



# Full wwPDB NMR Structure Validation Report ⓘ

Feb 28, 2026 – 06:59 PM UTC

PDB ID : 2KU6 / pdb\_00002ku6  
BMRB ID : 16723  
Title : Mouse Prion Protein (121-231) with mutations D167S and N173K  
Authors : Perez, D.R.; Damberger, F.F.; Wuthrich, K.  
Deposited on : 2010-02-12

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0  
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

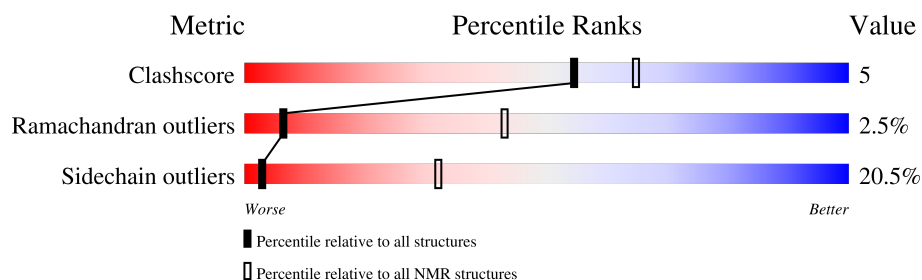
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 84%.

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     | 113    | <br>62% 23% • 12% |

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 9 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations*.

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:125-A:223 (99)      | 0.53              | 9            |

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 6 clusters and 6 single-model clusters were found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1809 atoms, of which 877 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Major prion protein.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|-------|
| 1   | A     | 113      | Total | C   | H   | N   | O   | S | 0     |
|     |       |          | 1809  | 579 | 877 | 164 | 180 | 9 |       |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| A     | 120     | SER      | -      | expression tag      | UNP P04925 |
| A     | 167     | SER      | ASP    | engineered mutation | UNP P04925 |
| A     | 173     | LYS      | ASN    | engineered mutation | UNP P04925 |

