:HIS:HD2  | 8        | 0.12          |
| (1,3667) | 1:37:A:HIS:H    | 1:37:A:HIS:HD2  | 10       | 0.12          |
| (1,3667) | 1:37:A:HIS:H    | 1:37:A:HIS:HD2  | 13       | 0.12          |
| (1,3667) | 1:37:A:HIS:H    | 1:37:A:HIS:HD2  | 17       | 0.12          |
| (1,3603) | 1:97:A:LEU:HA   | 1:97:A:LEU:HG   | 11       | 0.12          |
| (1,3599) | 1:92:A:ALA:HB3  | 1:113:A:ALA:HB1 | 15       | 0.12          |
| (1,3596) | 1:112:A:HIS:HA  | 1:115:A:LYS:HB3 | 12       | 0.12          |
| (1,3579) | 1:33:A:GLU:HB3  | 1:30:A:PHE:HA   | 10       | 0.12          |
| (1,3568) | 1:105:A:LEU:HB3 | 1:109:A:HIS:HB2 | 1        | 0.12          |
| (1,3568) | 1:105:A:LEU:HB3 | 1:109:A:HIS:HB2 | 3        | 0.12          |
| (1,3568) | 1:105:A:LEU:HB3 | 1:109:A:HIS:HB2 | 5        | 0.12          |
| (1,3568) | 1:105:A:LEU:HB3 | 1:109:A:HIS:HB2 | 6        | 0.12          |
| (1,3568) | 1:105:A:LEU:HB3 | 1:109:A:HIS:HB2 | 8        | 0.12          |
| (1,3568) | 1:105:A:LEU:HB3 | 1:109:A:HIS:HB2 | 10       | 0.12          |
| (1,3568) | 1:105:A:LEU:HB3 | 1:109:A:HIS:HB2 | 11       | 0.12          |
| (1,3568) | 1:105:A:LEU:HB3 | 1:109:A:HIS:HB2 | 12       | 0.12          |
| (1,3568) | 1:105:A:LEU:HB3 | 1:109:A:HIS:HB2 | 13       | 0.12          |
| (1,3568) | 1:105:A:LEU:HB3 | 1:109:A:HIS:HB2 | 16       | 0.12          |
| (1,3552) | 1:123:A:ARG:HG2 | 1:124:A:VAL:HA  | 3        | 0.12          |
| (1,3552) | 1:123:A:ARG:HG2 | 1:124:A:VAL:HA  | 6        | 0.12          |
| (1,3552) | 1:123:A:ARG:HG2 | 1:124:A:VAL:HA  | 8        | 0.12          |
| (1,3552) | 1:123:A:ARG:HG2 | 1:124:A:VAL:HA  | 12       | 0.12          |
| (1,3552) | 1:123:A:ARG:HG2 | 1:124:A:VAL:HA  | 16       | 0.12          |
| (1,3537) | 1:51:A:GLY:HA2  | 1:54:A:GLN:HB2  | 3        | 0.12          |
| (1,3523) | 1:56:A:LEU:HG   | 1:56:A:LEU:HB3  | 14       | 0.12          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3519) | 1:65:A:ASN:H    | 1:65:A:ASN:HB3   | 16       | 0.12          |
| (1,3514) | 1:83:A:ARG:HG3  | 1:84:A:TYR:H     | 16       | 0.12          |
| (1,3510) | 1:64:A:MET:HE3  | 1:21:A:LEU:H     | 8        | 0.12          |
| (1,3508) | 1:113:A:ALA:HB2 | 1:88:A:VAL:HA    | 8        | 0.12          |
| (1,3500) | 1:27:A:VAL:HG22 | 1:31:A:LEU:HD11  | 4        | 0.12          |
| (1,3500) | 1:27:A:VAL:HG23 | 1:31:A:LEU:HD12  | 5        | 0.12          |
| (1,3479) | 1:45:A:ALA:HB3  | 1:44:A:GLU:HB3   | 2        | 0.12          |
| (1,3465) | 1:88:A:VAL:HG22 | 1:85:A:LEU:HB3   | 11       | 0.12          |
| (1,3457) | 1:20:A:LYS:HE3  | 1:19:A:PRO:HA    | 1        | 0.12          |
| (1,3457) | 1:20:A:LYS:HE3  | 1:19:A:PRO:HA    | 2        | 0.12          |
| (1,3443) | 1:123:A:ARG:HG2 | 1:123:A:ARG:HD3  | 4        | 0.12          |
| (1,3443) | 1:123:A:ARG:HG2 | 1:123:A:ARG:HD3  | 5        | 0.12          |
| (1,3433) | 1:27:A:VAL:HA   | 1:21:A:LEU:HD13  | 9        | 0.12          |
| (1,3415) | 1:117:A:LEU:HA  | 1:117:A:LEU:HD12 | 6        | 0.12          |
| (1,3414) | 1:86:A:TYR:H    | 1:117:A:LEU:HD12 | 14       | 0.12          |
| (1,3414) | 1:86:A:TYR:H    | 1:117:A:LEU:HD11 | 16       | 0.12          |
| (1,3398) | 1:117:A:LEU:HA  | 1:120:A:ALA:HB2  | 9        | 0.12          |
| (1,3374) | 1:88:A:VAL:HA   | 1:88:A:VAL:HG12  | 5        | 0.12          |
| (1,3372) | 1:88:A:VAL:HA   | 1:47:A:PRO:HB3   | 9        | 0.12          |
| (1,3372) | 1:88:A:VAL:HA   | 1:47:A:PRO:HB3   | 13       | 0.12          |
| (1,3369) | 1:24:A:SER:HA   | 1:27:A:VAL:HG21  | 17       | 0.12          |
| (1,3335) | 1:71:A:LEU:HA   | 1:71:A:LEU:HD22  | 9        | 0.12          |
| (1,3316) | 1:66:A:LEU:HD11 | 1:30:A:PHE:HD2   | 3        | 0.12          |
| (1,3316) | 1:66:A:LEU:HD12 | 1:30:A:PHE:HD2   | 11       | 0.12          |
| (1,3315) | 1:66:A:LEU:HD13 | 1:66:A:LEU:HA    | 14       | 0.12          |
| (1,3314) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HG    | 7        | 0.12          |
| (1,3314) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HG    | 8        | 0.12          |
| (1,3306) | 1:128:A:ARG:HG2 | 1:128:A:ARG:HD2  | 4        | 0.12          |
| (1,3299) | 1:20:A:LYS:H    | 1:20:A:LYS:HD3   | 1        | 0.12          |
| (1,3291) | 1:72:A:ARG:HB3  | 1:53:A:PHE:HE2   | 12       | 0.12          |
| (1,3291) | 1:72:A:ARG:HB3  | 1:53:A:PHE:HE1   | 15       | 0.12          |
| (1,3275) | 1:119:A:GLU:HA  | 1:119:A:GLU:HG2  | 1        | 0.12          |
| (1,3275) | 1:119:A:GLU:HA  | 1:119:A:GLU:HG2  | 2        | 0.12          |
| (1,3275) | 1:119:A:GLU:HA  | 1:119:A:GLU:HG2  | 5        | 0.12          |
| (1,3275) | 1:119:A:GLU:HA  | 1:119:A:GLU:HG2  | 10       | 0.12          |
| (1,3275) | 1:119:A:GLU:HA  | 1:119:A:GLU:HG2  | 11       | 0.12          |
| (1,3275) | 1:119:A:GLU:HA  | 1:119:A:GLU:HG2  | 12       | 0.12          |
| (1,3275) | 1:119:A:GLU:HA  | 1:119:A:GLU:HG2  | 17       | 0.12          |
| (1,3273) | 1:42:A:GLU:HG2  | 1:43:A:GLY:H     | 3        | 0.12          |
| (1,3263) | 1:121:A:LYS:HG2 | 1:122:A:ALA:H    | 4        | 0.12          |
| (1,3263) | 1:121:A:LYS:HG2 | 1:122:A:ALA:H    | 7        | 0.12          |
| (1,3263) | 1:121:A:LYS:HG2 | 1:122:A:ALA:H    | 15       | 0.12          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3255) | 1:40:A:SER:HA    | 1:41:A:ALA:HB1  | 16       | 0.12          |
| (1,3244) | 1:78:A:TYR:HA    | 1:28:A:ILE:HG12 | 3        | 0.12          |
| (1,3244) | 1:78:A:TYR:HA    | 1:28:A:ILE:HG12 | 4        | 0.12          |
| (1,3244) | 1:78:A:TYR:HA    | 1:28:A:ILE:HG12 | 5        | 0.12          |
| (1,3244) | 1:78:A:TYR:HA    | 1:28:A:ILE:HG12 | 7        | 0.12          |
| (1,3244) | 1:78:A:TYR:HA    | 1:28:A:ILE:HG12 | 8        | 0.12          |
| (1,3244) | 1:78:A:TYR:HA    | 1:28:A:ILE:HG12 | 10       | 0.12          |
| (1,3244) | 1:78:A:TYR:HA    | 1:28:A:ILE:HG12 | 12       | 0.12          |
| (1,3244) | 1:78:A:TYR:HA    | 1:28:A:ILE:HG12 | 13       | 0.12          |
| (1,3244) | 1:78:A:TYR:HA    | 1:28:A:ILE:HG12 | 15       | 0.12          |
| (1,3244) | 1:78:A:TYR:HA    | 1:28:A:ILE:HG12 | 17       | 0.12          |
| (1,3241) | 1:52:A:ILE:HG13  | 1:97:A:LEU:HD23 | 2        | 0.12          |
| (1,3230) | 1:68:A:LYS:HB2   | 1:68:A:LYS:HA   | 3        | 0.12          |
| (1,3221) | 1:37:A:HIS:HB2   | 1:99:A:GLY:HA2  | 1        | 0.12          |
| (1,3221) | 1:37:A:HIS:HB2   | 1:99:A:GLY:HA2  | 4        | 0.12          |
| (1,3221) | 1:37:A:HIS:HB2   | 1:99:A:GLY:HA2  | 5        | 0.12          |
| (1,3208) | 1:124:A:VAL:HG13 | 1:124:A:VAL:HA  | 2        | 0.12          |
| (1,3205) | 1:124:A:VAL:HA   | 1:124:A:VAL:HB  | 2        | 0.12          |
| (1,3185) | 1:109:A:HIS:HB2  | 1:108:A:GLN:H   | 5        | 0.12          |
| (1,3183) | 1:124:A:VAL:HG22 | 1:121:A:LYS:HA  | 10       | 0.12          |
| (1,3172) | 1:25:A:LYS:HE3   | 1:25:A:LYS:HA   | 4        | 0.12          |
| (1,3172) | 1:25:A:LYS:HE3   | 1:25:A:LYS:HA   | 7        | 0.12          |
| (1,3169) | 1:53:A:PHE:HB3   | 1:75:A:LEU:HD23 | 1        | 0.12          |
| (1,3169) | 1:53:A:PHE:HB3   | 1:75:A:LEU:HD21 | 16       | 0.12          |
| (1,3164) | 1:120:A:ALA:HB1  | 1:120:A:ALA:H   | 4        | 0.12          |
| (1,3164) | 1:120:A:ALA:HB1  | 1:120:A:ALA:H   | 6        | 0.12          |
| (1,3160) | 1:74:A:ALA:HB2   | 1:74:A:ALA:HA   | 2        | 0.12          |
| (1,3160) | 1:74:A:ALA:HB3   | 1:74:A:ALA:HA   | 15       | 0.12          |
| (1,3151) | 1:97:A:LEU:HA    | 1:97:A:LEU:H    | 2        | 0.12          |
| (1,3151) | 1:97:A:LEU:HA    | 1:97:A:LEU:H    | 14       | 0.12          |
| (1,3147) | 1:23:A:SER:HB2   | 1:70:A:GLN:HB3  | 6        | 0.12          |
| (1,3147) | 1:23:A:SER:HB2   | 1:70:A:GLN:HB3  | 9        | 0.12          |
| (1,3130) | 1:123:A:ARG:HG2  | 1:123:A:ARG:H   | 16       | 0.12          |
| (1,3122) | 1:11:A:SER:HB2   | 1:11:A:SER:HA   | 4        | 0.12          |
| (1,3122) | 1:11:A:SER:HB2   | 1:11:A:SER:HA   | 12       | 0.12          |
| (1,3122) | 1:11:A:SER:HB2   | 1:11:A:SER:HA   | 17       | 0.12          |
| (1,3113) | 1:57:A:VAL:HG12  | 1:61:A:ALA:H    | 4        | 0.12          |
| (1,3113) | 1:57:A:VAL:HG12  | 1:61:A:ALA:H    | 9        | 0.12          |
| (1,3108) | 1:102:A:CYS:H    | 1:101:A:PRO:HB3 | 1        | 0.12          |
| (1,3108) | 1:102:A:CYS:H    | 1:101:A:PRO:HB3 | 3        | 0.12          |
| (1,3108) | 1:102:A:CYS:H    | 1:101:A:PRO:HB3 | 4        | 0.12          |
| (1,3108) | 1:102:A:CYS:H    | 1:101:A:PRO:HB3 | 8        | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3108) | 1:102:A:CYS:H   | 1:101:A:PRO:HB3 | 12       | 0.12          |
| (1,3108) | 1:102:A:CYS:H   | 1:101:A:PRO:HB3 | 13       | 0.12          |
| (1,3108) | 1:102:A:CYS:H   | 1:101:A:PRO:HB3 | 16       | 0.12          |
| (1,3104) | 1:56:A:LEU:HD13 | 1:52:A:ILE:HG13 | 2        | 0.12          |
| (1,3104) | 1:56:A:LEU:HD13 | 1:52:A:ILE:HG13 | 5        | 0.12          |
| (1,3104) | 1:56:A:LEU:HD13 | 1:52:A:ILE:HG13 | 14       | 0.12          |
| (1,3087) | 1:56:A:LEU:HG   | 1:56:A:LEU:HA   | 10       | 0.12          |
| (1,3087) | 1:56:A:LEU:HG   | 1:56:A:LEU:HA   | 12       | 0.12          |
| (1,3059) | 1:28:A:ILE:HB   | 1:28:A:ILE:HG23 | 5        | 0.12          |
| (1,3059) | 1:28:A:ILE:HB   | 1:28:A:ILE:HG22 | 11       | 0.12          |
| (1,3040) | 1:52:A:ILE:HA   | 1:52:A:ILE:HG12 | 11       | 0.12          |
| (1,3040) | 1:52:A:ILE:HA   | 1:52:A:ILE:HG12 | 15       | 0.12          |
| (1,3040) | 1:52:A:ILE:HA   | 1:52:A:ILE:HG12 | 17       | 0.12          |
| (1,3035) | 1:25:A:LYS:H    | 1:25:A:LYS:HG2  | 16       | 0.12          |
| (1,3019) | 1:64:A:MET:HE1  | 1:66:A:LEU:H    | 3        | 0.12          |
| (1,2988) | 1:68:A:LYS:HB2  | 1:68:A:LYS:H    | 5        | 0.12          |
| (1,2978) | 1:105:A:LEU:H   | 1:101:A:PRO:HD3 | 8        | 0.12          |
| (1,2978) | 1:105:A:LEU:H   | 1:101:A:PRO:HD3 | 16       | 0.12          |
| (1,2961) | 1:56:A:LEU:HD21 | 1:52:A:ILE:HB   | 3        | 0.12          |
| (1,2955) | 1:74:A:ALA:HB2  | 1:75:A:LEU:HD12 | 15       | 0.12          |
| (1,2950) | 1:75:A:LEU:HD12 | 1:75:A:LEU:H    | 17       | 0.12          |
| (1,2949) | 1:39:A:PHE:HZ   | 1:75:A:LEU:HD12 | 14       | 0.12          |
| (1,2899) | 1:28:A:ILE:HD12 | 1:75:A:LEU:H    | 6        | 0.12          |
| (1,2893) | 1:50:A:ILE:HB   | 1:50:A:ILE:HG21 | 12       | 0.12          |
| (1,2893) | 1:50:A:ILE:HB   | 1:50:A:ILE:HG21 | 15       | 0.12          |
| (1,2891) | 1:32:A:ALA:HB2  | 1:28:A:ILE:HG23 | 8        | 0.12          |
| (1,2882) | 1:32:A:ALA:HB1  | 1:33:A:GLU:H    | 8        | 0.12          |
| (1,2880) | 1:61:A:ALA:HB3  | 1:57:A:VAL:HG12 | 3        | 0.12          |
| (1,2875) | 1:122:A:ALA:HB3 | 1:122:A:ALA:H   | 3        | 0.12          |
| (1,2875) | 1:122:A:ALA:HB1 | 1:122:A:ALA:H   | 10       | 0.12          |
| (1,2875) | 1:122:A:ALA:HB1 | 1:122:A:ALA:H   | 15       | 0.12          |
| (1,2875) | 1:122:A:ALA:HB3 | 1:122:A:ALA:H   | 16       | 0.12          |
| (1,2871) | 1:129:A:ALA:HB3 | 1:129:A:ALA:H   | 8        | 0.12          |
| (1,2859) | 1:86:A:TYR:HE1  | 1:85:A:LEU:H    | 4        | 0.12          |
| (1,2859) | 1:86:A:TYR:HE1  | 1:85:A:LEU:H    | 14       | 0.12          |
| (1,2849) | 1:73:A:SER:HB3  | 1:74:A:ALA:H    | 1        | 0.12          |
| (1,2849) | 1:73:A:SER:HB3  | 1:74:A:ALA:H    | 2        | 0.12          |
| (1,2849) | 1:73:A:SER:HB3  | 1:74:A:ALA:H    | 6        | 0.12          |
| (1,2849) | 1:73:A:SER:HB3  | 1:74:A:ALA:H    | 8        | 0.12          |
| (1,2849) | 1:73:A:SER:HB3  | 1:74:A:ALA:H    | 14       | 0.12          |
| (1,2846) | 1:53:A:PHE:HE2  | 1:75:A:LEU:HB3  | 7        | 0.12          |
| (1,2846) | 1:53:A:PHE:HE1  | 1:75:A:LEU:HB3  | 8        | 0.12          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2846) | 1:53:A:PHE:HE2   | 1:75:A:LEU:HB3   | 13       | 0.12          |
| (1,2846) | 1:53:A:PHE:HE1   | 1:75:A:LEU:HB3   | 15       | 0.12          |
| (1,2846) | 1:53:A:PHE:HE1   | 1:75:A:LEU:HB3   | 16       | 0.12          |
| (1,2811) | 1:97:A:LEU:HD13  | 1:97:A:LEU:HB3   | 16       | 0.12          |
| (1,2786) | 1:82:A:TRP:HH2   | 1:82:A:TRP:HE1   | 1        | 0.12          |
| (1,2786) | 1:82:A:TRP:HH2   | 1:82:A:TRP:HE1   | 3        | 0.12          |
| (1,2786) | 1:82:A:TRP:HH2   | 1:82:A:TRP:HE1   | 4        | 0.12          |
| (1,2786) | 1:82:A:TRP:HH2   | 1:82:A:TRP:HE1   | 7        | 0.12          |
| (1,2786) | 1:82:A:TRP:HH2   | 1:82:A:TRP:HE1   | 8        | 0.12          |
| (1,2786) | 1:82:A:TRP:HH2   | 1:82:A:TRP:HE1   | 9        | 0.12          |
| (1,2786) | 1:82:A:TRP:HH2   | 1:82:A:TRP:HE1   | 10       | 0.12          |
| (1,2786) | 1:82:A:TRP:HH2   | 1:82:A:TRP:HE1   | 12       | 0.12          |
| (1,2786) | 1:82:A:TRP:HH2   | 1:82:A:TRP:HE1   | 15       | 0.12          |
| (1,2775) | 1:47:A:PRO:HB3   | 1:87:A:GLY:HA2   | 3        | 0.12          |
| (1,2775) | 1:47:A:PRO:HB3   | 1:87:A:GLY:HA2   | 7        | 0.12          |
| (1,2775) | 1:47:A:PRO:HB3   | 1:87:A:GLY:HA2   | 9        | 0.12          |
| (1,2775) | 1:47:A:PRO:HB3   | 1:87:A:GLY:HA2   | 13       | 0.12          |