## 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: Major prion protein

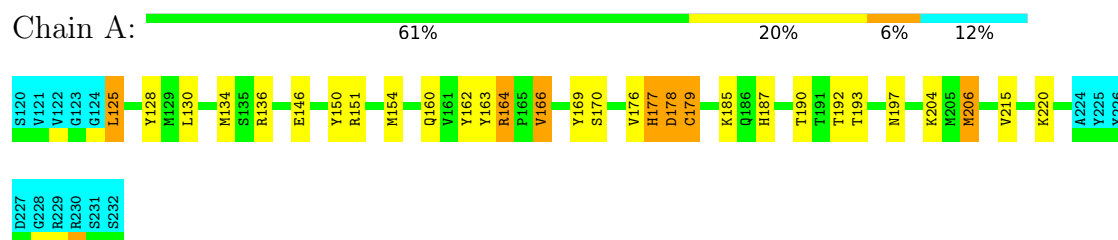


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

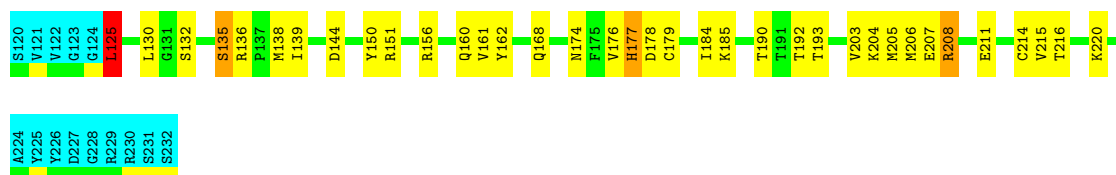
- Molecule 1: Major prion protein



#### 4.2.2 Score per residue for model 2

- Molecule 1: Major prion protein

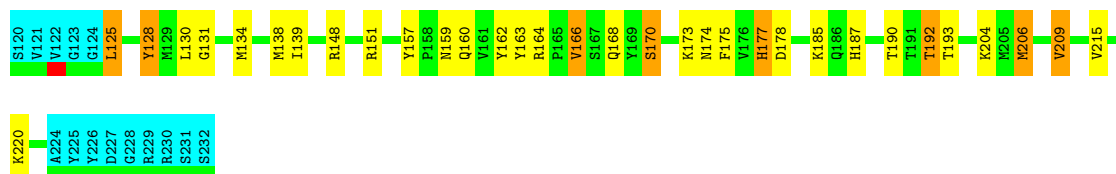




#### 4.2.3 Score per residue for model 3

- Molecule 1: Major prion protein

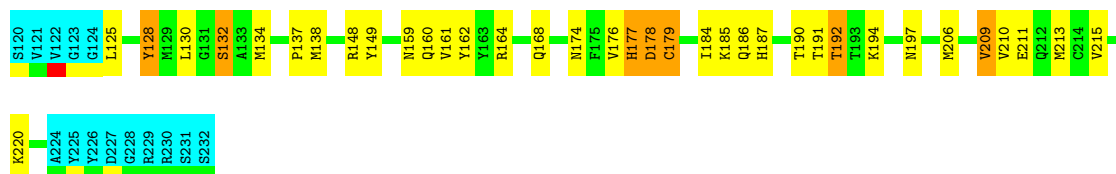
Chain A: 58% 22% 7% 12%



#### 4.2.4 Score per residue for model 4

- Molecule 1: Major prion protein

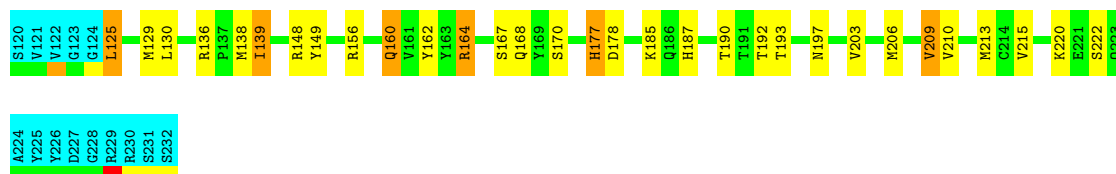
Chain A: 56% 26% 6% 12%



#### 4.2.5 Score per residue for model 5

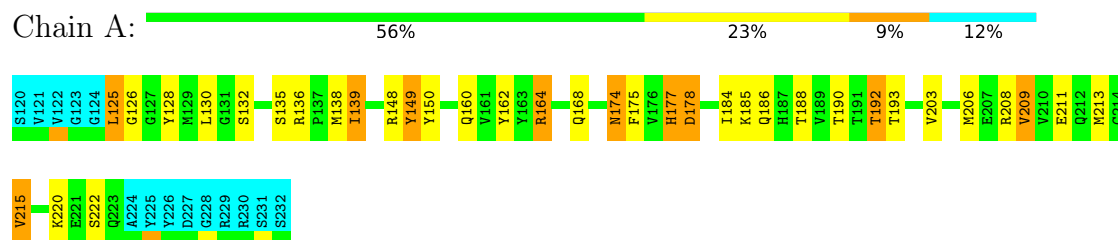
- Molecule 1: Major prion protein

Chain A: 60% 22% 5% 12%



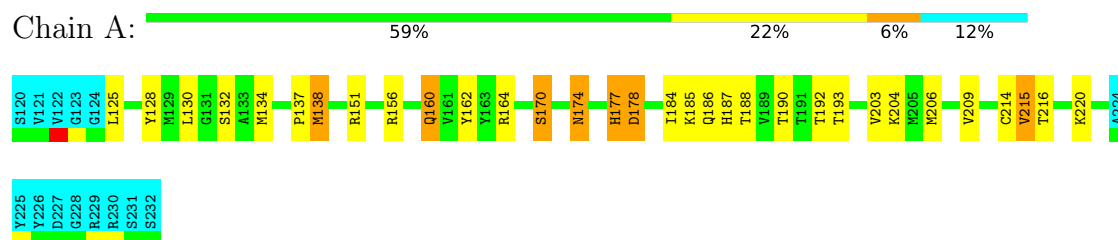
#### 4.2.6 Score per residue for model 6

- Molecule 1: Major prion protein



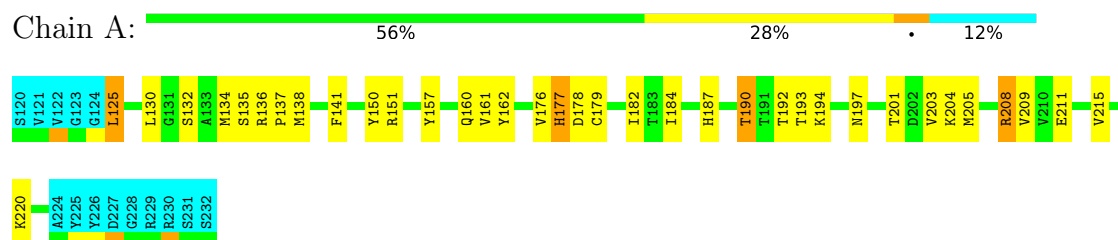
#### 4.2.7 Score per residue for model 7