| (1,2775) | 1:47:A:PRO:HB3   | 1:87:A:GLY:HA2   | 15       | 0.12          |
| (1,2774) | 1:91:A:GLY:HA3   | 1:90:A:PRO:HB2   | 12       | 0.12          |
| (1,2769) | 1:43:A:GLY:HA2   | 1:42:A:GLU:HB2   | 6        | 0.12          |
| (1,2743) | 1:34:A:ARG:HD3   | 1:30:A:PHE:HD1   | 11       | 0.12          |
| (1,2719) | 1:117:A:LEU:HD12 | 1:86:A:TYR:HB2   | 17       | 0.12          |
| (1,2707) | 1:35:A:PHE:HB2   | 1:97:A:LEU:HD21  | 5        | 0.12          |
| (1,2695) | 1:78:A:TYR:HA    | 1:81:A:SER:H     | 2        | 0.12          |
| (1,2695) | 1:78:A:TYR:HA    | 1:81:A:SER:H     | 12       | 0.12          |
| (1,2695) | 1:78:A:TYR:HA    | 1:81:A:SER:H     | 14       | 0.12          |
| (1,2695) | 1:78:A:TYR:HA    | 1:81:A:SER:H     | 17       | 0.12          |
| (1,2672) | 1:31:A:LEU:HD11  | 1:35:A:PHE:HD2   | 17       | 0.12          |
| (1,2665) | 1:86:A:TYR:HE1   | 1:86:A:TYR:HB3   | 16       | 0.12          |
| (1,2651) | 1:75:A:LEU:HB3   | 1:75:A:LEU:H     | 11       | 0.12          |
| (1,2648) | 1:56:A:LEU:HD12  | 1:52:A:ILE:HG12  | 12       | 0.12          |
| (1,2648) | 1:56:A:LEU:HD11  | 1:52:A:ILE:HG12  | 13       | 0.12          |
| (1,2648) | 1:56:A:LEU:HD11  | 1:52:A:ILE:HG12  | 15       | 0.12          |
| (1,2627) | 1:112:A:HIS:HA   | 1:112:A:HIS:HB2  | 12       | 0.12          |
| (1,2613) | 1:34:A:ARG:HG2   | 1:35:A:PHE:HD2   | 5        | 0.12          |
| (1,2612) | 1:30:A:PHE:HD1   | 1:34:A:ARG:HG2   | 8        | 0.12          |
| (1,2612) | 1:30:A:PHE:HD1   | 1:34:A:ARG:HG2   | 9        | 0.12          |
| (1,2586) | 1:93:A:THR:HG21  | 1:102:A:CYS:HA   | 2        | 0.12          |
| (1,2575) | 1:124:A:VAL:HA   | 1:124:A:VAL:HG21 | 3        | 0.12          |
| (1,2575) | 1:124:A:VAL:HA   | 1:124:A:VAL:HG22 | 9        | 0.12          |
| (1,2575) | 1:124:A:VAL:HA   | 1:124:A:VAL:HG21 | 17       | 0.12          |
| (1,2559) | 1:86:A:TYR:HE1   | 1:86:A:TYR:HB2   | 14       | 0.12          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2548) | 1:11:A:SER:HA    | 1:12:A:GLN:H    | 15       | 0.12          |
| (1,2519) | 1:55:A:ASP:HB3   | 1:55:A:ASP:HA   | 8        | 0.12          |
| (1,2505) | 1:126:A:ALA:HA   | 1:126:A:ALA:H   | 17       | 0.12          |
| (1,2497) | 1:30:A:PHE:HD1   | 1:31:A:LEU:HA   | 1        | 0.12          |
| (1,2469) | 1:53:A:PHE:HZ    | 1:72:A:ARG:HG3  | 8        | 0.12          |
| (1,2417) | 1:129:A:ALA:HB1  | 1:127:A:GLN:HB3 | 1        | 0.12          |
| (1,2416) | 1:45:A:ALA:HB1   | 1:45:A:ALA:H    | 10       | 0.12          |
| (1,2351) | 1:110:A:VAL:HG22 | 1:109:A:HIS:HA  | 14       | 0.12          |
| (1,2318) | 1:108:A:GLN:HA   | 1:108:A:GLN:HB3 | 5        | 0.12          |
| (1,2318) | 1:108:A:GLN:HA   | 1:108:A:GLN:HB3 | 12       | 0.12          |
| (1,2306) | 1:38:A:CYS:H     | 1:97:A:LEU:HA   | 3        | 0.12          |
| (1,2306) | 1:38:A:CYS:H     | 1:97:A:LEU:HA   | 5        | 0.12          |
| (1,2306) | 1:38:A:CYS:H     | 1:97:A:LEU:HA   | 9        | 0.12          |
| (1,2301) | 1:92:A:ALA:HA    | 1:93:A:THR:H    | 15       | 0.12          |
| (1,2299) | 1:55:A:ASP:HB3   | 1:96:A:ASP:HA   | 4        | 0.12          |
| (1,2299) | 1:55:A:ASP:HB3   | 1:96:A:ASP:HA   | 13       | 0.12          |
| (1,2295) | 1:121:A:LYS:HG2  | 1:121:A:LYS:HD3 | 3        | 0.12          |
| (1,2295) | 1:121:A:LYS:HG2  | 1:121:A:LYS:HD3 | 7        | 0.12          |
| (1,2295) | 1:121:A:LYS:HG2  | 1:121:A:LYS:HD3 | 12       | 0.12          |
| (1,2295) | 1:121:A:LYS:HG2  | 1:121:A:LYS:HD3 | 15       | 0.12          |
| (1,2288) | 1:70:A:GLN:HA    | 1:70:A:GLN:HG3  | 1        | 0.12          |
| (1,2288) | 1:70:A:GLN:HA    | 1:70:A:GLN:HG3  | 8        | 0.12          |
| (1,2288) | 1:70:A:GLN:HA    | 1:70:A:GLN:HG3  | 14       | 0.12          |
| (1,2283) | 1:33:A:GLU:HG2   | 1:33:A:GLU:HA   | 1        | 0.12          |
| (1,2283) | 1:33:A:GLU:HG2   | 1:33:A:GLU:HA   | 2        | 0.12          |
| (1,2270) | 1:113:A:ALA:HA   | 1:114:A:ARG:H   | 1        | 0.12          |
| (1,2257) | 1:69:A:THR:HB    | 1:72:A:ARG:HB3  | 3        | 0.12          |
| (1,2236) | 1:54:A:GLN:HB2   | 1:54:A:GLN:HG2  | 12       | 0.12          |
| (1,2221) | 1:31:A:LEU:HA    | 1:60:A:VAL:HB   | 1        | 0.12          |
| (1,2185) | 1:53:A:PHE:H     | 1:97:A:LEU:HD23 | 14       | 0.12          |
| (1,2185) | 1:53:A:PHE:H     | 1:97:A:LEU:HD23 | 15       | 0.12          |
| (1,2160) | 1:82:A:TRP:HZ3   | 1:82:A:TRP:HB2  | 1        | 0.12          |
| (1,2160) | 1:82:A:TRP:HZ3   | 1:82:A:TRP:HB2  | 3        | 0.12          |
| (1,2160) | 1:82:A:TRP:HZ3   | 1:82:A:TRP:HB2  | 6        | 0.12          |
| (1,2160) | 1:82:A:TRP:HZ3   | 1:82:A:TRP:HB2  | 15       | 0.12          |
| (1,2160) | 1:82:A:TRP:HZ3   | 1:82:A:TRP:HB2  | 16       | 0.12          |
| (1,2140) | 1:84:A:TYR:HB2   | 1:82:A:TRP:HA   | 1        | 0.12          |
| (1,2098) | 1:21:A:LEU:HD23  | 1:27:A:VAL:HG12 | 4        | 0.12          |
| (1,2094) | 1:95:A:VAL:HG22  | 1:97:A:LEU:HD23 | 1        | 0.12          |
| (1,2094) | 1:95:A:VAL:HG21  | 1:97:A:LEU:HD21 | 15       | 0.12          |
| (1,2089) | 1:49:A:LYS:HB2   | 1:52:A:ILE:H    | 1        | 0.12          |
| (1,2079) | 1:66:A:LEU:HD12  | 1:62:A:GLY:H    | 8        | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2079) | 1:66:A:LEU:HD11 | 1:62:A:GLY:H    | 14       | 0.12          |
| (1,2070) | 1:48:A:LEU:H    | 1:84:A:TYR:HE1  | 13       | 0.12          |
| (1,2047) | 1:60:A:VAL:H    | 1:61:A:ALA:H    | 7        | 0.12          |
| (1,2047) | 1:60:A:VAL:H    | 1:61:A:ALA:H    | 9        | 0.12          |
| (1,2047) | 1:60:A:VAL:H    | 1:61:A:ALA:H    | 13       | 0.12          |
| (1,2047) | 1:60:A:VAL:H    | 1:61:A:ALA:H    | 15       | 0.12          |
| (1,2045) | 1:77:A:LEU:H    | 1:78:A:TYR:H    | 6        | 0.12          |
| (1,2042) | 1:15:A:MET:H    | 1:16:A:GLU:H    | 2        | 0.12          |
| (1,2025) | 1:97:A:LEU:HD22 | 1:35:A:PHE:HD2  | 10       | 0.12          |
| (1,2025) | 1:97:A:LEU:HD22 | 1:35:A:PHE:HD2  | 17       | 0.12          |
| (1,2021) | 1:53:A:PHE:HE2  | 1:57:A:VAL:HG11 | 10       | 0.12          |
| (1,1954) | 1:116:A:GLN:H   | 1:113:A:ALA:HA  | 2        | 0.12          |
| (1,1952) | 1:112:A:HIS:HA  | 1:115:A:LYS:HB3 | 3        | 0.12          |
| (1,1952) | 1:112:A:HIS:HA  | 1:115:A:LYS:HB3 | 15       | 0.12          |
| (1,1938) | 1:97:A:LEU:HD23 | 1:38:A:CYS:HA   | 16       | 0.12          |
| (1,1906) | 1:105:A:LEU:HB3 | 1:101:A:PRO:HB3 | 1        | 0.12          |
| (1,1906) | 1:105:A:LEU:HB3 | 1:101:A:PRO:HB3 | 2        | 0.12          |
| (1,1906) | 1:105:A:LEU:HB3 | 1:101:A:PRO:HB3 | 15       | 0.12          |
| (1,1889) | 1:65:A:ASN:H    | 1:65:A:ASN:HB3  | 4        | 0.12          |
| (1,1847) | 1:36:A:PRO:HB2  | 1:36:A:PRO:HD2  | 15       | 0.12          |
| (1,1835) | 1:20:A:LYS:H    | 1:20:A:LYS:HG2  | 4        | 0.12          |
| (1,1835) | 1:20:A:LYS:H    | 1:20:A:LYS:HG2  | 9        | 0.12          |
| (1,1819) | 1:112:A:HIS:HA  | 1:112:A:HIS:H   | 6        | 0.12          |
| (1,1819) | 1:112:A:HIS:HA  | 1:112:A:HIS:H   | 7        | 0.12          |
| (1,1819) | 1:112:A:HIS:HA  | 1:112:A:HIS:H   | 8        | 0.12          |
| (1,1819) | 1:112:A:HIS:HA  | 1:112:A:HIS:H   | 9        | 0.12          |
| (1,1819) | 1:112:A:HIS:HA  | 1:112:A:HIS:H   | 10       | 0.12          |
| (1,1819) | 1:112:A:HIS:HA  | 1:112:A:HIS:H   | 11       | 0.12          |
| (1,1819) | 1:112:A:HIS:HA  | 1:112:A:HIS:H   | 16       | 0.12          |
| (1,1819) | 1:112:A:HIS:HA  | 1:112:A:HIS:H   | 17       | 0.12          |
| (1,1796) | 1:53:A:PHE:HE1  | 1:68:A:LYS:HA   | 2        | 0.12          |
| (1,1796) | 1:53:A:PHE:HE2  | 1:68:A:LYS:HA   | 6        | 0.12          |
| (1,1796) | 1:53:A:PHE:HE1  | 1:68:A:LYS:HA   | 8        | 0.12          |
| (1,1796) | 1:53:A:PHE:HE2  | 1:68:A:LYS:HA   | 11       | 0.12          |
| (1,1796) | 1:53:A:PHE:HE1  | 1:68:A:LYS:HA   | 14       | 0.12          |
| (1,1796) | 1:53:A:PHE:HE1  | 1:68:A:LYS:HA   | 15       | 0.12          |
| (1,1787) | 1:93:A:THR:HB   | 1:49:A:LYS:HB3  | 9        | 0.12          |
| (1,1775) | 1:88:A:VAL:HA   | 1:47:A:PRO:HB3  | 11       | 0.12          |
| (1,1768) | 1:72:A:ARG:HA   | 1:75:A:LEU:H    | 16       | 0.12          |
| (1,1768) | 1:72:A:ARG:HA   | 1:75:A:LEU:H    | 17       | 0.12          |
| (1,1756) | 1:79:A:THR:HG21 | 1:84:A:TYR:HE2  | 3        | 0.12          |
| (1,1756) | 1:79:A:THR:HG22 | 1:84:A:TYR:HE2  | 7        | 0.12          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1756) | 1:79:A:THR:HG23 | 1:84:A:TYR:HE1   | 8        | 0.12          |
| (1,1756) | 1:79:A:THR:HG21 | 1:84:A:TYR:HE1   | 9        | 0.12          |
| (1,1756) | 1:79:A:THR:HG23 | 1:84:A:TYR:HE2   | 15       | 0.12          |
| (1,1727) | 1:66:A:LEU:HD11 | 1:30:A:PHE:HD2   | 2        | 0.12          |
| (1,1727) | 1:66:A:LEU:HD12 | 1:30:A:PHE:HD1   | 17       | 0.12          |
| (1,1726) | 1:66:A:LEU:HD13 | 1:66:A:LEU:HA    | 16       | 0.12          |
| (1,1720) | 1:117:A:LEU:HG  | 1:117:A:LEU:HD11 | 11       | 0.12          |
| (1,1720) | 1:117:A:LEU:HG  | 1:117:A:LEU:HD13 | 12       | 0.12          |
| (1,1718) | 1:18:A:GLN:HB3  | 1:19:A:PRO:HD2   | 1        | 0.12          |
| (1,1718) | 1:18:A:GLN:HB3  | 1:19:A:PRO:HD2   | 9        | 0.12          |
| (1,1713) | 1:20:A:LYS:H    | 1:20:A:LYS:HD3   | 2        | 0.12          |
| (1,1713) | 1:20:A:LYS:H    | 1:20:A:LYS:HD3   | 7        | 0.12          |
| (1,1713) | 1:20:A:LYS:H    | 1:20:A:LYS:HD3   | 9        | 0.12          |
| (1,1707) | 1:70:A:GLN:HG3  | 1:70:A:GLN:HB3   | 5        | 0.12          |
| (1,1701) | 1:130:A:GLU:HG3 | 1:131:A:GLN:H    | 5        | 0.12          |
| (1,1683) | 1:48:A:LEU:HD12 | 1:38:A:CYS:HA    | 11       | 0.12          |
| (1,1640) | 1:33:A:GLU:HG3  | 1:33:A:GLU:H     | 14       | 0.12          |
| (1,1636) | 1:124:A:VAL:HA  | 1:125:A:GLN:HG3  | 10       | 0.12          |
| (1,1636) | 1:124:A:VAL:HA  | 1:125:A:GLN:HG3  | 15       | 0.12          |
| (1,1636) | 1:124:A:VAL:HA  | 1:125:A:GLN:HG3  | 17       | 0.12          |
| (1,1599) | 1:53:A:PHE:HB3  | 1:75:A:LEU:HD22  | 2        | 0.12          |
| (1,1599) | 1:53:A:PHE:HB3  | 1:75:A:LEU:HD22  | 4        | 0.12          |
| (1,1599) | 1:53:A:PHE:HB3  | 1:75:A:LEU:HD21  | 8        | 0.12          |
| (1,1589) | 1:120:A:ALA:HB3 | 1:121:A:LYS:H    | 11       | 0.12          |
| (1,1588) | 1:74:A:ALA:HB1  | 1:74:A:ALA:HA    | 14       | 0.12          |
| (1,1578) | 1:70:A:GLN:HB3  | 1:66:A:LEU:HA    | 1        | 0.12          |
| (1,1553) | 1:57:A:VAL:HG12 | 1:61:A:ALA:H     | 15       | 0.12          |
| (1,1546) | 1:56:A:LEU:HD13 | 1:52:A:ILE:HG13  | 1        | 0.12          |
| (1,1546) | 1:56:A:LEU:HD11 | 1:52:A:ILE:HG13  | 7        | 0.12          |
| (1,1536) | 1:53:A:PHE:HA   | 1:56:A:LEU:HB3   | 3        | 0.12          |
| (1,1536) | 1:53:A:PHE:HA   | 1:56:A:LEU:HB3   | 6        | 0.12          |
| (1,1536) | 1:53:A:PHE:HA   | 1:56:A:LEU:HB3   | 9        | 0.12          |
| (1,1536) | 1:53:A:PHE:HA   | 1:56:A:LEU:HB3   | 11       | 0.12          |
| (1,1526) | 1:54:A:GLN:HB3  | 1:54:A:GLN:HA    | 6        | 0.12          |
| (1,1526) | 1:54:A:GLN:HB3  | 1:54:A:GLN:HA    | 7        | 0.12          |
| (1,1526) | 1:54:A:GLN:HB3  | 1:54:A:GLN:HA    | 12       | 0.12          |
| (1,1526) | 1:54:A:GLN:HB3  | 1:54:A:GLN:HA    | 13       | 0.12          |
| (1,1526) | 1:54:A:GLN:HB3  | 1:54:A:GLN:HA    | 14       | 0.12          |
| (1,1526) | 1:54:A:GLN:HB3  | 1:54:A:GLN:HA    | 17       | 0.12          |
| (1,1486) | 1:25:A:LYS:HG3  | 1:26:A:GLU:HA    | 3        | 0.12          |
| (1,1486) | 1:25:A:LYS:HG3  | 1:26:A:GLU:HA    | 7        | 0.12          |
| (1,1486) | 1:25:A:LYS:HG3  | 1:26:A:GLU:HA    | 8        | 0.12          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1486) | 1:25:A:LYS:HG3   | 1:26:A:GLU:HA   | 9        | 0.12          |
| (1,1486) | 1:25:A:LYS:HG3   | 1:26:A:GLU:HA   | 10       | 0.12          |
| (1,1486) | 1:25:A:LYS:HG3   | 1:26:A:GLU:HA   | 17       | 0.12          |
| (1,1464) | 1:102:A:CYS:HB3  | 1:103:A:GLY:H   | 11       | 0.12          |
| (1,1464) | 1:102:A:CYS:HB3  | 1:103:A:GLY:H   | 15       | 0.12          |
| (1,1457) | 1:60:A:VAL:HG13  | 1:60:A:VAL:HB   | 3        | 0.12          |
| (1,1445) | 1:15:A:MET:H     | 1:15:A:MET:HB2  | 8        | 0.12          |
| (1,1445) | 1:15:A:MET:H     | 1:15:A:MET:HB2  | 12       | 0.12          |
| (1,1414) | 1:74:A:ALA:HB3   | 1:75:A:LEU:HD12 | 8        | 0.12          |
| (1,1412) | 1:39:A:PHE:HZ    | 1:75:A:LEU:HD11 | 7        | 0.12          |
| (1,1410) | 1:110:A:VAL:HG21 | 1:108:A:GLN:H   | 12       | 0.12          |
| (1,1409) | 1:57:A:VAL:HG22  | 1:57:A:VAL:HG13 | 14       | 0.12          |
| (1,1382) | 1:57:A:VAL:HG22  | 1:53:A:PHE:HE1  | 6        | 0.12          |
| (1,1358) | 1:32:A:ALA:HB3   | 1:33:A:GLU:H    | 3        | 0.12          |
| (1,1352) | 1:122:A:ALA:HB2  | 1:122:A:ALA:H   | 4        | 0.12          |
| (1,1352) | 1:122:A:ALA:HB2  | 1:122:A:ALA:H   | 9        | 0.12          |
| (1,1352) | 1:122:A:ALA:HB2  | 1:122:A:ALA:H   | 12       | 0.12          |