- Molecule 1: Major prion protein



#### 4.2.8 Score per residue for model 8

- Molecule 1: Major prion protein



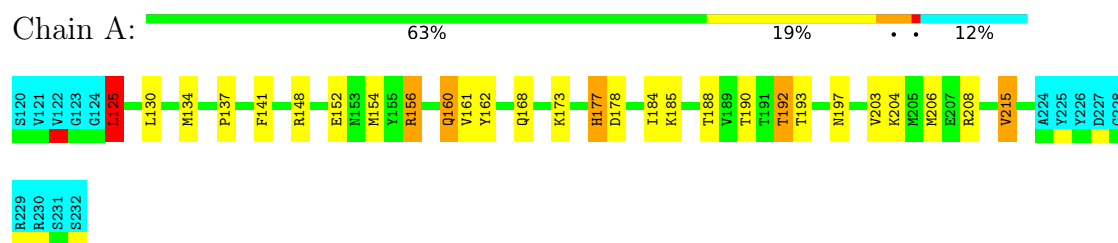
#### 4.2.9 Score per residue for model 9 (medoid)

- Molecule 1: Major prion protein



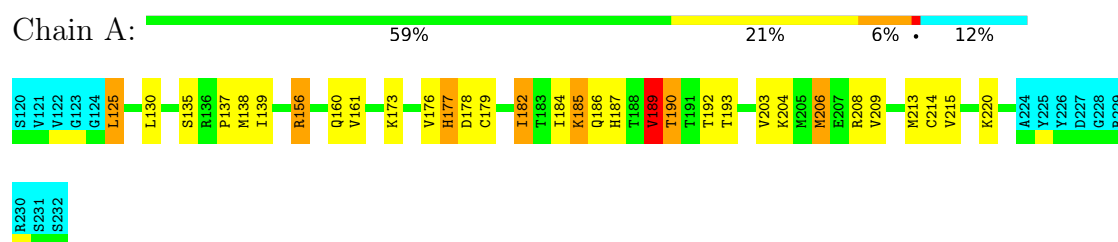
### 4.2.10 Score per residue for model 10

- Molecule 1: Major prion protein



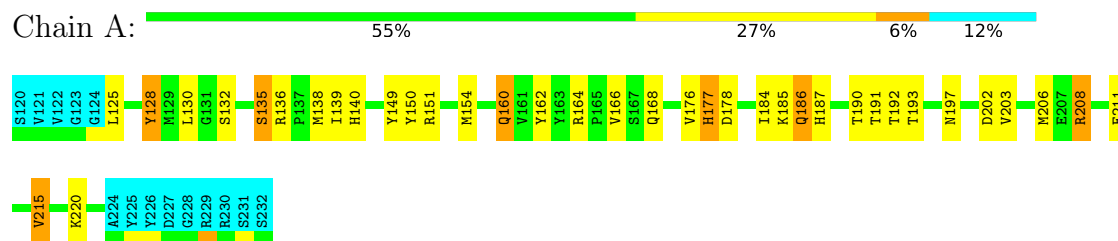
### 4.2.11 Score per residue for model 11

- Molecule 1: Major prion protein



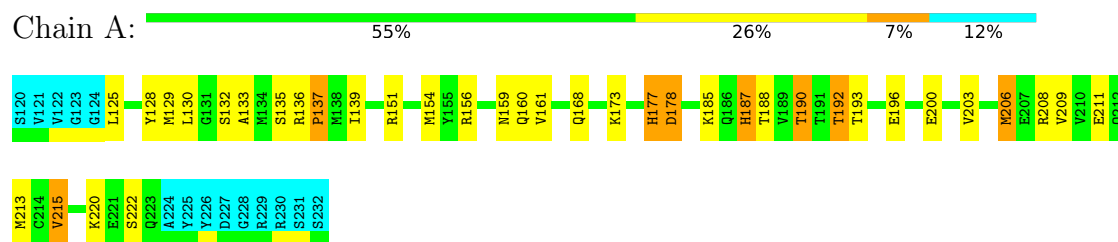
### 4.2.12 Score per residue for model 12

- Molecule 1: Major prion protein



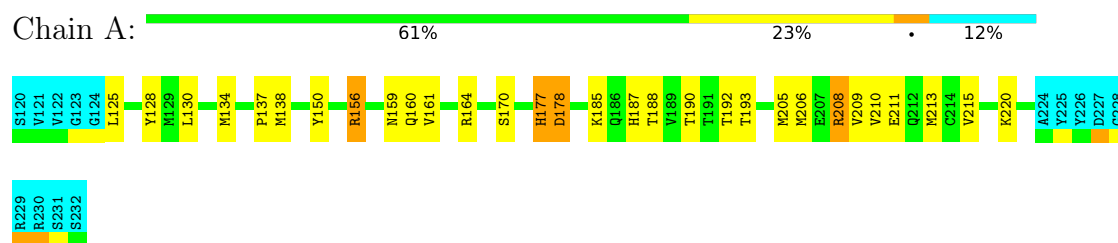
### 4.2.13 Score per residue for model 13