| (1,1351) | 1:127:A:GLN:H    | 1:126:A:ALA:HB1 | 5        | 0.12          |
| (1,1303) | 1:97:A:LEU:HD13  | 1:35:A:PHE:HE1  | 13       | 0.12          |
| (1,1285) | 1:48:A:LEU:HD23  | 1:48:A:LEU:HB3  | 2        | 0.12          |
| (1,1275) | 1:84:A:TYR:HE2   | 1:84:A:TYR:HB3  | 5        | 0.12          |
| (1,1275) | 1:84:A:TYR:HE2   | 1:84:A:TYR:HB3  | 9        | 0.12          |
| (1,1275) | 1:84:A:TYR:HE2   | 1:84:A:TYR:HB3  | 11       | 0.12          |
| (1,1273) | 1:45:A:ALA:HB1   | 1:84:A:TYR:HB3  | 16       | 0.12          |
| (1,1247) | 1:42:A:GLU:HB3   | 1:43:A:GLY:HA2  | 6        | 0.12          |
| (1,1247) | 1:42:A:GLU:HB3   | 1:43:A:GLY:HA2  | 12       | 0.12          |
| (1,1240) | 1:78:A:TYR:HE2   | 1:79:A:THR:HB   | 8        | 0.12          |
| (1,1240) | 1:78:A:TYR:HE1   | 1:79:A:THR:HB   | 10       | 0.12          |
| (1,1240) | 1:78:A:TYR:HE1   | 1:79:A:THR:HB   | 12       | 0.12          |
| (1,1240) | 1:78:A:TYR:HE1   | 1:79:A:THR:HB   | 14       | 0.12          |
| (1,1239) | 1:79:A:THR:H     | 1:78:A:TYR:HE2  | 6        | 0.12          |
| (1,1239) | 1:79:A:THR:H     | 1:78:A:TYR:HE1  | 12       | 0.12          |
| (1,1239) | 1:79:A:THR:H     | 1:78:A:TYR:HE1  | 16       | 0.12          |
| (1,1136) | 1:31:A:LEU:HD12  | 1:35:A:PHE:HD1  | 12       | 0.12          |
| (1,1111) | 1:75:A:LEU:HB3   | 1:75:A:LEU:H    | 3        | 0.12          |
| (1,1111) | 1:75:A:LEU:HB3   | 1:75:A:LEU:H    | 5        | 0.12          |
| (1,1111) | 1:75:A:LEU:HB3   | 1:75:A:LEU:H    | 7        | 0.12          |
| (1,1074) | 1:34:A:ARG:HG2   | 1:35:A:PHE:HD2  | 15       | 0.12          |
| (1,1073) | 1:97:A:LEU:HD11  | 1:97:A:LEU:H    | 4        | 0.12          |
| (1,1052) | 1:69:A:THR:HG21  | 1:69:A:THR:HA   | 3        | 0.12          |
| (1,1052) | 1:69:A:THR:HG22  | 1:69:A:THR:HA   | 5        | 0.12          |
| (1,1052) | 1:69:A:THR:HG21  | 1:69:A:THR:HA   | 8        | 0.12          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1047) | 1:124:A:VAL:HA  | 1:124:A:VAL:HG21 | 5        | 0.12          |
| (1,1032) | 1:85:A:LEU:H    | 1:84:A:TYR:HE2   | 14       | 0.12          |
| (1,1009) | 1:37:A:HIS:HD2  | 1:38:A:CYS:HA    | 1        | 0.12          |
| (1,1009) | 1:37:A:HIS:HD2  | 1:38:A:CYS:HA    | 5        | 0.12          |
| (1,1009) | 1:37:A:HIS:HD2  | 1:38:A:CYS:HA    | 9        | 0.12          |
| (1,1004) | 1:82:A:TRP:HA   | 1:86:A:TYR:HD2   | 3        | 0.12          |
| (1,1004) | 1:82:A:TRP:HA   | 1:86:A:TYR:HD1   | 7        | 0.12          |
| (1,1004) | 1:82:A:TRP:HA   | 1:86:A:TYR:HD1   | 9        | 0.12          |
| (1,1004) | 1:82:A:TRP:HA   | 1:86:A:TYR:HD1   | 11       | 0.12          |
| (1,1004) | 1:82:A:TRP:HA   | 1:86:A:TYR:HD2   | 12       | 0.12          |
| (1,1004) | 1:82:A:TRP:HA   | 1:86:A:TYR:HD2   | 17       | 0.12          |
| (1,983)  | 1:55:A:ASP:HB3  | 1:55:A:ASP:HA    | 16       | 0.12          |
| (1,982)  | 1:20:A:LYS:HA   | 1:20:A:LYS:HG2   | 5        | 0.12          |
| (1,959)  | 1:30:A:PHE:HD1  | 1:31:A:LEU:HA    | 12       | 0.12          |
| (1,872)  | 1:56:A:LEU:HB3  | 1:56:A:LEU:HA    | 1        | 0.12          |
| (1,872)  | 1:56:A:LEU:HB3  | 1:56:A:LEU:HA    | 6        | 0.12          |
| (1,872)  | 1:56:A:LEU:HB3  | 1:56:A:LEU:HA    | 10       | 0.12          |
| (1,872)  | 1:56:A:LEU:HB3  | 1:56:A:LEU:HA    | 12       | 0.12          |
| (1,872)  | 1:56:A:LEU:HB3  | 1:56:A:LEU:HA    | 14       | 0.12          |
| (1,872)  | 1:56:A:LEU:HB3  | 1:56:A:LEU:HA    | 17       | 0.12          |
| (1,856)  | 1:13:A:ASP:HB3  | 1:14:A:PRO:HD3   | 17       | 0.12          |
| (1,847)  | 1:49:A:LYS:HB2  | 1:102:A:CYS:HB3  | 8        | 0.12          |
| (1,818)  | 1:28:A:ILE:HD12 | 1:78:A:TYR:HB3   | 4        | 0.12          |
| (1,762)  | 1:65:A:ASN:HA   | 1:66:A:LEU:H     | 15       | 0.12          |
| (1,756)  | 1:93:A:THR:HB   | 1:102:A:CYS:H    | 15       | 0.12          |
| (1,714)  | 1:12:A:GLN:HA   | 1:13:A:ASP:H     | 15       | 0.12          |
| (1,709)  | 1:73:A:SER:HA   | 1:75:A:LEU:H     | 6        | 0.12          |
| (1,709)  | 1:73:A:SER:HA   | 1:75:A:LEU:H     | 14       | 0.12          |
| (1,707)  | 1:75:A:LEU:HB3  | 1:74:A:ALA:H     | 1        | 0.12          |
| (1,707)  | 1:75:A:LEU:HB3  | 1:74:A:ALA:H     | 2        | 0.12          |
| (1,665)  | 1:122:A:ALA:HB2 | 1:123:A:ARG:H    | 1        | 0.12          |
| (1,645)  | 1:115:A:LYS:HE3 | 1:115:A:LYS:H    | 3        | 0.12          |
| (1,645)  | 1:115:A:LYS:HE3 | 1:115:A:LYS:H    | 11       | 0.12          |
| (1,645)  | 1:115:A:LYS:HE3 | 1:115:A:LYS:H    | 12       | 0.12          |
| (1,645)  | 1:115:A:LYS:HE3 | 1:115:A:LYS:H    | 14       | 0.12          |
| (1,645)  | 1:115:A:LYS:HE3 | 1:115:A:LYS:H    | 15       | 0.12          |
| (1,645)  | 1:115:A:LYS:HE3 | 1:115:A:LYS:H    | 16       | 0.12          |
| (1,635)  | 1:127:A:GLN:H   | 1:127:A:GLN:HB3  | 10       | 0.12          |
| (1,630)  | 1:61:A:ALA:HB1  | 1:67:A:SER:H     | 13       | 0.12          |
| (1,609)  | 1:49:A:LYS:HB2  | 1:49:A:LYS:H     | 7        | 0.12          |
| (1,587)  | 1:25:A:LYS:HB2  | 1:26:A:GLU:H     | 3        | 0.12          |
| (1,587)  | 1:25:A:LYS:HB2  | 1:26:A:GLU:H     | 10       | 0.12          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,587) | 1:25:A:LYS:HB2  | 1:26:A:GLU:H    | 17       | 0.12          |
| (1,582) | 1:37:A:HIS:HA   | 1:39:A:PHE:H    | 6        | 0.12          |
| (1,550) | 1:40:A:SER:HA   | 1:42:A:GLU:H    | 11       | 0.12          |
| (1,483) | 1:25:A:LYS:HG3  | 1:25:A:LYS:H    | 3        | 0.12          |
| (1,483) | 1:25:A:LYS:HG3  | 1:25:A:LYS:H    | 4        | 0.12          |
| (1,483) | 1:25:A:LYS:HG3  | 1:25:A:LYS:H    | 6        | 0.12          |
| (1,483) | 1:25:A:LYS:HG3  | 1:25:A:LYS:H    | 7        | 0.12          |
| (1,483) | 1:25:A:LYS:HG3  | 1:25:A:LYS:H    | 9        | 0.12          |
| (1,483) | 1:25:A:LYS:HG3  | 1:25:A:LYS:H    | 10       | 0.12          |
| (1,483) | 1:25:A:LYS:HG3  | 1:25:A:LYS:H    | 11       | 0.12          |
| (1,483) | 1:25:A:LYS:HG3  | 1:25:A:LYS:H    | 13       | 0.12          |
| (1,483) | 1:25:A:LYS:HG3  | 1:25:A:LYS:H    | 15       | 0.12          |
| (1,483) | 1:25:A:LYS:HG3  | 1:25:A:LYS:H    | 16       | 0.12          |
| (1,483) | 1:25:A:LYS:HG3  | 1:25:A:LYS:H    | 17       | 0.12          |
| (1,451) | 1:32:A:ALA:HB2  | 1:35:A:PHE:H    | 2        | 0.12          |
| (1,451) | 1:32:A:ALA:HB2  | 1:35:A:PHE:H    | 13       | 0.12          |
| (1,423) | 1:50:A:ILE:HG21 | 1:50:A:ILE:H    | 11       | 0.12          |
| (1,397) | 1:57:A:VAL:H    | 1:56:A:LEU:HB3  | 11       | 0.12          |
| (1,359) | 1:62:A:GLY:HA3  | 1:63:A:GLU:H    | 2        | 0.12          |
| (1,359) | 1:62:A:GLY:HA3  | 1:63:A:GLU:H    | 4        | 0.12          |
| (1,359) | 1:62:A:GLY:HA3  | 1:63:A:GLU:H    | 8        | 0.12          |
| (1,359) | 1:62:A:GLY:HA3  | 1:63:A:GLU:H    | 13       | 0.12          |
| (1,351) | 1:63:A:GLU:HB3  | 1:65:A:ASN:H    | 6        | 0.12          |
| (1,351) | 1:63:A:GLU:HB3  | 1:65:A:ASN:H    | 13       | 0.12          |
| (1,297) | 1:81:A:SER:HB2  | 1:82:A:TRP:H    | 2        | 0.12          |
| (1,287) | 1:127:A:GLN:H   | 1:127:A:GLN:HG2 | 9        | 0.12          |
| (1,280) | 1:86:A:TYR:H    | 1:86:A:TYR:HB2  | 8        | 0.12          |
| (1,219) | 1:102:A:CYS:H   | 1:100:A:ASN:HB3 | 6        | 0.12          |
| (1,193) | 1:108:A:GLN:HB3 | 1:108:A:GLN:H   | 7        | 0.12          |
| (1,156) | 1:126:A:ALA:HB3 | 1:126:A:ALA:H   | 10       | 0.12          |
| (1,153) | 1:129:A:ALA:HA  | 1:129:A:ALA:H   | 10       | 0.12          |
| (1,152) | 1:128:A:ARG:HB3 | 1:129:A:ALA:H   | 6        | 0.12          |
| (1,128) | 1:35:A:PHE:HD2  | 1:39:A:PHE:H    | 10       | 0.12          |
| (1,128) | 1:35:A:PHE:HD2  | 1:39:A:PHE:H    | 15       | 0.12          |
| (3,149) | 1:82:A:TRP:HE1  | 1:82:A:TRP:HE3  | 3        | 0.11          |
| (3,149) | 1:82:A:TRP:HE1  | 1:82:A:TRP:HE3  | 12       | 0.11          |
| (3,149) | 1:82:A:TRP:HE1  | 1:86:A:TYR:HD1  | 13       | 0.11          |
| (3,149) | 1:82:A:TRP:HE1  | 1:82:A:TRP:HE3  | 15       | 0.11          |
| (3,122) | 1:27:A:VAL:HG23 | 1:28:A:ILE:HD11 | 8        | 0.11          |
| (3,122) | 1:27:A:VAL:HG23 | 1:28:A:ILE:HD13 | 16       | 0.11          |
| (3,103) | 1:123:A:ARG:HG2 | 1:123:A:ARG:HA  | 5        | 0.11          |
| (3,92)  | 1:88:A:VAL:HG23 | 1:87:A:GLY:HA2  | 10       | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,92)   | 1:88:A:VAL:HG21 | 1:87:A:GLY:HA2  | 17       | 0.11          |
| (3,90)   | 1:115:A:LYS:HG3 | 1:116:A:GLN:HG3 | 10       | 0.11          |
| (3,90)   | 1:115:A:LYS:HG3 | 1:116:A:GLN:HG3 | 15       | 0.11          |
| (3,90)   | 1:115:A:LYS:HG3 | 1:116:A:GLN:HG3 | 17       | 0.11          |
| (3,81)   | 1:74:A:ALA:HA   | 1:77:A:LEU:HD13 | 11       | 0.11          |
| (3,48)   | 1:72:A:ARG:HD3  | 1:72:A:ARG:HB3  | 3        | 0.11          |
| (3,48)   | 1:72:A:ARG:HD3  | 1:72:A:ARG:HB3  | 4        | 0.11          |
| (3,48)   | 1:72:A:ARG:HD3  | 1:72:A:ARG:HB3  | 6        | 0.11          |
| (3,48)   | 1:72:A:ARG:HD3  | 1:72:A:ARG:HB3  | 10       | 0.11          |
| (3,48)   | 1:72:A:ARG:HD3  | 1:72:A:ARG:HB3  | 13       | 0.11          |
| (3,48)   | 1:72:A:ARG:HD3  | 1:72:A:ARG:HB3  | 15       | 0.11          |
| (3,38)   | 1:32:A:ALA:HB3  | 1:33:A:GLU:HG2  | 5        | 0.11          |
| (3,34)   | 1:97:A:LEU:HD21 | 1:31:A:LEU:HD13 | 11       | 0.11          |
| (3,29)   | 1:48:A:LEU:HD22 | 1:39:A:PHE:HD2  | 14       | 0.11          |
| (3,22)   | 1:48:A:LEU:HD13 | 1:97:A:LEU:H    | 4        | 0.11          |
| (1,4344) | 1:120:A:ALA:H   | 1:119:A:GLU:HG2 | 7        | 0.11          |
| (1,4339) | 1:116:A:GLN:HG3 | 1:115:A:LYS:H   | 4        | 0.11          |
| (1,4339) | 1:116:A:GLN:HG3 | 1:115:A:LYS:H   | 7        | 0.11          |
| (1,4339) | 1:116:A:GLN:HG3 | 1:115:A:LYS:H   | 8        | 0.11          |
| (1,4339) | 1:116:A:GLN:HG3 | 1:115:A:LYS:H   | 9        | 0.11          |
| (1,4339) | 1:116:A:GLN:HG3 | 1:115:A:LYS:H   | 11       | 0.11          |
| (1,4339) | 1:116:A:GLN:HG3 | 1:115:A:LYS:H   | 15       | 0.11          |
| (1,4339) | 1:116:A:GLN:HG3 | 1:115:A:LYS:H   | 16       | 0.11          |
| (1,4331) | 1:104:A:GLU:HG2 | 1:104:A:GLU:H   | 1        | 0.11          |
| (1,4331) | 1:104:A:GLU:HG2 | 1:104:A:GLU:H   | 2        | 0.11          |
| (1,4331) | 1:104:A:GLU:HG2 | 1:104:A:GLU:H   | 3        | 0.11          |
| (1,4331) | 1:104:A:GLU:HG2 | 1:104:A:GLU:H   | 5        | 0.11          |
| (1,4331) | 1:104:A:GLU:HG2 | 1:104:A:GLU:H   | 9        | 0.11          |
| (1,4331) | 1:104:A:GLU:HG2 | 1:104:A:GLU:H   | 11       | 0.11          |
| (1,4331) | 1:104:A:GLU:HG2 | 1:104:A:GLU:H   | 13       | 0.11          |
| (1,4331) | 1:104:A:GLU:HG2 | 1:104:A:GLU:H   | 15       | 0.11          |
| (1,4326) | 1:65:A:ASN:HA   | 1:66:A:LEU:H    | 16       | 0.11          |
| (1,4320) | 1:62:A:GLY:H    | 1:66:A:LEU:H    | 11       | 0.11          |
| (1,4295) | 1:116:A:GLN:HA  | 1:117:A:LEU:H   | 5        | 0.11          |
| (1,4295) | 1:116:A:GLN:HA  | 1:117:A:LEU:H   | 9        | 0.11          |
| (1,4295) | 1:116:A:GLN:HA  | 1:117:A:LEU:H   | 13       | 0.11          |
| (1,4287) | 1:84:A:TYR:H    | 1:82:A:TRP:HB2  | 16       | 0.11          |
| (1,4281) | 1:118:A:GLU:HA  | 1:119:A:GLU:H   | 8        | 0.11          |
| (1,4281) | 1:118:A:GLU:HA  | 1:119:A:GLU:H   | 13       | 0.11          |
| (1,4273) | 1:73:A:SER:HA   | 1:75:A:LEU:H    | 4        | 0.11          |
| (1,4271) | 1:78:A:TYR:HE2  | 1:75:A:LEU:H    | 13       | 0.11          |
| (1,4271) | 1:78:A:TYR:HE1  | 1:75:A:LEU:H    | 14       | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,4271) | 1:78:A:TYR:HE1  | 1:75:A:LEU:H    | 15       | 0.11          |
| (1,4270) | 1:75:A:LEU:HB3  | 1:74:A:ALA:H    | 11       | 0.11          |
| (1,4258) | 1:52:A:ILE:HG12 | 1:56:A:LEU:H    | 4        | 0.11          |
| (1,4258) | 1:52:A:ILE:HG12 | 1:56:A:LEU:H    | 6        | 0.11          |
| (1,4258) | 1:52:A:ILE:HG12 | 1:56:A:LEU:H    | 13       | 0.11          |
| (1,4258) | 1:52:A:ILE:HG12 | 1:56:A:LEU:H    | 14       | 0.11          |
| (1,4238) | 1:97:A:LEU:H    | 1:96:A:ASP:H    | 2        | 0.11          |
| (1,4238) | 1:97:A:LEU:H    | 1:96:A:ASP:H    | 14       | 0.11          |
| (1,4223) | 1:123:A:ARG:H   | 1:125:A:GLN:HG3 | 16       | 0.11          |
| (1,4212) | 1:115:A:LYS:HE3 | 1:115:A:LYS:H   | 13       | 0.11          |
| (1,4203) | 1:106:A:ASP:HB2 | 1:109:A:HIS:H   | 1        | 0.11          |
| (1,4203) | 1:106:A:ASP:HB2 | 1:109:A:HIS:H   | 13       | 0.11          |
| (1,4203) | 1:106:A:ASP:HB2 | 1:109:A:HIS:H   | 17       | 0.11          |
| (1,4202) | 1:127:A:GLN:H   | 1:127:A:GLN:HB3 | 9        | 0.11          |
| (1,4202) | 1:127:A:GLN:H   | 1:127:A:GLN:HB3 | 11       | 0.11          |
| (1,4198) | 1:127:A:GLN:HA  | 1:127:A:GLN:H   | 2        | 0.11          |
| (1,4198) | 1:127:A:GLN:HA  | 1:127:A:GLN:H   | 11       | 0.11          |
| (1,4194) | 1:107:A:GLU:H   | 1:106:A:ASP:HA  | 5        | 0.11          |
| (1,4194) | 1:107:A:GLU:H   | 1:106:A:ASP:HA  | 12       | 0.11          |
| (1,4194) | 1:107:A:GLU:H   | 1:106:A:ASP:HA  | 15       | 0.11          |
| (1,4170) | 1:49:A:LYS:HB2  | 1:49:A:LYS:H    | 17       | 0.11          |
| (1,4165) | 1:40:A:SER:HA   | 1:43:A:GLY:H    | 7        | 0.11          |
| (1,4151) | 1:18:A:GLN:HG2  | 1:18:A:GLN:H    | 9        | 0.11          |
| (1,4148) | 1:25:A:LYS:HB2  | 1:26:A:GLU:H    | 14       | 0.11          |
| (1,4143) | 1:37:A:HIS:HA   | 1:39:A:PHE:H    | 14       | 0.11          |
| (1,4119) | 1:66:A:LEU:HB2  | 1:70:A:GLN:HE22 | 1        | 0.11          |
| (1,4110) | 1:40:A:SER:HA   | 1:42:A:GLU:H    | 1        | 0.11          |
| (1,4110) | 1:40:A:SER:HA   | 1:42:A:GLU:H    | 13       | 0.11          |
| (1,4106) | 1:99:A:GLY:HA3  | 1:98:A:ASP:H    | 3        | 0.11          |
| (1,4106) | 1:99:A:GLY:HA3  | 1:98:A:ASP:H    | 11       | 0.11          |
| (1,4084) | 1:20:A:LYS:HB3  | 1:22:A:ASN:HD22 | 1        | 0.11          |
| (1,4063) | 1:37:A:HIS:HB2  | 1:37:A:HIS:H    | 3        | 0.11          |
| (1,4060) | 1:97:A:LEU:HD21 | 1:39:A:PHE:H    | 5        | 0.11          |
| (1,4060) | 1:97:A:LEU:HD22 | 1:39:A:PHE:H    | 9        | 0.11          |
| (1,4060) | 1:97:A:LEU:HD21 | 1:39:A:PHE:H    | 10       | 0.11          |
| (1,4060) | 1:97:A:LEU:HD23 | 1:39:A:PHE:H    | 16       | 0.11          |
| (1,4060) | 1:97:A:LEU:HD21 | 1:39:A:PHE:H    | 17       | 0.11          |
| (1,4041) | 1:21:A:LEU:HA   | 1:23:A:SER:H    | 15       | 0.11          |
| (1,4004) | 1:42:A:GLU:HB3  | 1:42:A:GLU:H    | 2        | 0.11          |
| (1,3991) | 1:85:A:LEU:H    | 1:84:A:TYR:HA   | 2        | 0.11          |
| (1,3991) | 1:85:A:LEU:H    | 1:84:A:TYR:HA   | 5        | 0.11          |
| (1,3991) | 1:85:A:LEU:H    | 1:84:A:TYR:HA   | 7        | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3991) | 1:85:A:LEU:H    | 1:84:A:TYR:HA   | 17       | 0.11          |
| (1,3979) | 1:50:A:ILE:HA   | 1:51:A:GLY:H    | 11       | 0.11          |
| (1,3976) | 1:52:A:ILE:H    | 1:49:A:LYS:HB3  | 7        | 0.11          |
| (1,3956) | 1:58:A:ASP:H    | 1:54:A:GLN:HA   | 1        | 0.11          |
| (1,3941) | 1:63:A:GLU:H    | 1:61:A:ALA:HB2  | 9        | 0.11          |
| (1,3941) | 1:63:A:GLU:H    | 1:61:A:ALA:HB2  | 16       | 0.11          |
| (1,3931) | 1:67:A:SER:H    | 1:66:A:LEU:H    | 11       | 0.11          |
| (1,3911) | 1:71:A:LEU:HD22 | 1:75:A:LEU:H    | 17       | 0.11          |
| (1,3907) | 1:76:A:ARG:HD2  | 1:77:A:LEU:H    | 13       | 0.11          |
| (1,3898) | 1:79:A:THR:HG21 | 1:80:A:SER:H    | 1        | 0.11          |
| (1,3884) | 1:83:A:ARG:H    | 1:83:A:ARG:HB2  | 5        | 0.11          |
| (1,3880) | 1:83:A:ARG:HB3  | 1:84:A:TYR:H    | 9        | 0.11          |
| (1,3879) | 1:127:A:GLN:H   | 1:127:A:GLN:HG2 | 3        | 0.11          |
| (1,3879) | 1:127:A:GLN:H   | 1:127:A:GLN:HG2 | 4        | 0.11          |
| (1,3879) | 1:127:A:GLN:H   | 1:127:A:GLN:HG2 | 5        | 0.11          |
| (1,3879) | 1:127:A:GLN:H   | 1:127:A:GLN:HG2 | 12       | 0.11          |
| (1,3859) | 1:90:A:PRO:HB2  | 1:91:A:GLY:H    | 2        | 0.11          |
| (1,3859) | 1:90:A:PRO:HB2  | 1:91:A:GLY:H    | 3        | 0.11          |
| (1,3859) | 1:90:A:PRO:HB2  | 1:91:A:GLY:H    | 9        | 0.11          |
| (1,3859) | 1:90:A:PRO:HB2  | 1:91:A:GLY:H    | 16       | 0.11          |
| (1,3859) | 1:90:A:PRO:HB2  | 1:91:A:GLY:H    | 17       | 0.11          |
| (1,3824) | 1:102:A:CYS:H   | 1:100:A:ASN:HB3 | 4        | 0.11          |
| (1,3824) | 1:102:A:CYS:H   | 1:100:A:ASN:HB3 | 8        | 0.11          |
| (1,3824) | 1:102:A:CYS:H   | 1:100:A:ASN:HB3 | 14       | 0.11          |
| (1,3803) | 1:108:A:GLN:HB3 | 1:108:A:GLN:H   | 10       | 0.11          |
| (1,3801) | 1:108:A:GLN:HA  | 1:108:A:GLN:H   | 3        | 0.11          |
| (1,3801) | 1:108:A:GLN:HA  | 1:108:A:GLN:H   | 4        | 0.11          |
| (1,3801) | 1:108:A:GLN:HA  | 1:108:A:GLN:H   | 6        | 0.11          |
| (1,3801) | 1:108:A:GLN:HA  | 1:108:A:GLN:H   | 9        | 0.11          |
| (1,3801) | 1:108:A:GLN:HA  | 1:108:A:GLN:H   | 11       | 0.11          |
| (1,3801) | 1:108:A:GLN:HA  | 1:108:A:GLN:H   | 12       | 0.11          |
| (1,3801) | 1:108:A:GLN:HA  | 1:108:A:GLN:H   | 16       | 0.11          |
| (1,3801) | 1:108:A:GLN:HA  | 1:108:A:GLN:H   | 17       | 0.11          |
| (1,3797) | 1:44:A:GLU:HA   | 1:44:A:GLU:H    | 12       | 0.11          |
| (1,3786) | 1:27:A:VAL:HG13 | 1:21:A:LEU:H    | 17       | 0.11          |
| (1,3783) | 1:117:A:LEU:HB3 | 1:117:A:LEU:H   | 14       | 0.11          |
| (1,3783) | 1:117:A:LEU:HB3 | 1:117:A:LEU:H   | 16       | 0.11          |
| (1,3779) | 1:121:A:LYS:HB2 | 1:120:A:ALA:H   | 2        | 0.11          |
| (1,3779) | 1:121:A:LYS:HB2 | 1:120:A:ALA:H   | 11       | 0.11          |
| (1,3767) | 1:129:A:ALA:HA  | 1:129:A:ALA:H   | 9        | 0.11          |
| (1,3766) | 1:128:A:ARG:HB3 | 1:129:A:ALA:H   | 11       | 0.11          |
| (1,3757) | 1:116:A:GLN:H   | 1:117:A:LEU:H   | 2        | 0.11          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3757) | 1:116:A:GLN:H   | 1:117:A:LEU:H    | 16       | 0.11          |
| (1,3744) | 1:35:A:PHE:HD1  | 1:39:A:PHE:H     | 16       | 0.11          |
| (1,3736) | 1:41:A:ALA:HA   | 1:29:A:ALA:H     | 8        | 0.11          |
| (1,3736) | 1:41:A:ALA:HA   | 1:29:A:ALA:H     | 10       | 0.11          |
| (1,3736) | 1:41:A:ALA:HA   | 1:29:A:ALA:H     | 16       | 0.11          |
| (1,3733) | 1:27:A:VAL:HG12 | 1:26:A:GLU:H     | 2        | 0.11          |
| (1,3699) | 1:88:A:VAL:HA   | 1:89:A:LYS:H     | 11       | 0.11          |
| (1,3685) | 1:81:A:SER:H    | 1:84:A:TYR:H     | 2        | 0.11          |
| (1,3685) | 1:81:A:SER:H    | 1:84:A:TYR:H     | 17       | 0.11          |
| (1,3667) | 1:37:A:HIS:H    | 1:37:A:HIS:HD2   | 12       | 0.11          |
| (1,3647) | 1:59:A:ARG:H    | 1:61:A:ALA:H     | 16       | 0.11          |
| (1,3568) | 1:105:A:LEU:HB3 | 1:109:A:HIS:HB2  | 2        | 0.11          |
| (1,3568) | 1:105:A:LEU:HB3 | 1:109:A:HIS:HB2  | 4        | 0.11          |
| (1,3568) | 1:105:A:LEU:HB3 | 1:109:A:HIS:HB2  | 15       | 0.11          |
| (1,3542) | 1:105:A:LEU:HB3 | 1:101:A:PRO:HB3  | 7        | 0.11          |
| (1,3542) | 1:105:A:LEU:HB3 | 1:101:A:PRO:HB3  | 10       | 0.11          |
| (1,3537) | 1:51:A:GLY:HA2  | 1:54:A:GLN:HB2   | 1        | 0.11          |
| (1,3523) | 1:56:A:LEU:HG   | 1:56:A:LEU:HB3   | 3        | 0.11          |
| (1,3523) | 1:56:A:LEU:HG   | 1:56:A:LEU:HB3   | 4        | 0.11          |
| (1,3523) | 1:56:A:LEU:HG   | 1:56:A:LEU:HB3   | 6        | 0.11          |
| (1,3523) | 1:56:A:LEU:HG   | 1:56:A:LEU:HB3   | 7        | 0.11          |
| (1,3523) | 1:56:A:LEU:HG   | 1:56:A:LEU:HB3   | 9        | 0.11          |
| (1,3523) | 1:56:A:LEU:HG   | 1:56:A:LEU:HB3   | 11       | 0.11          |
| (1,3519) | 1:65:A:ASN:H    | 1:65:A:ASN:HB3   | 13       | 0.11          |
| (1,3516) | 1:21:A:LEU:HG   | 1:65:A:ASN:HB3   | 4        | 0.11          |
| (1,3511) | 1:50:A:ILE:HG13 | 1:49:A:LYS:HA    | 10       | 0.11          |
| (1,3510) | 1:64:A:MET:HE1  | 1:21:A:LEU:H     | 16       | 0.11          |
| (1,3502) | 1:27:A:VAL:HG21 | 1:27:A:VAL:H     | 6        | 0.11          |
| (1,3502) | 1:27:A:VAL:HG23 | 1:27:A:VAL:H     | 13       | 0.11          |
| (1,3500) | 1:27:A:VAL:HG23 | 1:31:A:LEU:HD12  | 15       | 0.11          |
| (1,3477) | 1:15:A:MET:HG3  | 1:15:A:MET:HB2   | 14       | 0.11          |
| (1,3477) | 1:15:A:MET:HG3  | 1:15:A:MET:HB2   | 16       | 0.11          |
| (1,3460) | 1:36:A:PRO:HB2  | 1:36:A:PRO:HD2   | 6        | 0.11          |
| (1,3457) | 1:20:A:LYS:HE3  | 1:19:A:PRO:HA    | 8        | 0.11          |
| (1,3457) | 1:20:A:LYS:HE3  | 1:19:A:PRO:HA    | 9        | 0.11          |
| (1,3448) | 1:20:A:LYS:H    | 1:20:A:LYS:HG2   | 2        | 0.11          |
| (1,3443) | 1:123:A:ARG:HG2 | 1:123:A:ARG:HD3  | 3        | 0.11          |
| (1,3443) | 1:123:A:ARG:HG2 | 1:123:A:ARG:HD3  | 15       | 0.11          |
| (1,3443) | 1:123:A:ARG:HG2 | 1:123:A:ARG:HD3  | 17       | 0.11          |
| (1,3424) | 1:118:A:GLU:HA  | 1:122:A:ALA:H    | 13       | 0.11          |
| (1,3415) | 1:117:A:LEU:HA  | 1:117:A:LEU:HD12 | 10       | 0.11          |
| (1,3414) | 1:86:A:TYR:H    | 1:117:A:LEU:HD11 | 8        | 0.11          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3372) | 1:88:A:VAL:HA    | 1:47:A:PRO:HB3  | 3        | 0.11          |
| (1,3372) | 1:88:A:VAL:HA    | 1:47:A:PRO:HB3  | 8        | 0.11          |
| (1,3372) | 1:88:A:VAL:HA    | 1:47:A:PRO:HB3  | 10       | 0.11          |
| (1,3370) | 1:24:A:SER:HA    | 1:27:A:VAL:HG13 | 1        | 0.11          |
| (1,3370) | 1:24:A:SER:HA    | 1:27:A:VAL:HG12 | 15       | 0.11          |
| (1,3369) | 1:24:A:SER:HA    | 1:27:A:VAL:HG23 | 13       | 0.11          |
| (1,3348) | 1:79:A:THR:HG22  | 1:84:A:TYR:HE2  | 1        | 0.11          |
| (1,3315) | 1:66:A:LEU:HD12  | 1:66:A:LEU:HA   | 12       | 0.11          |
| (1,3314) | 1:71:A:LEU:HD13  | 1:71:A:LEU:HG   | 9        | 0.11          |
| (1,3314) | 1:71:A:LEU:HD13  | 1:71:A:LEU:HG   | 13       | 0.11          |
| (1,3299) | 1:20:A:LYS:H     | 1:20:A:LYS:HD3  | 5        | 0.11          |
| (1,3291) | 1:72:A:ARG:HB3   | 1:53:A:PHE:HE1  | 4        | 0.11          |
| (1,3291) | 1:72:A:ARG:HB3   | 1:53:A:PHE:HE2  | 9        | 0.11          |
| (1,3275) | 1:119:A:GLU:HA   | 1:119:A:GLU:HG2 | 3        | 0.11          |
| (1,3275) | 1:119:A:GLU:HA   | 1:119:A:GLU:HG2 | 14       | 0.11          |
| (1,3275) | 1:119:A:GLU:HA   | 1:119:A:GLU:HG2 | 15       | 0.11          |
| (1,3273) | 1:42:A:GLU:HG2   | 1:43:A:GLY:H    | 14       | 0.11          |
| (1,3270) | 1:42:A:GLU:HG2   | 1:41:A:ALA:HB2  | 3        | 0.11          |
| (1,3270) | 1:42:A:GLU:HG2   | 1:41:A:ALA:HB1  | 16       | 0.11          |
| (1,3269) | 1:33:A:GLU:HB3   | 1:17:A:ASN:HB2  | 1        | 0.11          |
| (1,3269) | 1:33:A:GLU:HB3   | 1:17:A:ASN:HB2  | 10       | 0.11          |
| (1,3263) | 1:121:A:LYS:HG2  | 1:122:A:ALA:H   | 2        | 0.11          |
| (1,3263) | 1:121:A:LYS:HG2  | 1:122:A:ALA:H   | 3        | 0.11          |
| (1,3263) | 1:121:A:LYS:HG2  | 1:122:A:ALA:H   | 5        | 0.11          |
| (1,3263) | 1:121:A:LYS:HG2  | 1:122:A:ALA:H   | 10       | 0.11          |
| (1,3263) | 1:121:A:LYS:HG2  | 1:122:A:ALA:H   | 12       | 0.11          |
| (1,3263) | 1:121:A:LYS:HG2  | 1:122:A:ALA:H   | 14       | 0.11          |
| (1,3263) | 1:121:A:LYS:HG2  | 1:122:A:ALA:H   | 17       | 0.11          |
| (1,3244) | 1:78:A:TYR:HA    | 1:28:A:ILE:HG12 | 16       | 0.11          |
| (1,3241) | 1:52:A:ILE:HG13  | 1:97:A:LEU:HD22 | 1        | 0.11          |
| (1,3240) | 1:52:A:ILE:HG13  | 1:48:A:LEU:HD12 | 7        | 0.11          |
| (1,3208) | 1:124:A:VAL:HG12 | 1:124:A:VAL:HA  | 13       | 0.11          |
| (1,3200) | 1:116:A:GLN:HG3  | 1:113:A:ALA:HB2 | 13       | 0.11          |
| (1,3200) | 1:116:A:GLN:HG3  | 1:113:A:ALA:HB3 | 16       | 0.11          |
| (1,3172) | 1:25:A:LYS:HE3   | 1:25:A:LYS:HA   | 3        | 0.11          |
| (1,3172) | 1:25:A:LYS:HE3   | 1:25:A:LYS:HA   | 13       | 0.11          |
| (1,3172) | 1:25:A:LYS:HE3   | 1:25:A:LYS:HA   | 16       | 0.11          |
| (1,3169) | 1:53:A:PHE:HB3   | 1:75:A:LEU:HD23 | 6        | 0.11          |
| (1,3164) | 1:120:A:ALA:HB1  | 1:120:A:ALA:H   | 14       | 0.11          |
| (1,3162) | 1:120:A:ALA:HB3  | 1:121:A:LYS:H   | 2        | 0.11          |
| (1,3147) | 1:23:A:SER:HB2   | 1:70:A:GLN:HB3  | 2        | 0.11          |
| (1,3147) | 1:23:A:SER:HB2   | 1:70:A:GLN:HB3  | 4        | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3147) | 1:23:A:SER:HB2  | 1:70:A:GLN:HB3  | 13       | 0.11          |
| (1,3134) | 1:15:A:MET:HB2  | 1:15:A:MET:HG2  | 10       | 0.11          |
| (1,3113) | 1:57:A:VAL:HG12 | 1:61:A:ALA:H    | 1        | 0.11          |
| (1,3108) | 1:102:A:CYS:H   | 1:101:A:PRO:HB3 | 2        | 0.11          |
| (1,3108) | 1:102:A:CYS:H   | 1:101:A:PRO:HB3 | 6        | 0.11          |
| (1,3108) | 1:102:A:CYS:H   | 1:101:A:PRO:HB3 | 7        | 0.11          |
| (1,3108) | 1:102:A:CYS:H   | 1:101:A:PRO:HB3 | 10       | 0.11          |
| (1,3108) | 1:102:A:CYS:H   | 1:101:A:PRO:HB3 | 11       | 0.11          |
| (1,3108) | 1:102:A:CYS:H   | 1:101:A:PRO:HB3 | 14       | 0.11          |
| (1,3108) | 1:102:A:CYS:H   | 1:101:A:PRO:HB3 | 15       | 0.11          |
| (1,3087) | 1:56:A:LEU:HG   | 1:56:A:LEU:HA   | 8        | 0.11          |
| (1,3059) | 1:28:A:ILE:HB   | 1:28:A:ILE:HG23 | 13       | 0.11          |
| (1,3059) | 1:28:A:ILE:HB   | 1:28:A:ILE:HG23 | 15       | 0.11          |
| (1,3040) | 1:52:A:ILE:HA   | 1:52:A:ILE:HG12 | 12       | 0.11          |
| (1,3035) | 1:25:A:LYS:H    | 1:25:A:LYS:HG2  | 4        | 0.11          |
| (1,3035) | 1:25:A:LYS:H    | 1:25:A:LYS:HG2  | 9        | 0.11          |
| (1,3035) | 1:25:A:LYS:H    | 1:25:A:LYS:HG2  | 11       | 0.11          |
| (1,3035) | 1:25:A:LYS:H    | 1:25:A:LYS:HG2  | 12       | 0.11          |
| (1,3035) | 1:25:A:LYS:H    | 1:25:A:LYS:HG2  | 13       | 0.11          |
| (1,3035) | 1:25:A:LYS:H    | 1:25:A:LYS:HG2  | 15       | 0.11          |
| (1,3031) | 1:25:A:LYS:HG3  | 1:25:A:LYS:HD2  | 3        | 0.11          |
| (1,3029) | 1:25:A:LYS:HG3  | 1:26:A:GLU:HA   | 4        | 0.11          |
| (1,3029) | 1:25:A:LYS:HG3  | 1:26:A:GLU:HA   | 6        | 0.11          |
| (1,3029) | 1:25:A:LYS:HG3  | 1:26:A:GLU:HA   | 11       | 0.11          |
| (1,3029) | 1:25:A:LYS:HG3  | 1:26:A:GLU:HA   | 13       | 0.11          |
| (1,3029) | 1:25:A:LYS:HG3  | 1:26:A:GLU:HA   | 15       | 0.11          |
| (1,3029) | 1:25:A:LYS:HG3  | 1:26:A:GLU:HA   | 16       | 0.11          |
| (1,3021) | 1:64:A:MET:HE2  | 1:63:A:GLU:H    | 16       | 0.11          |
| (1,2988) | 1:68:A:LYS:HB2  | 1:68:A:LYS:H    | 3        | 0.11          |
| (1,2986) | 1:115:A:LYS:HB3 | 1:115:A:LYS:H   | 10       | 0.11          |
| (1,2986) | 1:115:A:LYS:HB3 | 1:115:A:LYS:H   | 16       | 0.11          |
| (1,2978) | 1:105:A:LEU:H   | 1:101:A:PRO:HD3 | 1        | 0.11          |
| (1,2978) | 1:105:A:LEU:H   | 1:101:A:PRO:HD3 | 2        | 0.11          |
| (1,2978) | 1:105:A:LEU:H   | 1:101:A:PRO:HD3 | 5        | 0.11          |
| (1,2978) | 1:105:A:LEU:H   | 1:101:A:PRO:HD3 | 6        | 0.11          |
| (1,2978) | 1:105:A:LEU:H   | 1:101:A:PRO:HD3 | 9        | 0.11          |
| (1,2978) | 1:105:A:LEU:H   | 1:101:A:PRO:HD3 | 10       | 0.11          |
| (1,2978) | 1:105:A:LEU:H   | 1:101:A:PRO:HD3 | 13       | 0.11          |
| (1,2978) | 1:105:A:LEU:H   | 1:101:A:PRO:HD3 | 15       | 0.11          |
| (1,2978) | 1:105:A:LEU:H   | 1:101:A:PRO:HD3 | 17       | 0.11          |
| (1,2955) | 1:74:A:ALA:HB3  | 1:75:A:LEU:HD11 | 9        | 0.11          |
| (1,2955) | 1:74:A:ALA:HB2  | 1:75:A:LEU:HD13 | 12       | 0.11          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2949) | 1:39:A:PHE:HZ    | 1:75:A:LEU:HD12 | 1        | 0.11          |
| (1,2949) | 1:39:A:PHE:HZ    | 1:75:A:LEU:HD13 | 8        | 0.11          |
| (1,2949) | 1:39:A:PHE:HZ    | 1:75:A:LEU:HD12 | 9        | 0.11          |
| (1,2949) | 1:39:A:PHE:HZ    | 1:75:A:LEU:HD11 | 10       | 0.11          |
| (1,2943) | 1:110:A:VAL:HG21 | 1:108:A:GLN:H   | 3        | 0.11          |
| (1,2932) | 1:95:A:VAL:HG21  | 1:95:A:VAL:H    | 12       | 0.11          |
| (1,2930) | 1:31:A:LEU:HD21  | 1:60:A:VAL:HG12 | 4        | 0.11          |
| (1,2930) | 1:31:A:LEU:HD22  | 1:60:A:VAL:HG12 | 9        | 0.11          |
| (1,2915) | 1:38:A:CYS:HB2   | 1:39:A:PHE:HE1  | 8        | 0.11          |
| (1,2899) | 1:28:A:ILE:HD11  | 1:75:A:LEU:H    | 2        | 0.11          |
| (1,2881) | 1:74:A:ALA:HB2   | 1:31:A:LEU:HD13 | 17       | 0.11          |
| (1,2875) | 1:122:A:ALA:HB3  | 1:122:A:ALA:H   | 7        | 0.11          |
| (1,2875) | 1:122:A:ALA:HB2  | 1:122:A:ALA:H   | 8        | 0.11          |
| (1,2871) | 1:129:A:ALA:HB2  | 1:129:A:ALA:H   | 4        | 0.11          |
| (1,2871) | 1:129:A:ALA:HB2  | 1:129:A:ALA:H   | 12       | 0.11          |
| (1,2871) | 1:129:A:ALA:HB2  | 1:129:A:ALA:H   | 16       | 0.11          |
| (1,2859) | 1:86:A:TYR:HE1   | 1:85:A:LEU:H    | 13       | 0.11          |
| (1,2849) | 1:73:A:SER:HB3   | 1:74:A:ALA:H    | 9        | 0.11          |
| (1,2846) | 1:53:A:PHE:HE1   | 1:75:A:LEU:HB3  | 1        | 0.11          |
| (1,2846) | 1:53:A:PHE:HE2   | 1:75:A:LEU:HB3  | 3        | 0.11          |
| (1,2846) | 1:53:A:PHE:HE1   | 1:75:A:LEU:HB3  | 5        | 0.11          |
| (1,2836) | 1:95:A:VAL:HG22  | 1:97:A:LEU:HD21 | 12       | 0.11          |
| (1,2811) | 1:97:A:LEU:HD12  | 1:97:A:LEU:HB3  | 7        | 0.11          |
| (1,2786) | 1:82:A:TRP:HH2   | 1:82:A:TRP:HE1  | 14       | 0.11          |
| (1,2775) | 1:47:A:PRO:HB3   | 1:87:A:GLY:HA2  | 12       | 0.11          |
| (1,2774) | 1:91:A:GLY:HA3   | 1:90:A:PRO:HB2  | 7        | 0.11          |
| (1,2774) | 1:91:A:GLY:HA3   | 1:90:A:PRO:HB2  | 13       | 0.11          |
| (1,2774) | 1:91:A:GLY:HA3   | 1:90:A:PRO:HB2  | 15       | 0.11          |
| (1,2774) | 1:91:A:GLY:HA3   | 1:90:A:PRO:HB2  | 17       | 0.11          |
| (1,2744) | 1:13:A:ASP:HB2   | 1:16:A:GLU:H    | 8        | 0.11          |
| (1,2744) | 1:13:A:ASP:HB2   | 1:16:A:GLU:H    | 17       | 0.11          |
| (1,2743) | 1:34:A:ARG:HD3   | 1:30:A:PHE:HD2  | 16       | 0.11          |
| (1,2719) | 1:117:A:LEU:HD13 | 1:86:A:TYR:HB2  | 3        | 0.11          |
| (1,2707) | 1:35:A:PHE:HB2   | 1:97:A:LEU:HD22 | 7        | 0.11          |
| (1,2689) | 1:34:A:ARG:HB3   | 1:30:A:PHE:HD1  | 9        | 0.11          |
| (1,2665) | 1:86:A:TYR:HE1   | 1:86:A:TYR:HB3  | 1        | 0.11          |
| (1,2665) | 1:86:A:TYR:HE2   | 1:86:A:TYR:HB3  | 13       | 0.11          |
| (1,2627) | 1:112:A:HIS:HA   | 1:112:A:HIS:HB2 | 14       | 0.11          |
| (1,2613) | 1:34:A:ARG:HG2   | 1:35:A:PHE:HD1  | 13       | 0.11          |
| (1,2612) | 1:30:A:PHE:HD1   | 1:34:A:ARG:HG2  | 4        | 0.11          |
| (1,2587) | 1:68:A:LYS:HB2   | 1:69:A:THR:HG22 | 12       | 0.11          |
| (1,2587) | 1:68:A:LYS:HB2   | 1:69:A:THR:HG21 | 13       | 0.11          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2586) | 1:93:A:THR:HG23 | 1:102:A:CYS:HA   | 1        | 0.11          |
| (1,2583) | 1:60:A:VAL:HG11 | 1:34:A:ARG:HG2   | 16       | 0.11          |
| (1,2569) | 1:82:A:TRP:HZ2  | 1:124:A:VAL:HG22 | 14       | 0.11          |
| (1,2569) | 1:82:A:TRP:HZ2  | 1:124:A:VAL:HG23 | 16       | 0.11          |
| (1,2561) | 1:85:A:LEU:H    | 1:84:A:TYR:HE1   | 17       | 0.11          |
| (1,2519) | 1:55:A:ASP:HB3  | 1:55:A:ASP:HA    | 12       | 0.11          |
| (1,2516) | 1:132:A:GLN:HG2 | 1:132:A:GLN:HA   | 15       | 0.11          |
| (1,2501) | 1:42:A:GLU:HA   | 1:42:A:GLU:HB3   | 16       | 0.11          |
| (1,2436) | 1:13:A:ASP:HB3  | 1:33:A:GLU:HB3   | 5        | 0.11          |
| (1,2435) | 1:33:A:GLU:HB3  | 1:13:A:ASP:HB2   | 3        | 0.11          |
| (1,2417) | 1:129:A:ALA:HB1 | 1:127:A:GLN:HB3  | 2        | 0.11          |
| (1,2417) | 1:129:A:ALA:HB1 | 1:127:A:GLN:HB3  | 3        | 0.11          |
| (1,2318) | 1:108:A:GLN:HA  | 1:108:A:GLN:HB3  | 1        | 0.11          |
| (1,2318) | 1:108:A:GLN:HA  | 1:108:A:GLN:HB3  | 2        | 0.11          |
| (1,2318) | 1:108:A:GLN:HA  | 1:108:A:GLN:HB3  | 4        | 0.11          |
| (1,2318) | 1:108:A:GLN:HA  | 1:108:A:GLN:HB3  | 6        | 0.11          |
| (1,2318) | 1:108:A:GLN:HA  | 1:108:A:GLN:HB3  | 9        | 0.11          |
| (1,2318) | 1:108:A:GLN:HA  | 1:108:A:GLN:HB3  | 13       | 0.11          |
| (1,2318) | 1:108:A:GLN:HA  | 1:108:A:GLN:HB3  | 14       | 0.11          |
| (1,2318) | 1:108:A:GLN:HA  | 1:108:A:GLN:HB3  | 16       | 0.11          |
| (1,2318) | 1:108:A:GLN:HA  | 1:108:A:GLN:HB3  | 17       | 0.11          |
| (1,2312) | 1:77:A:LEU:HG   | 1:77:A:LEU:H     | 2        | 0.11          |
| (1,2312) | 1:77:A:LEU:HG   | 1:77:A:LEU:H     | 11       | 0.11          |
| (1,2312) | 1:77:A:LEU:HG   | 1:77:A:LEU:H     | 14       | 0.11          |
| (1,2312) | 1:77:A:LEU:HG   | 1:77:A:LEU:H     | 15       | 0.11          |
| (1,2295) | 1:121:A:LYS:HG2 | 1:121:A:LYS:HD3  | 17       | 0.11          |
| (1,2283) | 1:33:A:GLU:HG2  | 1:33:A:GLU:HA    | 8        | 0.11          |
| (1,2270) | 1:113:A:ALA:HA  | 1:114:A:ARG:H    | 2        | 0.11          |
| (1,2270) | 1:113:A:ALA:HA  | 1:114:A:ARG:H    | 7        | 0.11          |
| (1,2270) | 1:113:A:ALA:HA  | 1:114:A:ARG:H    | 11       | 0.11          |
| (1,2270) | 1:113:A:ALA:HA  | 1:114:A:ARG:H    | 13       | 0.11          |
| (1,2270) | 1:113:A:ALA:HA  | 1:114:A:ARG:H    | 15       | 0.11          |
| (1,2264) | 1:85:A:LEU:HB3  | 1:82:A:TRP:HA    | 4        | 0.11          |
| (1,2257) | 1:69:A:THR:HB   | 1:72:A:ARG:HB3   | 17       | 0.11          |
| (1,2245) | 1:57:A:VAL:HA   | 1:58:A:ASP:HB2   | 1        | 0.11          |
| (1,2236) | 1:54:A:GLN:HB2  | 1:54:A:GLN:HG2   | 8        | 0.11          |
| (1,2236) | 1:54:A:GLN:HB2  | 1:54:A:GLN:HG2   | 13       | 0.11          |
| (1,2236) | 1:54:A:GLN:HB2  | 1:54:A:GLN:HG2   | 15       | 0.11          |
| (1,2197) | 1:39:A:PHE:HD1  | 1:56:A:LEU:HA    | 8        | 0.11          |
| (1,2160) | 1:82:A:TRP:HZ3  | 1:82:A:TRP:HB2   | 8        | 0.11          |
| (1,2160) | 1:82:A:TRP:HZ3  | 1:82:A:TRP:HB2   | 13       | 0.11          |
| (1,2070) | 1:48:A:LEU:H    | 1:84:A:TYR:HE1   | 6        | 0.11          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2070) | 1:48:A:LEU:H     | 1:84:A:TYR:HE2   | 7        | 0.11          |
| (1,2070) | 1:48:A:LEU:H     | 1:84:A:TYR:HE1   | 8        | 0.11          |
| (1,2070) | 1:48:A:LEU:H     | 1:84:A:TYR:HE1   | 10       | 0.11          |
| (1,2070) | 1:48:A:LEU:H     | 1:84:A:TYR:HE1   | 12       | 0.11          |
| (1,2058) | 1:12:A:GLN:H     | 1:13:A:ASP:H     | 17       | 0.11          |
| (1,2052) | 1:65:A:ASN:H     | 1:66:A:LEU:H     | 14       | 0.11          |
| (1,2047) | 1:60:A:VAL:H     | 1:61:A:ALA:H     | 6        | 0.11          |
| (1,2047) | 1:60:A:VAL:H     | 1:61:A:ALA:H     | 10       | 0.11          |
| (1,2047) | 1:60:A:VAL:H     | 1:61:A:ALA:H     | 12       | 0.11          |
| (1,2047) | 1:60:A:VAL:H     | 1:61:A:ALA:H     | 17       | 0.11          |
| (1,2045) | 1:77:A:LEU:H     | 1:78:A:TYR:H     | 12       | 0.11          |
| (1,1960) | 1:121:A:LYS:HG3  | 1:117:A:LEU:HD11 | 14       | 0.11          |
| (1,1956) | 1:19:A:PRO:HB2   | 1:19:A:PRO:HD2   | 12       | 0.11          |
| (1,1955) | 1:92:A:ALA:HB1   | 1:113:A:ALA:HB3  | 1        | 0.11          |
| (1,1954) | 1:116:A:GLN:H    | 1:113:A:ALA:HA   | 5        | 0.11          |
| (1,1954) | 1:116:A:GLN:H    | 1:113:A:ALA:HA   | 6        | 0.11          |
| (1,1954) | 1:116:A:GLN:H    | 1:113:A:ALA:HA   | 10       | 0.11          |
| (1,1954) | 1:116:A:GLN:H    | 1:113:A:ALA:HA   | 14       | 0.11          |
| (1,1954) | 1:116:A:GLN:H    | 1:113:A:ALA:HA   | 17       | 0.11          |
| (1,1949) | 1:92:A:ALA:HB3   | 1:110:A:VAL:HG11 | 4        | 0.11          |
| (1,1946) | 1:110:A:VAL:HG22 | 1:110:A:VAL:HB   | 12       | 0.11          |
| (1,1946) | 1:110:A:VAL:HG23 | 1:110:A:VAL:HB   | 13       | 0.11          |
| (1,1946) | 1:110:A:VAL:HG23 | 1:110:A:VAL:HB   | 15       | 0.11          |
| (1,1939) | 1:33:A:GLU:HB3   | 1:30:A:PHE:HA    | 2        | 0.11          |
| (1,1939) | 1:33:A:GLU:HB3   | 1:30:A:PHE:HA    | 6        | 0.11          |
| (1,1920) | 1:101:A:PRO:HG3  | 1:101:A:PRO:HD2  | 2        | 0.11          |
| (1,1920) | 1:101:A:PRO:HG3  | 1:101:A:PRO:HD2  | 5        | 0.11          |
| (1,1920) | 1:101:A:PRO:HG3  | 1:101:A:PRO:HD2  | 8        | 0.11          |
| (1,1920) | 1:101:A:PRO:HG3  | 1:101:A:PRO:HD2  | 10       | 0.11          |
| (1,1920) | 1:101:A:PRO:HG3  | 1:101:A:PRO:HD2  | 11       | 0.11          |
| (1,1920) | 1:101:A:PRO:HG3  | 1:101:A:PRO:HD2  | 12       | 0.11          |
| (1,1920) | 1:101:A:PRO:HG3  | 1:101:A:PRO:HD2  | 13       | 0.11          |
| (1,1920) | 1:101:A:PRO:HG3  | 1:101:A:PRO:HD2  | 14       | 0.11          |
| (1,1920) | 1:101:A:PRO:HG3  | 1:101:A:PRO:HD2  | 17       | 0.11          |
| (1,1911) | 1:114:A:ARG:HB2  | 1:111:A:GLU:HA   | 11       | 0.11          |
| (1,1911) | 1:114:A:ARG:HB2  | 1:111:A:GLU:HA   | 14       | 0.11          |
| (1,1906) | 1:105:A:LEU:HB3  | 1:101:A:PRO:HB3  | 6        | 0.11          |
| (1,1887) | 1:65:A:ASN:HB2   | 1:66:A:LEU:H     | 3        | 0.11          |
| (1,1887) | 1:65:A:ASN:HB2   | 1:66:A:LEU:H     | 10       | 0.11          |
| (1,1887) | 1:65:A:ASN:HB2   | 1:66:A:LEU:H     | 17       | 0.11          |
| (1,1886) | 1:102:A:CYS:HB3  | 1:49:A:LYS:HA    | 16       | 0.11          |
| (1,1847) | 1:36:A:PRO:HB2   | 1:36:A:PRO:HD2   | 4        | 0.11          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1847) | 1:36:A:PRO:HB2  | 1:36:A:PRO:HD2   | 17       | 0.11          |
| (1,1835) | 1:20:A:LYS:H    | 1:20:A:LYS:HG2   | 8        | 0.11          |
| (1,1819) | 1:112:A:HIS:HA  | 1:112:A:HIS:H    | 4        | 0.11          |
| (1,1819) | 1:112:A:HIS:HA  | 1:112:A:HIS:H    | 5        | 0.11          |
| (1,1818) | 1:118:A:GLU:HA  | 1:122:A:ALA:H    | 1        | 0.11          |
| (1,1801) | 1:117:A:LEU:HA  | 1:120:A:ALA:HB3  | 11       | 0.11          |
| (1,1793) | 1:88:A:VAL:HG22 | 1:84:A:TYR:HA    | 14       | 0.11          |
| (1,1787) | 1:93:A:THR:HB   | 1:49:A:LYS:HB3   | 14       | 0.11          |
| (1,1775) | 1:88:A:VAL:HA   | 1:47:A:PRO:HB3   | 17       | 0.11          |
| (1,1769) | 1:72:A:ARG:HD3  | 1:72:A:ARG:HA    | 12       | 0.11          |
| (1,1769) | 1:72:A:ARG:HD3  | 1:72:A:ARG:HA    | 17       | 0.11          |
| (1,1768) | 1:72:A:ARG:HA   | 1:75:A:LEU:H     | 10       | 0.11          |
| (1,1768) | 1:72:A:ARG:HA   | 1:75:A:LEU:H     | 12       | 0.11          |
| (1,1761) | 1:92:A:ALA:HB2  | 1:92:A:ALA:HA    | 10       | 0.11          |
| (1,1756) | 1:79:A:THR:HG23 | 1:84:A:TYR:HE1   | 13       | 0.11          |
| (1,1727) | 1:66:A:LEU:HD11 | 1:30:A:PHE:HD2   | 4        | 0.11          |
| (1,1727) | 1:66:A:LEU:HD13 | 1:30:A:PHE:HD1   | 7        | 0.11          |
| (1,1727) | 1:66:A:LEU:HD13 | 1:30:A:PHE:HD2   | 8        | 0.11          |
| (1,1727) | 1:66:A:LEU:HD13 | 1:30:A:PHE:HD2   | 9        | 0.11          |
| (1,1727) | 1:66:A:LEU:HD11 | 1:30:A:PHE:HD2   | 10       | 0.11          |
| (1,1727) | 1:66:A:LEU:HD11 | 1:30:A:PHE:HD1   | 12       | 0.11          |
| (1,1725) | 1:71:A:LEU:HD13 | 1:71:A:LEU:HG    | 4        | 0.11          |
| (1,1725) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HG    | 6        | 0.11          |
| (1,1725) | 1:71:A:LEU:HD12 | 1:71:A:LEU:HG    | 14       | 0.11          |
| (1,1720) | 1:117:A:LEU:HG  | 1:117:A:LEU:HD13 | 5        | 0.11          |
| (1,1720) | 1:117:A:LEU:HG  | 1:117:A:LEU:HD12 | 16       | 0.11          |
| (1,1718) | 1:18:A:GLN:HB3  | 1:19:A:PRO:HD2   | 5        | 0.11          |
| (1,1713) | 1:20:A:LYS:H    | 1:20:A:LYS:HD3   | 4        | 0.11          |
| (1,1711) | 1:25:A:LYS:HD3  | 1:25:A:LYS:HA    | 7        | 0.11          |
| (1,1711) | 1:25:A:LYS:HD3  | 1:25:A:LYS:HA    | 10       | 0.11          |
| (1,1709) | 1:72:A:ARG:HB3  | 1:53:A:PHE:HE1   | 14       | 0.11          |
| (1,1690) | 1:42:A:GLU:HG2  | 1:41:A:ALA:HB3   | 4        | 0.11          |
| (1,1690) | 1:42:A:GLU:HG2  | 1:41:A:ALA:HB1   | 10       | 0.11          |
| (1,1681) | 1:40:A:SER:HA   | 1:41:A:ALA:HB1   | 10       | 0.11          |
| (1,1640) | 1:33:A:GLU:HG3  | 1:33:A:GLU:H     | 10       | 0.11          |
| (1,1636) | 1:124:A:VAL:HA  | 1:125:A:GLN:HG3  | 1        | 0.11          |
| (1,1636) | 1:124:A:VAL:HA  | 1:125:A:GLN:HG3  | 4        | 0.11          |
| (1,1636) | 1:124:A:VAL:HA  | 1:125:A:GLN:HG3  | 8        | 0.11          |
| (1,1599) | 1:53:A:PHE:HB3  | 1:75:A:LEU:HD21  | 12       | 0.11          |
| (1,1599) | 1:53:A:PHE:HB3  | 1:75:A:LEU:HD22  | 13       | 0.11          |
| (1,1590) | 1:61:A:ALA:HB3  | 1:61:A:ALA:H     | 9        | 0.11          |
| (1,1590) | 1:61:A:ALA:HB3  | 1:61:A:ALA:H     | 13       | 0.11          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1588) | 1:74:A:ALA:HB3   | 1:74:A:ALA:HA   | 12       | 0.11          |
| (1,1583) | 1:36:A:PRO:HD2   | 1:34:A:ARG:HA   | 14       | 0.11          |
| (1,1583) | 1:36:A:PRO:HD2   | 1:34:A:ARG:HA   | 17       | 0.11          |
| (1,1580) | 1:97:A:LEU:HA    | 1:97:A:LEU:H    | 1        | 0.11          |
| (1,1578) | 1:70:A:GLN:HB3   | 1:66:A:LEU:HA   | 2        | 0.11          |
| (1,1578) | 1:70:A:GLN:HB3   | 1:66:A:LEU:HA   | 6        | 0.11          |
| (1,1578) | 1:70:A:GLN:HB3   | 1:66:A:LEU:HA   | 7        | 0.11          |
| (1,1578) | 1:70:A:GLN:HB3   | 1:66:A:LEU:HA   | 9        | 0.11          |
| (1,1578) | 1:70:A:GLN:HB3   | 1:66:A:LEU:HA   | 13       | 0.11          |
| (1,1578) | 1:70:A:GLN:HB3   | 1:66:A:LEU:HA   | 15       | 0.11          |
| (1,1578) | 1:70:A:GLN:HB3   | 1:66:A:LEU:HA   | 16       | 0.11          |
| (1,1567) | 1:68:A:LYS:HB2   | 1:68:A:LYS:HA   | 16       | 0.11          |
| (1,1553) | 1:57:A:VAL:HG13  | 1:61:A:ALA:H    | 5        | 0.11          |
| (1,1549) | 1:107:A:GLU:H    | 1:107:A:GLU:HB3 | 5        | 0.11          |
| (1,1546) | 1:56:A:LEU:HD11  | 1:52:A:ILE:HG13 | 4        | 0.11          |
| (1,1536) | 1:53:A:PHE:HA    | 1:56:A:LEU:HB3  | 5        | 0.11          |
| (1,1526) | 1:54:A:GLN:HB3   | 1:54:A:GLN:HA   | 2        | 0.11          |
| (1,1526) | 1:54:A:GLN:HB3   | 1:54:A:GLN:HA   | 3        | 0.11          |
| (1,1526) | 1:54:A:GLN:HB3   | 1:54:A:GLN:HA   | 4        | 0.11          |
| (1,1511) | 1:28:A:ILE:HA    | 1:28:A:ILE:HG21 | 11       | 0.11          |
| (1,1504) | 1:121:A:LYS:HD3  | 1:121:A:LYS:H   | 1        | 0.11          |
| (1,1504) | 1:121:A:LYS:HD3  | 1:121:A:LYS:H   | 5        | 0.11          |
| (1,1504) | 1:121:A:LYS:HD3  | 1:121:A:LYS:H   | 6        | 0.11          |
| (1,1504) | 1:121:A:LYS:HD3  | 1:121:A:LYS:H   | 11       | 0.11          |
| (1,1486) | 1:25:A:LYS:HG3   | 1:26:A:GLU:HA   | 5        | 0.11          |
| (1,1486) | 1:25:A:LYS:HG3   | 1:26:A:GLU:HA   | 12       | 0.11          |
| (1,1464) | 1:102:A:CYS:HB3  | 1:103:A:GLY:H   | 1        | 0.11          |
| (1,1464) | 1:102:A:CYS:HB3  | 1:103:A:GLY:H   | 16       | 0.11          |
| (1,1457) | 1:60:A:VAL:HG13  | 1:60:A:VAL:HB   | 11       | 0.11          |
| (1,1455) | 1:132:A:GLN:HG2  | 1:129:A:ALA:HA  | 15       | 0.11          |
| (1,1412) | 1:39:A:PHE:HZ    | 1:75:A:LEU:HD11 | 11       | 0.11          |
| (1,1410) | 1:110:A:VAL:HG21 | 1:108:A:GLN:H   | 9        | 0.11          |
| (1,1410) | 1:110:A:VAL:HG21 | 1:108:A:GLN:H   | 16       | 0.11          |
| (1,1403) | 1:95:A:VAL:HG23  | 1:95:A:VAL:HG12 | 6        | 0.11          |
| (1,1403) | 1:95:A:VAL:HG23  | 1:95:A:VAL:HG11 | 15       | 0.11          |
| (1,1399) | 1:95:A:VAL:HG22  | 1:95:A:VAL:H    | 16       | 0.11          |
| (1,1397) | 1:31:A:LEU:HD23  | 1:60:A:VAL:HG13 | 7        | 0.11          |
| (1,1391) | 1:54:A:GLN:HB3   | 1:53:A:PHE:HD1  | 6        | 0.11          |
| (1,1391) | 1:54:A:GLN:HB3   | 1:53:A:PHE:HD1  | 9        | 0.11          |
| (1,1389) | 1:68:A:LYS:HD3   | 1:53:A:PHE:HZ   | 6        | 0.11          |
| (1,1389) | 1:68:A:LYS:HD3   | 1:53:A:PHE:HZ   | 14       | 0.11          |
| (1,1358) | 1:32:A:ALA:HB1   | 1:33:A:GLU:H    | 4        | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1358) | 1:32:A:ALA:HB1  | 1:33:A:GLU:H    | 9        | 0.11          |
| (1,1357) | 1:74:A:ALA:HB2  | 1:31:A:LEU:HD13 | 16       | 0.11          |
| (1,1350) | 1:129:A:ALA:HB1 | 1:129:A:ALA:H   | 6        | 0.11          |
| (1,1327) | 1:73:A:SER:HB2  | 1:73:A:SER:H    | 1        | 0.11          |
| (1,1327) | 1:73:A:SER:HB2  | 1:73:A:SER:H    | 8        | 0.11          |
| (1,1327) | 1:73:A:SER:HB2  | 1:73:A:SER:H    | 14       | 0.11          |
| (1,1315) | 1:95:A:VAL:HG23 | 1:97:A:LEU:HD22 | 9        | 0.11          |
| (1,1275) | 1:84:A:TYR:HE1  | 1:84:A:TYR:HB3  | 3        | 0.11          |
| (1,1275) | 1:84:A:TYR:HE1  | 1:84:A:TYR:HB3  | 7        | 0.11          |
| (1,1275) | 1:84:A:TYR:HE2  | 1:84:A:TYR:HB3  | 12       | 0.11          |
| (1,1247) | 1:42:A:GLU:HB3  | 1:43:A:GLY:HA2  | 2        | 0.11          |
| (1,1244) | 1:43:A:GLY:HA3  | 1:44:A:GLU:H    | 15       | 0.11          |
| (1,1229) | 1:83:A:ARG:HD3  | 1:83:A:ARG:HB2  | 5        | 0.11          |
| (1,1143) | 1:86:A:TYR:HE2  | 1:86:A:TYR:HD2  | 5        | 0.11          |
| (1,1143) | 1:86:A:TYR:HE1  | 1:86:A:TYR:HD1  | 8        | 0.11          |
| (1,1143) | 1:86:A:TYR:HE1  | 1:86:A:TYR:HD1  | 14       | 0.11          |
| (1,1121) | 1:101:A:PRO:HD2 | 1:100:A:ASN:HA  | 12       | 0.11          |
| (1,1121) | 1:101:A:PRO:HD2 | 1:100:A:ASN:HA  | 14       | 0.11          |
| (1,1111) | 1:75:A:LEU:HB3  | 1:75:A:LEU:H    | 10       | 0.11          |
| (1,1111) | 1:75:A:LEU:HB3  | 1:75:A:LEU:H    | 13       | 0.11          |
| (1,1074) | 1:34:A:ARG:HG2  | 1:35:A:PHE:HD2  | 4        | 0.11          |
| (1,1074) | 1:34:A:ARG:HG2  | 1:35:A:PHE:HD2  | 14       | 0.11          |
| (1,1074) | 1:34:A:ARG:HG2  | 1:35:A:PHE:HD1  | 16       | 0.11          |
| (1,1053) | 1:93:A:THR:HG23 | 1:102:A:CYS:HA  | 14       | 0.11          |
| (1,1052) | 1:69:A:THR:HG21 | 1:69:A:THR:HA   | 4        | 0.11          |
| (1,1052) | 1:69:A:THR:HG22 | 1:69:A:THR:HA   | 6        | 0.11          |
| (1,1052) | 1:69:A:THR:HG22 | 1:69:A:THR:HA   | 11       | 0.11          |
| (1,1032) | 1:85:A:LEU:H    | 1:84:A:TYR:HE2  | 12       | 0.11          |
| (1,1032) | 1:85:A:LEU:H    | 1:84:A:TYR:HE2  | 13       | 0.11          |
| (1,1013) | 1:11:A:SER:HA   | 1:12:A:GLN:H    | 2        | 0.11          |
| (1,1009) | 1:37:A:HIS:HD2  | 1:38:A:CYS:HA   | 3        | 0.11          |
| (1,1009) | 1:37:A:HIS:HD2  | 1:38:A:CYS:HA   | 4        | 0.11          |
| (1,1009) | 1:37:A:HIS:HD2  | 1:38:A:CYS:HA   | 7        | 0.11          |
| (1,983)  | 1:55:A:ASP:HB3  | 1:55:A:ASP:HA   | 5        | 0.11          |
| (1,983)  | 1:55:A:ASP:HB3  | 1:55:A:ASP:HA   | 6        | 0.11          |
| (1,983)  | 1:55:A:ASP:HB3  | 1:55:A:ASP:HA   | 11       | 0.11          |
| (1,983)  | 1:55:A:ASP:HB3  | 1:55:A:ASP:HA   | 14       | 0.11          |
| (1,983)  | 1:55:A:ASP:HB3  | 1:55:A:ASP:HA   | 15       | 0.11          |
| (1,959)  | 1:30:A:PHE:HD1  | 1:31:A:LEU:HA   | 7        | 0.11          |
| (1,959)  | 1:30:A:PHE:HD2  | 1:31:A:LEU:HA   | 8        | 0.11          |
| (1,959)  | 1:30:A:PHE:HD2  | 1:31:A:LEU:HA   | 9        | 0.11          |
| (1,925)  | 1:28:A:ILE:HB   | 1:25:A:LYS:HA   | 2        | 0.11          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,925) | 1:28:A:ILE:HB   | 1:25:A:LYS:HA   | 4        | 0.11          |
| (1,925) | 1:28:A:ILE:HB   | 1:25:A:LYS:HA   | 9        | 0.11          |
| (1,925) | 1:28:A:ILE:HB   | 1:25:A:LYS:HA   | 17       | 0.11          |
| (1,917) | 1:15:A:MET:HG3  | 1:15:A:MET:H    | 4        | 0.11          |
| (1,917) | 1:15:A:MET:HG3  | 1:15:A:MET:H    | 14       | 0.11          |
| (1,872) | 1:56:A:LEU:HB3  | 1:56:A:LEU:HA   | 2        | 0.11          |
| (1,872) | 1:56:A:LEU:HB3  | 1:56:A:LEU:HA   | 16       | 0.11          |
| (1,853) | 1:65:A:ASN:HB2  | 1:65:A:ASN:HD21 | 10       | 0.11          |
| (1,853) | 1:65:A:ASN:HB2  | 1:65:A:ASN:HD21 | 12       | 0.11          |
| (1,853) | 1:65:A:ASN:HB2  | 1:65:A:ASN:HD21 | 17       | 0.11          |
| (1,847) | 1:49:A:LYS:HB2  | 1:102:A:CYS:HB3 | 7        | 0.11          |
| (1,847) | 1:49:A:LYS:HB2  | 1:102:A:CYS:HB3 | 13       | 0.11          |
| (1,847) | 1:49:A:LYS:HB2  | 1:102:A:CYS:HB3 | 16       | 0.11          |
| (1,847) | 1:49:A:LYS:HB2  | 1:102:A:CYS:HB3 | 17       | 0.11          |
| (1,830) | 1:129:A:ALA:HB2 | 1:127:A:GLN:HB3 | 9        | 0.11          |
| (1,830) | 1:129:A:ALA:HB1 | 1:127:A:GLN:HB3 | 12       | 0.11          |
| (1,830) | 1:129:A:ALA:HB1 | 1:127:A:GLN:HB3 | 17       | 0.11          |
| (1,818) | 1:28:A:ILE:HD11 | 1:78:A:TYR:HB3  | 7        | 0.11          |
| (1,762) | 1:65:A:ASN:HA   | 1:66:A:LEU:H    | 5        | 0.11          |
| (1,756) | 1:93:A:THR:HB   | 1:102:A:CYS:H   | 8        | 0.11          |
| (1,756) | 1:93:A:THR:HB   | 1:102:A:CYS:H   | 11       | 0.11          |
| (1,756) | 1:93:A:THR:HB   | 1:102:A:CYS:H   | 13       | 0.11          |
| (1,756) | 1:93:A:THR:HB   | 1:102:A:CYS:H   | 14       | 0.11          |
| (1,755) | 1:95:A:VAL:H    | 1:94:A:ARG:HB3  | 4        | 0.11          |
| (1,755) | 1:95:A:VAL:H    | 1:94:A:ARG:HB3  | 10       | 0.11          |
| (1,734) | 1:116:A:GLN:HA  | 1:117:A:LEU:H   | 7        | 0.11          |
| (1,709) | 1:73:A:SER:HA   | 1:75:A:LEU:H    | 1        | 0.11          |
| (1,709) | 1:73:A:SER:HA   | 1:75:A:LEU:H    | 9        | 0.11          |
| (1,707) | 1:75:A:LEU:HB3  | 1:74:A:ALA:H    | 8        | 0.11          |
| (1,707) | 1:75:A:LEU:HB3  | 1:74:A:ALA:H    | 15       | 0.11          |
| (1,665) | 1:122:A:ALA:HB1 | 1:123:A:ARG:H   | 4        | 0.11          |
| (1,665) | 1:122:A:ALA:HB1 | 1:123:A:ARG:H   | 9        | 0.11          |
| (1,645) | 1:115:A:LYS:HE3 | 1:115:A:LYS:H   | 1        | 0.11          |
| (1,645) | 1:115:A:LYS:HE3 | 1:115:A:LYS:H   | 2        | 0.11          |
| (1,645) | 1:115:A:LYS:HE3 | 1:115:A:LYS:H   | 4        | 0.11          |
| (1,645) | 1:115:A:LYS:HE3 | 1:115:A:LYS:H   | 7        | 0.11          |
| (1,645) | 1:115:A:LYS:HE3 | 1:115:A:LYS:H   | 10       | 0.11          |
| (1,645) | 1:115:A:LYS:HE3 | 1:115:A:LYS:H   | 17       | 0.11          |
| (1,635) | 1:127:A:GLN:H   | 1:127:A:GLN:HB3 | 8        | 0.11          |
| (1,618) | 1:95:A:VAL:H    | 1:48:A:LEU:HD11 | 14       | 0.11          |
| (1,609) | 1:49:A:LYS:HB2  | 1:49:A:LYS:H    | 10       | 0.11          |
| (1,609) | 1:49:A:LYS:HB2  | 1:49:A:LYS:H    | 12       | 0.11          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,609) | 1:49:A:LYS:HB2  | 1:49:A:LYS:H    | 13       | 0.11          |
| (1,609) | 1:49:A:LYS:HB2  | 1:49:A:LYS:H    | 16       | 0.11          |
| (1,605) | 1:40:A:SER:HA   | 1:43:A:GLY:H    | 6        | 0.11          |
| (1,587) | 1:25:A:LYS:HB2  | 1:26:A:GLU:H    | 4        | 0.11          |
| (1,587) | 1:25:A:LYS:HB2  | 1:26:A:GLU:H    | 5        | 0.11          |
| (1,587) | 1:25:A:LYS:HB2  | 1:26:A:GLU:H    | 6        | 0.11          |
| (1,587) | 1:25:A:LYS:HB2  | 1:26:A:GLU:H    | 7        | 0.11          |
| (1,587) | 1:25:A:LYS:HB2  | 1:26:A:GLU:H    | 9        | 0.11          |
| (1,587) | 1:25:A:LYS:HB2  | 1:26:A:GLU:H    | 11       | 0.11          |
| (1,587) | 1:25:A:LYS:HB2  | 1:26:A:GLU:H    | 12       | 0.11          |
| (1,587) | 1:25:A:LYS:HB2  | 1:26:A:GLU:H    | 13       | 0.11          |
| (1,587) | 1:25:A:LYS:HB2  | 1:26:A:GLU:H    | 15       | 0.11          |
| (1,587) | 1:25:A:LYS:HB2  | 1:26:A:GLU:H    | 16       | 0.11          |
| (1,564) | 1:59:A:ARG:HE   | 1:97:A:LEU:HD11 | 3        | 0.11          |
| (1,550) | 1:40:A:SER:HA   | 1:42:A:GLU:H    | 14       | 0.11          |
| (1,549) | 1:97:A:LEU:HD12 | 1:98:A:ASP:H    | 10       | 0.11          |
| (1,549) | 1:97:A:LEU:HD13 | 1:98:A:ASP:H    | 12       | 0.11          |
| (1,549) | 1:97:A:LEU:HD11 | 1:98:A:ASP:H    | 13       | 0.11          |
| (1,484) | 1:21:A:LEU:HA   | 1:23:A:SER:H    | 8        | 0.11          |
| (1,483) | 1:25:A:LYS:HG3  | 1:25:A:LYS:H    | 8        | 0.11          |
| (1,478) | 1:27:A:VAL:HG22 | 1:29:A:ALA:H    | 1        | 0.11          |
| (1,435) | 1:42:A:GLU:HB2  | 1:43:A:GLY:H    | 6        | 0.11          |
| (1,423) | 1:50:A:ILE:HG21 | 1:50:A:ILE:H    | 7        | 0.11          |
| (1,359) | 1:62:A:GLY:HA3  | 1:63:A:GLU:H    | 3        | 0.11          |
| (1,359) | 1:62:A:GLY:HA3  | 1:63:A:GLU:H    | 5        | 0.11          |
| (1,359) | 1:62:A:GLY:HA3  | 1:63:A:GLU:H    | 6        | 0.11          |
| (1,359) | 1:62:A:GLY:HA3  | 1:63:A:GLU:H    | 10       | 0.11          |
| (1,359) | 1:62:A:GLY:HA3  | 1:63:A:GLU:H    | 11       | 0.11          |
| (1,359) | 1:62:A:GLY:HA3  | 1:63:A:GLU:H    | 14       | 0.11          |
| (1,359) | 1:62:A:GLY:HA3  | 1:63:A:GLU:H    | 17       | 0.11          |
| (1,351) | 1:63:A:GLU:HB3  | 1:65:A:ASN:H    | 2        | 0.11          |
| (1,351) | 1:63:A:GLU:HB3  | 1:65:A:ASN:H    | 8        | 0.11          |
| (1,351) | 1:63:A:GLU:HB3  | 1:65:A:ASN:H    | 12       | 0.11          |
| (1,319) | 1:76:A:ARG:HD2  | 1:77:A:LEU:H    | 5        | 0.11          |
| (1,319) | 1:76:A:ARG:HD2  | 1:77:A:LEU:H    | 14       | 0.11          |
| (1,294) | 1:83:A:ARG:H    | 1:83:A:ARG:HB2  | 9        | 0.11          |
| (1,294) | 1:83:A:ARG:H    | 1:83:A:ARG:HB2  | 11       | 0.11          |
| (1,287) | 1:127:A:GLN:H   | 1:127:A:GLN:HG2 | 10       | 0.11          |
| (1,280) | 1:86:A:TYR:H    | 1:86:A:TYR:HB2  | 4        | 0.11          |
| (1,280) | 1:86:A:TYR:H    | 1:86:A:TYR:HB2  | 13       | 0.11          |
| (1,252) | 1:97:A:LEU:HG   | 1:97:A:LEU:H    | 1        | 0.11          |
| (1,226) | 1:100:A:ASN:HB3 | 1:100:A:ASN:H   | 11       | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,172)  | 1:27:A:VAL:HG12 | 1:21:A:LEU:H    | 11       | 0.11          |
| (1,158)  | 1:126:A:ALA:HA  | 1:126:A:ALA:H   | 4        | 0.11          |
| (1,158)  | 1:126:A:ALA:HA  | 1:126:A:ALA:H   | 5        | 0.11          |
| (1,156)  | 1:126:A:ALA:HB3 | 1:126:A:ALA:H   | 8        | 0.11          |
| (1,116)  | 1:21:A:LEU:HD11 | 1:30:A:PHE:H    | 4        | 0.11          |
| (1,91)   | 1:62:A:GLY:H    | 1:62:A:GLY:HA3  | 11       | 0.11          |
| (1,81)   | 1:88:A:VAL:HA   | 1:89:A:LYS:H    | 5        | 0.11          |
| (3,149)  | 1:82:A:TRP:HE1  | 1:82:A:TRP:HE3  | 7        | 0.1           |
| (3,149)  | 1:82:A:TRP:HE1  | 1:86:A:TYR:HD1  | 10       | 0.1           |
| (3,149)  | 1:82:A:TRP:HE1  | 1:86:A:TYR:HD2  | 16       | 0.1           |
| (3,90)   | 1:115:A:LYS:HG3 | 1:116:A:GLN:HG3 | 11       | 0.1           |
| (3,48)   | 1:72:A:ARG:HD3  | 1:72:A:ARG:HB3  | 7        | 0.1           |
| (3,48)   | 1:72:A:ARG:HD3  | 1:72:A:ARG:HB3  | 16       | 0.1           |
| (3,48)   | 1:72:A:ARG:HD3  | 1:72:A:ARG:HB3  | 17       | 0.1           |
| (1,4345) | 1:117:A:LEU:HA  | 1:121:A:LYS:H   | 3        | 0.1           |
| (1,4345) | 1:117:A:LEU:HA  | 1:121:A:LYS:H   | 12       | 0.1           |
| (1,4339) | 1:116:A:GLN:HG3 | 1:115:A:LYS:H   | 1        | 0.1           |
| (1,4331) | 1:104:A:GLU:HG2 | 1:104:A:GLU:H   | 14       | 0.1           |
| (1,4320) | 1:62:A:GLY:H    | 1:66:A:LEU:H    | 1        | 0.1           |
| (1,4316) | 1:95:A:VAL:H    | 1:94:A:ARG:HB3  | 1        | 0.1           |
| (1,4314) | 1:87:A:GLY:HA2  | 1:89:A:LYS:H    | 12       | 0.1           |
| (1,4302) | 1:94:A:ARG:H    | 1:94:A:ARG:HB3  | 2        | 0.1           |
| (1,4302) | 1:94:A:ARG:H    | 1:94:A:ARG:HB3  | 6        | 0.1           |
| (1,4302) | 1:94:A:ARG:H    | 1:94:A:ARG:HB3  | 14       | 0.1           |
| (1,4302) | 1:94:A:ARG:H    | 1:94:A:ARG:HB3  | 16       | 0.1           |
| (1,4263) | 1:66:A:LEU:HA   | 1:70:A:GLN:H    | 5        | 0.1           |
| (1,4258) | 1:52:A:ILE:HG12 | 1:56:A:LEU:H    | 5        | 0.1           |
| (1,4223) | 1:123:A:ARG:H   | 1:125:A:GLN:HG3 | 2        | 0.1           |
| (1,4202) | 1:127:A:GLN:H   | 1:127:A:GLN:HB3 | 14       | 0.1           |
| (1,4165) | 1:40:A:SER:HA   | 1:43:A:GLY:H    | 1        | 0.1           |
| (1,4165) | 1:40:A:SER:HA   | 1:43:A:GLY:H    | 15       | 0.1           |
| (1,4165) | 1:40:A:SER:HA   | 1:43:A:GLY:H    | 16       | 0.1           |
| (1,4143) | 1:37:A:HIS:HA   | 1:39:A:PHE:H    | 16       | 0.1           |
| (1,4112) | 1:54:A:GLN:HE22 | 1:57:A:VAL:H    | 5        | 0.1           |
| (1,4109) | 1:97:A:LEU:HD12 | 1:98:A:ASP:H    | 6        | 0.1           |
| (1,4106) | 1:99:A:GLY:HA3  | 1:98:A:ASP:H    | 6        | 0.1           |
| (1,4106) | 1:99:A:GLY:HA3  | 1:98:A:ASP:H    | 7        | 0.1           |
| (1,4060) | 1:97:A:LEU:HD21 | 1:39:A:PHE:H    | 15       | 0.1           |
| (1,4045) | 1:21:A:LEU:HD11 | 1:23:A:SER:H    | 5        | 0.1           |
| (1,4000) | 1:42:A:GLU:HB2  | 1:43:A:GLY:H    | 6        | 0.1           |
| (1,3994) | 1:45:A:ALA:H    | 1:83:A:ARG:HB2  | 17       | 0.1           |
| (1,3991) | 1:85:A:LEU:H    | 1:84:A:TYR:HA   | 3        | 0.1           |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3991) | 1:85:A:LEU:H    | 1:84:A:TYR:HA    | 11       | 0.1           |
| (1,3979) | 1:50:A:ILE:HA   | 1:51:A:GLY:H     | 5        | 0.1           |
| (1,3979) | 1:50:A:ILE:HA   | 1:51:A:GLY:H     | 7        | 0.1           |
| (1,3934) | 1:65:A:ASN:H    | 1:64:A:MET:HG2   | 16       | 0.1           |
| (1,3931) | 1:67:A:SER:H    | 1:66:A:LEU:H     | 5        | 0.1           |
| (1,3887) | 1:81:A:SER:HB2  | 1:82:A:TRP:H     | 13       | 0.1           |
| (1,3859) | 1:90:A:PRO:HB2  | 1:91:A:GLY:H     | 4        | 0.1           |
| (1,3859) | 1:90:A:PRO:HB2  | 1:91:A:GLY:H     | 8        | 0.1           |
| (1,3859) | 1:90:A:PRO:HB2  | 1:91:A:GLY:H     | 10       | 0.1           |
| (1,3853) | 1:97:A:LEU:HG   | 1:97:A:LEU:H     | 1        | 0.1           |
| (1,3846) | 1:94:A:ARG:HA   | 1:95:A:VAL:H     | 11       | 0.1           |
| (1,3845) | 1:95:A:VAL:HG12 | 1:96:A:ASP:H     | 7        | 0.1           |
| (1,3824) | 1:102:A:CYS:H   | 1:100:A:ASN:HB3  | 3        | 0.1           |
| (1,3824) | 1:102:A:CYS:H   | 1:100:A:ASN:HB3  | 9        | 0.1           |
| (1,3803) | 1:108:A:GLN:HB3 | 1:108:A:GLN:H    | 8        | 0.1           |
| (1,3801) | 1:108:A:GLN:HA  | 1:108:A:GLN:H    | 10       | 0.1           |
| (1,3784) | 1:21:A:LEU:HG   | 1:21:A:LEU:H     | 7        | 0.1           |
| (1,3779) | 1:121:A:LYS:HB2 | 1:120:A:ALA:H    | 9        | 0.1           |
| (1,3767) | 1:129:A:ALA:HA  | 1:129:A:ALA:H    | 4        | 0.1           |
| (1,3736) | 1:41:A:ALA:HA   | 1:29:A:ALA:H     | 5        | 0.1           |
| (1,3731) | 1:66:A:LEU:HB3  | 1:66:A:LEU:H     | 9        | 0.1           |
| (1,3667) | 1:37:A:HIS:H    | 1:37:A:HIS:HD2   | 14       | 0.1           |
| (1,3647) | 1:59:A:ARG:H    | 1:61:A:ALA:H     | 6        | 0.1           |
| (1,3647) | 1:59:A:ARG:H    | 1:61:A:ALA:H     | 14       | 0.1           |
| (1,3603) | 1:97:A:LEU:HA   | 1:97:A:LEU:HG    | 10       | 0.1           |
| (1,3568) | 1:105:A:LEU:HB3 | 1:109:A:HIS:HB2  | 17       | 0.1           |
| (1,3546) | 1:128:A:ARG:HB3 | 1:128:A:ARG:HD2  | 5        | 0.1           |
| (1,3542) | 1:105:A:LEU:HB3 | 1:101:A:PRO:HB3  | 4        | 0.1           |
| (1,3542) | 1:105:A:LEU:HB3 | 1:101:A:PRO:HB3  | 8        | 0.1           |
| (1,3542) | 1:105:A:LEU:HB3 | 1:101:A:PRO:HB3  | 13       | 0.1           |
| (1,3542) | 1:105:A:LEU:HB3 | 1:101:A:PRO:HB3  | 16       | 0.1           |
| (1,3508) | 1:113:A:ALA:HB2 | 1:88:A:VAL:HA    | 13       | 0.1           |
| (1,3501) | 1:27:A:VAL:HG23 | 1:28:A:ILE:HA    | 5        | 0.1           |
| (1,3500) | 1:27:A:VAL:HG23 | 1:31:A:LEU:HD11  | 3        | 0.1           |
| (1,3456) | 1:95:A:VAL:HG22 | 1:96:A:ASP:HA    | 13       | 0.1           |
| (1,3443) | 1:123:A:ARG:HG2 | 1:123:A:ARG:HD3  | 6        | 0.1           |
| (1,3443) | 1:123:A:ARG:HG2 | 1:123:A:ARG:HD3  | 16       | 0.1           |
| (1,3415) | 1:117:A:LEU:HA  | 1:117:A:LEU:HD13 | 5        | 0.1           |
| (1,3415) | 1:117:A:LEU:HA  | 1:117:A:LEU:HD12 | 8        | 0.1           |
| (1,3415) | 1:117:A:LEU:HA  | 1:117:A:LEU:HD12 | 13       | 0.1           |
| (1,3415) | 1:117:A:LEU:HA  | 1:117:A:LEU:HD13 | 14       | 0.1           |
| (1,3415) | 1:117:A:LEU:HA  | 1:117:A:LEU:HD12 | 16       | 0.1           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3392) | 1:53:A:PHE:HE1  | 1:68:A:LYS:HA   | 1        | 0.1           |
| (1,3390) | 1:88:A:VAL:HG22 | 1:84:A:TYR:HA   | 11       | 0.1           |
| (1,3372) | 1:88:A:VAL:HA   | 1:47:A:PRO:HB3  | 2        | 0.1           |
| (1,3369) | 1:24:A:SER:HA   | 1:27:A:VAL:HG21 | 3        | 0.1           |
| (1,3335) | 1:71:A:LEU:HA   | 1:71:A:LEU:HD23 | 1        | 0.1           |
| (1,3316) | 1:66:A:LEU:HD13 | 1:30:A:PHE:HD1  | 1        | 0.1           |
| (1,3314) | 1:71:A:LEU:HD11 | 1:71:A:LEU:HG   | 2        | 0.1           |
| (1,3275) | 1:119:A:GLU:HA  | 1:119:A:GLU:HG2 | 4        | 0.1           |
| (1,3273) | 1:42:A:GLU:HG2  | 1:43:A:GLY:H    | 8        | 0.1           |
| (1,3263) | 1:121:A:LYS:HG2 | 1:122:A:ALA:H   | 6        | 0.1           |
| (1,3263) | 1:121:A:LYS:HG2 | 1:122:A:ALA:H   | 9        | 0.1           |
| (1,3255) | 1:40:A:SER:HA   | 1:41:A:ALA:HB1  | 1        | 0.1           |
| (1,3241) | 1:52:A:ILE:HG13 | 1:97:A:LEU:HD22 | 16       | 0.1           |
| (1,3230) | 1:68:A:LYS:HB2  | 1:68:A:LYS:HA   | 5        | 0.1           |
| (1,3213) | 1:33:A:GLU:HG3  | 1:33:A:GLU:H    | 17       | 0.1           |
| (1,3206) | 1:124:A:VAL:HA  | 1:125:A:GLN:HG3 | 6        | 0.1           |
| (1,3172) | 1:25:A:LYS:HE3  | 1:25:A:LYS:HA   | 11       | 0.1           |
| (1,3172) | 1:25:A:LYS:HE3  | 1:25:A:LYS:HA   | 17       | 0.1           |
| (1,3169) | 1:53:A:PHE:HB3  | 1:75:A:LEU:HD23 | 3        | 0.1           |
| (1,3169) | 1:53:A:PHE:HB3  | 1:75:A:LEU:HD23 | 9        | 0.1           |
| (1,3164) | 1:120:A:ALA:HB3 | 1:120:A:ALA:H   | 9        | 0.1           |
| (1,3164) | 1:120:A:ALA:HB3 | 1:120:A:ALA:H   | 17       | 0.1           |
| (1,3122) | 1:11:A:SER:HB2  | 1:11:A:SER:HA   | 6        | 0.1           |
| (1,3108) | 1:102:A:CYS:H   | 1:101:A:PRO:HB3 | 5        | 0.1           |
| (1,3059) | 1:28:A:ILE:HB   | 1:28:A:ILE:HG22 | 1        | 0.1           |
| (1,3059) | 1:28:A:ILE:HB   | 1:28:A:ILE:HG22 | 14       | 0.1           |
| (1,3035) | 1:25:A:LYS:H    | 1:25:A:LYS:HG2  | 3        | 0.1           |
| (1,3035) | 1:25:A:LYS:H    | 1:25:A:LYS:HG2  | 5        | 0.1           |
| (1,3035) | 1:25:A:LYS:H    | 1:25:A:LYS:HG2  | 17       | 0.1           |
| (1,3031) | 1:25:A:LYS:HG3  | 1:25:A:LYS:HD2  | 7        | 0.1           |
| (1,3031) | 1:25:A:LYS:HG3  | 1:25:A:LYS:HD2  | 8        | 0.1           |
| (1,3031) | 1:25:A:LYS:HG3  | 1:25:A:LYS:HD2  | 9        | 0.1           |
| (1,3031) | 1:25:A:LYS:HG3  | 1:25:A:LYS:HD2  | 10       | 0.1           |
| (1,3031) | 1:25:A:LYS:HG3  | 1:25:A:LYS:HD2  | 17       | 0.1           |
| (1,2986) | 1:115:A:LYS:HB3 | 1:115:A:LYS:H   | 7        | 0.1           |
| (1,2978) | 1:105:A:LEU:H   | 1:101:A:PRO:HD3 | 4        | 0.1           |
| (1,2978) | 1:105:A:LEU:H   | 1:101:A:PRO:HD3 | 14       | 0.1           |
| (1,2976) | 1:103:A:GLY:HA3 | 1:101:A:PRO:HD3 | 7        | 0.1           |
| (1,2955) | 1:74:A:ALA:HB3  | 1:75:A:LEU:HD12 | 13       | 0.1           |
| (1,2949) | 1:39:A:PHE:HZ   | 1:75:A:LEU:HD11 | 5        | 0.1           |
| (1,2949) | 1:39:A:PHE:HZ   | 1:75:A:LEU:HD12 | 6        | 0.1           |
| (1,2899) | 1:28:A:ILE:HD13 | 1:75:A:LEU:H    | 13       | 0.1           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2899) | 1:28:A:ILE:HD13 | 1:75:A:LEU:H    | 14       | 0.1           |
| (1,2899) | 1:28:A:ILE:HD12 | 1:75:A:LEU:H    | 16       | 0.1           |
| (1,2875) | 1:122:A:ALA:HB2 | 1:122:A:ALA:H   | 12       | 0.1           |
| (1,2859) | 1:86:A:TYR:HE1  | 1:85:A:LEU:H    | 2        | 0.1           |
| (1,2846) | 1:53:A:PHE:HE1  | 1:75:A:LEU:HB3  | 2        | 0.1           |
| (1,2846) | 1:53:A:PHE:HE2  | 1:75:A:LEU:HB3  | 4        | 0.1           |
| (1,2846) | 1:53:A:PHE:HE2  | 1:75:A:LEU:HB3  | 17       | 0.1           |
| (1,2811) | 1:97:A:LEU:HD13 | 1:97:A:LEU:HB3  | 1        | 0.1           |
| (1,2791) | 1:84:A:TYR:HE2  | 1:84:A:TYR:HB3  | 6        | 0.1           |
| (1,2786) | 1:82:A:TRP:HH2  | 1:82:A:TRP:HE1  | 11       | 0.1           |
| (1,2765) | 1:79:A:THR:H    | 1:78:A:TYR:HE1  | 11       | 0.1           |
| (1,2695) | 1:78:A:TYR:HA   | 1:81:A:SER:H    | 5        | 0.1           |
| (1,2689) | 1:34:A:ARG:HB3  | 1:30:A:PHE:HD1  | 15       | 0.1           |
| (1,2648) | 1:56:A:LEU:HD12 | 1:52:A:ILE:HG12 | 10       | 0.1           |
| (1,2627) | 1:112:A:HIS:HA  | 1:112:A:HIS:HB2 | 4        | 0.1           |
| (1,2627) | 1:112:A:HIS:HA  | 1:112:A:HIS:HB2 | 17       | 0.1           |
| (1,2584) | 1:69:A:THR:HG22 | 1:69:A:THR:HA   | 2        | 0.1           |
| (1,2583) | 1:60:A:VAL:HG13 | 1:34:A:ARG:HG2  | 7        | 0.1           |
| (1,2579) | 1:59:A:ARG:HB2  | 1:60:A:VAL:HG12 | 3        | 0.1           |
| (1,2579) | 1:59:A:ARG:HB2  | 1:60:A:VAL:HG12 | 11       | 0.1           |
| (1,2547) | 1:11:A:SER:HA   | 1:12:A:GLN:HG3  | 10       | 0.1           |
| (1,2544) | 1:37:A:HIS:HD2  | 1:38:A:CYS:HA   | 15       | 0.1           |
| (1,2519) | 1:55:A:ASP:HB3  | 1:55:A:ASP:HA   | 7        | 0.1           |
| (1,2519) | 1:55:A:ASP:HB3  | 1:55:A:ASP:HA   | 10       | 0.1           |
| (1,2501) | 1:42:A:GLU:HA   | 1:42:A:GLU:HB3  | 10       | 0.1           |
| (1,2489) | 1:28:A:ILE:HA   | 1:28:A:ILE:HG21 | 11       | 0.1           |
| (1,2480) | 1:71:A:LEU:HB2  | 1:27:A:VAL:HG13 | 10       | 0.1           |
| (1,2469) | 1:53:A:PHE:HZ   | 1:72:A:ARG:HG3  | 2        | 0.1           |
| (1,2428) | 1:52:A:ILE:HG13 | 1:52:A:ILE:HG23 | 2        | 0.1           |
| (1,2417) | 1:129:A:ALA:HB3 | 1:127:A:GLN:HB3 | 10       | 0.1           |
| (1,2416) | 1:45:A:ALA:HB2  | 1:45:A:ALA:H    | 17       | 0.1           |
| (1,2415) | 1:45:A:ALA:HB3  | 1:84:A:TYR:HD2  | 3        | 0.1           |
| (1,2411) | 1:45:A:ALA:HB3  | 1:84:A:TYR:HB3  | 7        | 0.1           |
| (1,2397) | 1:50:A:ILE:HD11 | 1:50:A:ILE:HA   | 17       | 0.1           |
| (1,2367) | 1:52:A:ILE:H    | 1:52:A:ILE:HD12 | 10       | 0.1           |
| (1,2336) | 1:64:A:MET:HE2  | 1:31:A:LEU:HA   | 11       | 0.1           |
| (1,2318) | 1:108:A:GLN:HA  | 1:108:A:GLN:HB3 | 3        | 0.1           |
| (1,2318) | 1:108:A:GLN:HA  | 1:108:A:GLN:HB3 | 11       | 0.1           |
| (1,2318) | 1:108:A:GLN:HA  | 1:108:A:GLN:HB3 | 15       | 0.1           |
| (1,2312) | 1:77:A:LEU:HG   | 1:77:A:LEU:H    | 1        | 0.1           |
| (1,2312) | 1:77:A:LEU:HG   | 1:77:A:LEU:H    | 4        | 0.1           |
| (1,2312) | 1:77:A:LEU:HG   | 1:77:A:LEU:H    | 6        | 0.1           |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2312) | 1:77:A:LEU:HG    | 1:77:A:LEU:H    | 9        | 0.1           |
| (1,2312) | 1:77:A:LEU:HG    | 1:77:A:LEU:H    | 12       | 0.1           |
| (1,2312) | 1:77:A:LEU:HG    | 1:77:A:LEU:H    | 16       | 0.1           |
| (1,2312) | 1:77:A:LEU:HG    | 1:77:A:LEU:H    | 17       | 0.1           |
| (1,2301) | 1:92:A:ALA:HA    | 1:93:A:THR:H    | 6        | 0.1           |
| (1,2295) | 1:121:A:LYS:HG2  | 1:121:A:LYS:HD3 | 4        | 0.1           |
| (1,2283) | 1:33:A:GLU:HG2   | 1:33:A:GLU:HA   | 12       | 0.1           |
| (1,2270) | 1:113:A:ALA:HA   | 1:114:A:ARG:H   | 14       | 0.1           |
| (1,2257) | 1:69:A:THR:HB    | 1:72:A:ARG:HB3  | 11       | 0.1           |
| (1,2257) | 1:69:A:THR:HB    | 1:72:A:ARG:HB3  | 14       | 0.1           |
| (1,2236) | 1:54:A:GLN:HB2   | 1:54:A:GLN:HG2  | 6        | 0.1           |
| (1,2236) | 1:54:A:GLN:HB2   | 1:54:A:GLN:HG2  | 7        | 0.1           |
| (1,2236) | 1:54:A:GLN:HB2   | 1:54:A:GLN:HG2  | 17       | 0.1           |
| (1,2228) | 1:25:A:LYS:HD3   | 1:25:A:LYS:HG3  | 12       | 0.1           |
| (1,2203) | 1:21:A:LEU:HB2   | 1:21:A:LEU:HD22 | 1        | 0.1           |
| (1,2160) | 1:82:A:TRP:HZ3   | 1:82:A:TRP:HB2  | 4        | 0.1           |
| (1,2160) | 1:82:A:TRP:HZ3   | 1:82:A:TRP:HB2  | 10       | 0.1           |
| (1,2089) | 1:49:A:LYS:HB2   | 1:52:A:ILE:H    | 3        | 0.1           |
| (1,2089) | 1:49:A:LYS:HB2   | 1:52:A:ILE:H    | 6        | 0.1           |
| (1,2070) | 1:48:A:LEU:H     | 1:84:A:TYR:HE1  | 5        | 0.1           |
| (1,2070) | 1:48:A:LEU:H     | 1:84:A:TYR:HE2  | 15       | 0.1           |
| (1,2052) | 1:65:A:ASN:H     | 1:66:A:LEU:H    | 1        | 0.1           |
| (1,2052) | 1:65:A:ASN:H     | 1:66:A:LEU:H    | 15       | 0.1           |
| (1,2047) | 1:60:A:VAL:H     | 1:61:A:ALA:H    | 1        | 0.1           |
| (1,2047) | 1:60:A:VAL:H     | 1:61:A:ALA:H    | 16       | 0.1           |
| (1,2044) | 1:22:A:ASN:H     | 1:23:A:SER:H    | 11       | 0.1           |
| (1,2025) | 1:97:A:LEU:HD22  | 1:35:A:PHE:HD1  | 12       | 0.1           |
| (1,1997) | 1:107:A:GLU:HG2  | 1:107:A:GLU:H   | 3        | 0.1           |
| (1,1954) | 1:116:A:GLN:H    | 1:113:A:ALA:HA  | 8        | 0.1           |
| (1,1954) | 1:116:A:GLN:H    | 1:113:A:ALA:HA  | 11       | 0.1           |
| (1,1954) | 1:116:A:GLN:H    | 1:113:A:ALA:HA  | 13       | 0.1           |
| (1,1952) | 1:112:A:HIS:HA   | 1:115:A:LYS:HB3 | 16       | 0.1           |
| (1,1946) | 1:110:A:VAL:HG21 | 1:110:A:VAL:HB  | 2        | 0.1           |
| (1,1946) | 1:110:A:VAL:HG22 | 1:110:A:VAL:HB  | 8        | 0.1           |
| (1,1946) | 1:110:A:VAL:HG22 | 1:110:A:VAL:HB  | 9        | 0.1           |
| (1,1946) | 1:110:A:VAL:HG21 | 1:110:A:VAL:HB  | 10       | 0.1           |
| (1,1920) | 1:101:A:PRO:HG3  | 1:101:A:PRO:HD2 | 1        | 0.1           |
| (1,1920) | 1:101:A:PRO:HG3  | 1:101:A:PRO:HD2 | 3        | 0.1           |
| (1,1920) | 1:101:A:PRO:HG3  | 1:101:A:PRO:HD2 | 4        | 0.1           |
| (1,1920) | 1:101:A:PRO:HG3  | 1:101:A:PRO:HD2 | 7        | 0.1           |
| (1,1920) | 1:101:A:PRO:HG3  | 1:101:A:PRO:HD2 | 15       | 0.1           |
| (1,1920) | 1:101:A:PRO:HG3  | 1:101:A:PRO:HD2 | 16       | 0.1           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1910) | 1:128:A:ARG:HB3 | 1:128:A:ARG:HD2 | 4        | 0.1           |
| (1,1887) | 1:65:A:ASN:HB2  | 1:66:A:LEU:H    | 14       | 0.1           |
| (1,1886) | 1:102:A:CYS:HB3 | 1:49:A:LYS:HA   | 7        | 0.1           |
| (1,1876) | 1:27:A:VAL:HG22 | 1:31:A:LEU:HD12 | 1        | 0.1           |
| (1,1847) | 1:36:A:PRO:HB2  | 1:36:A:PRO:HD2  | 5        | 0.1           |
| (1,1845) | 1:95:A:VAL:HG21 | 1:96:A:ASP:HA   | 16       | 0.1           |
| (1,1819) | 1:112:A:HIS:HA  | 1:112:A:HIS:H   | 12       | 0.1           |
| (1,1819) | 1:112:A:HIS:HA  | 1:112:A:HIS:H   | 14       | 0.1           |
| (1,1769) | 1:72:A:ARG:HD3  | 1:72:A:ARG:HA   | 2        | 0.1           |
| (1,1769) | 1:72:A:ARG:HD3  | 1:72:A:ARG:HA   | 3        | 0.1           |
| (1,1769) | 1:72:A:ARG:HD3  | 1:72:A:ARG:HA   | 4        | 0.1           |
| (1,1769) | 1:72:A:ARG:HD3  | 1:72:A:ARG:HA   | 5        | 0.1           |
| (1,1769) | 1:72:A:ARG:HD3  | 1:72:A:ARG:HA   | 8        | 0.1           |
| (1,1769) | 1:72:A:ARG:HD3  | 1:72:A:ARG:HA   | 10       | 0.1           |
| (1,1769) | 1:72:A:ARG:HD3  | 1:72:A:ARG:HA   | 13       | 0.1           |
| (1,1769) | 1:72:A:ARG:HD3  | 1:72:A:ARG:HA   | 15       | 0.1           |
| (1,1769) | 1:72:A:ARG:HD3  | 1:72:A:ARG:HA   | 16       | 0.1           |
| (1,1768) | 1:72:A:ARG:HA   | 1:75:A:LEU:H    | 6        | 0.1           |
| (1,1768) | 1:72:A:ARG:HA   | 1:75:A:LEU:H    | 14       | 0.1           |
| (1,1756) | 1:79:A:THR:HG21 | 1:84:A:TYR:HE1  | 10       | 0.1           |
| (1,1756) | 1:79:A:THR:HG23 | 1:84:A:TYR:HE1  | 14       | 0.1           |
| (1,1727) | 1:66:A:LEU:HD12 | 1:30:A:PHE:HD2  | 15       | 0.1           |
| (1,1716) | 1:84:A:TYR:H    | 1:83:A:ARG:HB2  | 6        | 0.1           |
| (1,1716) | 1:84:A:TYR:H    | 1:83:A:ARG:HB2  | 12       | 0.1           |
| (1,1711) | 1:25:A:LYS:HD3  | 1:25:A:LYS:HA   | 8        | 0.1           |
| (1,1711) | 1:25:A:LYS:HD3  | 1:25:A:LYS:HA   | 9        | 0.1           |
| (1,1709) | 1:72:A:ARG:HB3  | 1:53:A:PHE:HE2  | 7        | 0.1           |
| (1,1709) | 1:72:A:ARG:HB3  | 1:53:A:PHE:HE1  | 8        | 0.1           |
| (1,1681) | 1:40:A:SER:HA   | 1:41:A:ALA:HB1  | 9        | 0.1           |
| (1,1640) | 1:33:A:GLU:HG3  | 1:33:A:GLU:H    | 2        | 0.1           |
| (1,1636) | 1:124:A:VAL:HA  | 1:125:A:GLN:HG3 | 9        | 0.1           |
| (1,1608) | 1:76:A:ARG:HA   | 1:76:A:ARG:HD2  | 11       | 0.1           |
| (1,1590) | 1:61:A:ALA:HB2  | 1:61:A:ALA:H    | 2        | 0.1           |
| (1,1590) | 1:61:A:ALA:HB3  | 1:61:A:ALA:H    | 16       | 0.1           |
| (1,1583) | 1:36:A:PRO:HD2  | 1:34:A:ARG:HA   | 6        | 0.1           |
| (1,1583) | 1:36:A:PRO:HD2  | 1:34:A:ARG:HA   | 12       | 0.1           |
| (1,1578) | 1:70:A:GLN:HB3  | 1:66:A:LEU:HA   | 5        | 0.1           |
| (1,1578) | 1:70:A:GLN:HB3  | 1:66:A:LEU:HA   | 8        | 0.1           |
| (1,1553) | 1:57:A:VAL:HG12 | 1:61:A:ALA:H    | 2        | 0.1           |
| (1,1549) | 1:107:A:GLU:H   | 1:107:A:GLU:HB3 | 15       | 0.1           |
| (1,1546) | 1:56:A:LEU:HD12 | 1:52:A:ILE:HG13 | 12       | 0.1           |
| (1,1536) | 1:53:A:PHE:HA   | 1:56:A:LEU:HB3  | 4        | 0.1           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1536) | 1:53:A:PHE:HA    | 1:56:A:LEU:HB3   | 8        | 0.1           |
| (1,1536) | 1:53:A:PHE:HA    | 1:56:A:LEU:HB3   | 13       | 0.1           |
| (1,1526) | 1:54:A:GLN:HB3   | 1:54:A:GLN:HA    | 9        | 0.1           |
| (1,1526) | 1:54:A:GLN:HB3   | 1:54:A:GLN:HA    | 16       | 0.1           |
| (1,1512) | 1:52:A:ILE:HG21  | 1:53:A:PHE:HB2   | 6        | 0.1           |
| (1,1504) | 1:121:A:LYS:HD3  | 1:121:A:LYS:H    | 10       | 0.1           |
| (1,1465) | 1:102:A:CYS:HB3  | 1:49:A:LYS:HB3   | 3        | 0.1           |
| (1,1464) | 1:102:A:CYS:HB3  | 1:103:A:GLY:H    | 3        | 0.1           |
| (1,1457) | 1:60:A:VAL:HG11  | 1:60:A:VAL:HB    | 5        | 0.1           |
| (1,1454) | 1:60:A:VAL:HB    | 1:61:A:ALA:H     | 3        | 0.1           |
| (1,1454) | 1:60:A:VAL:HB    | 1:61:A:ALA:H     | 5        | 0.1           |
| (1,1441) | 1:42:A:GLU:HB2   | 1:43:A:GLY:H     | 6        | 0.1           |
| (1,1410) | 1:110:A:VAL:HG23 | 1:108:A:GLN:H    | 7        | 0.1           |
| (1,1391) | 1:54:A:GLN:HB3   | 1:53:A:PHE:HD1   | 4        | 0.1           |
| (1,1389) | 1:68:A:LYS:HD3   | 1:53:A:PHE:HZ    | 4        | 0.1           |
| (1,1374) | 1:88:A:VAL:HG21  | 1:47:A:PRO:HB3   | 5        | 0.1           |
| (1,1275) | 1:84:A:TYR:HE1   | 1:84:A:TYR:HB3   | 15       | 0.1           |
| (1,1214) | 1:17:A:ASN:HB3   | 1:17:A:ASN:H     | 8        | 0.1           |
| (1,1176) | 1:40:A:SER:HB2   | 1:42:A:GLU:H     | 7        | 0.1           |
| (1,1143) | 1:86:A:TYR:HE1   | 1:86:A:TYR:HD1   | 10       | 0.1           |
| (1,1121) | 1:101:A:PRO:HD2  | 1:100:A:ASN:HA   | 6        | 0.1           |
| (1,1121) | 1:101:A:PRO:HD2  | 1:100:A:ASN:HA   | 15       | 0.1           |
| (1,1121) | 1:101:A:PRO:HD2  | 1:100:A:ASN:HA   | 16       | 0.1           |
| (1,1074) | 1:34:A:ARG:HG2   | 1:35:A:PHE:HD1   | 6        | 0.1           |
| (1,1053) | 1:93:A:THR:HG22  | 1:102:A:CYS:HA   | 3        | 0.1           |
| (1,1047) | 1:124:A:VAL:HA   | 1:124:A:VAL:HG23 | 6        | 0.1           |
| (1,1047) | 1:124:A:VAL:HA   | 1:124:A:VAL:HG23 | 12       | 0.1           |
| (1,1042) | 1:78:A:TYR:HE2   | 1:48:A:LEU:HG    | 8        | 0.1           |
| (1,1030) | 1:86:A:TYR:HE1   | 1:86:A:TYR:HB2   | 9        | 0.1           |
| (1,1013) | 1:11:A:SER:HA    | 1:12:A:GLN:H     | 14       | 0.1           |
| (1,1004) | 1:82:A:TRP:HA    | 1:86:A:TYR:HD1   | 6        | 0.1           |
| (1,1004) | 1:82:A:TRP:HA    | 1:86:A:TYR:HD1   | 15       | 0.1           |
| (1,983)  | 1:55:A:ASP:HB3   | 1:55:A:ASP:HA    | 2        | 0.1           |
| (1,983)  | 1:55:A:ASP:HB3   | 1:55:A:ASP:HA    | 9        | 0.1           |
| (1,982)  | 1:20:A:LYS:HA    | 1:20:A:LYS:HG2   | 15       | 0.1           |
| (1,981)  | 1:132:A:GLN:HB3  | 1:132:A:GLN:HA   | 17       | 0.1           |
| (1,830)  | 1:129:A:ALA:HB2  | 1:127:A:GLN:HB3  | 8        | 0.1           |
| (1,773)  | 1:116:A:GLN:HG3  | 1:115:A:LYS:H    | 5        | 0.1           |
| (1,762)  | 1:65:A:ASN:HA    | 1:66:A:LEU:H     | 11       | 0.1           |
| (1,756)  | 1:93:A:THR:HB    | 1:102:A:CYS:H    | 9        | 0.1           |
| (1,756)  | 1:93:A:THR:HB    | 1:102:A:CYS:H    | 12       | 0.1           |
| (1,734)  | 1:116:A:GLN:HA   | 1:117:A:LEU:H    | 17       | 0.1           |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,732) | 1:130:A:GLU:H   | 1:132:A:GLN:HB2 | 15       | 0.1           |
| (1,683) | 1:54:A:GLN:HB3  | 1:54:A:GLN:H    | 9        | 0.1           |
| (1,645) | 1:115:A:LYS:HE3 | 1:115:A:LYS:H   | 5        | 0.1           |
| (1,609) | 1:49:A:LYS:HB2  | 1:49:A:LYS:H    | 8        | 0.1           |
| (1,587) | 1:25:A:LYS:HB2  | 1:26:A:GLU:H    | 8        | 0.1           |
| (1,552) | 1:65:A:ASN:H    | 1:65:A:ASN:HD21 | 17       | 0.1           |
| (1,550) | 1:40:A:SER:HA   | 1:42:A:GLU:H    | 9        | 0.1           |
| (1,483) | 1:25:A:LYS:HG3  | 1:25:A:LYS:H    | 5        | 0.1           |
| (1,483) | 1:25:A:LYS:HG3  | 1:25:A:LYS:H    | 12       | 0.1           |
| (1,477) | 1:31:A:LEU:H    | 1:31:A:LEU:HD11 | 10       | 0.1           |
| (1,363) | 1:66:A:LEU:HD13 | 1:62:A:GLY:H    | 5        | 0.1           |
| (1,359) | 1:62:A:GLY:HA3  | 1:63:A:GLU:H    | 12       | 0.1           |
| (1,297) | 1:81:A:SER:HB2  | 1:82:A:TRP:H    | 14       | 0.1           |
| (1,287) | 1:127:A:GLN:H   | 1:127:A:GLN:HG2 | 2        | 0.1           |
| (1,287) | 1:127:A:GLN:H   | 1:127:A:GLN:HG2 | 8        | 0.1           |
| (1,280) | 1:86:A:TYR:H    | 1:86:A:TYR:HB2  | 5        | 0.1           |
| (1,280) | 1:86:A:TYR:H    | 1:86:A:TYR:HB2  | 10       | 0.1           |
| (1,280) | 1:86:A:TYR:H    | 1:86:A:TYR:HB2  | 14       | 0.1           |
| (1,280) | 1:86:A:TYR:H    | 1:86:A:TYR:HB2  | 16       | 0.1           |
| (1,184) | 1:43:A:GLY:HA3  | 1:44:A:GLU:H    | 9        | 0.1           |
| (1,158) | 1:126:A:ALA:HA  | 1:126:A:ALA:H   | 12       | 0.1           |
| (1,158) | 1:126:A:ALA:HA  | 1:126:A:ALA:H   | 15       | 0.1           |
| (1,116) | 1:21:A:LEU:HD13 | 1:30:A:PHE:H    | 9        | 0.1           |

## 10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found