- Molecule 1: Major prion protein



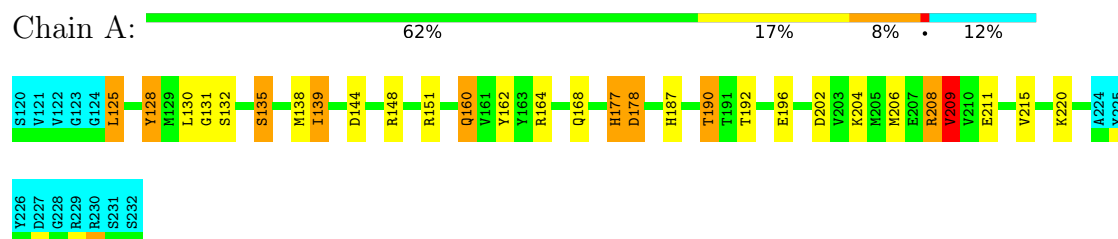
### 4.2.14 Score per residue for model 14

- Molecule 1: Major prion protein



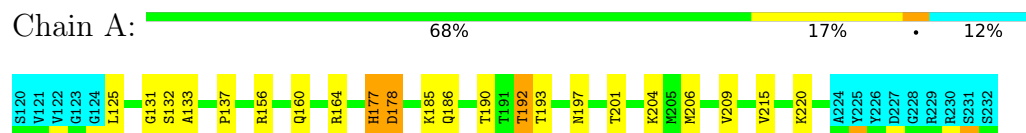
### 4.2.15 Score per residue for model 15

- Molecule 1: Major prion protein



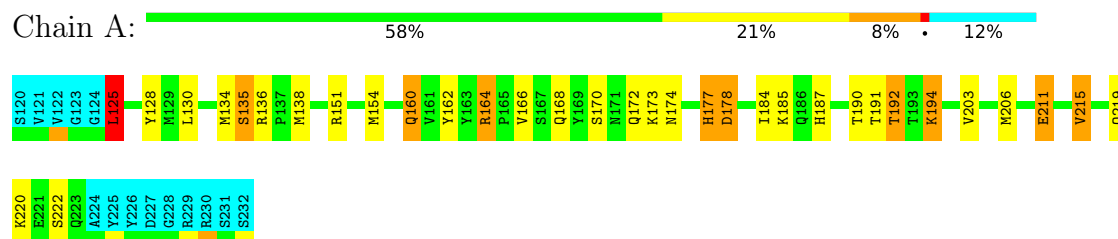
### 4.2.16 Score per residue for model 16

- Molecule 1: Major prion protein



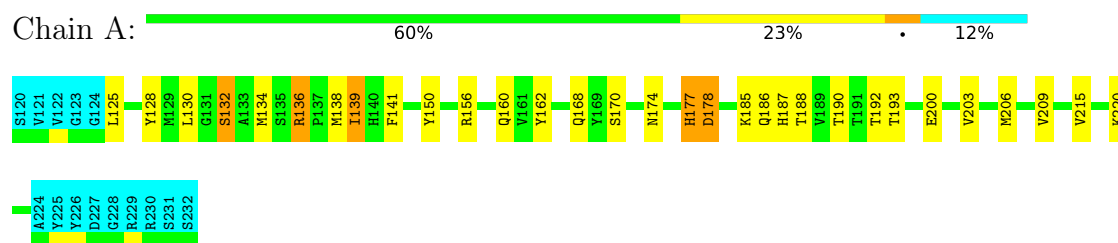
### 4.2.17 Score per residue for model 17

- Molecule 1: Major prion protein



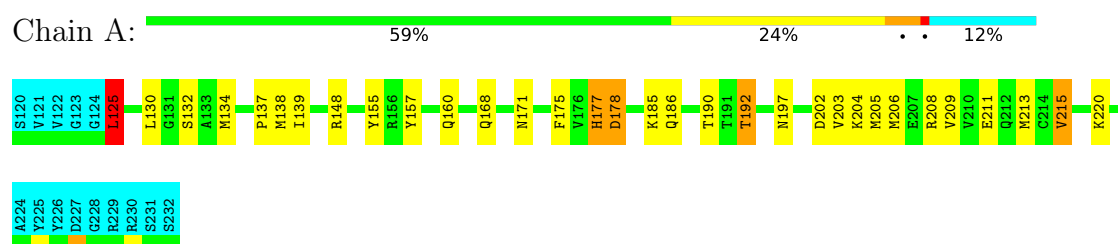
### 4.2.18 Score per residue for model 18

- Molecule 1: Major prion protein



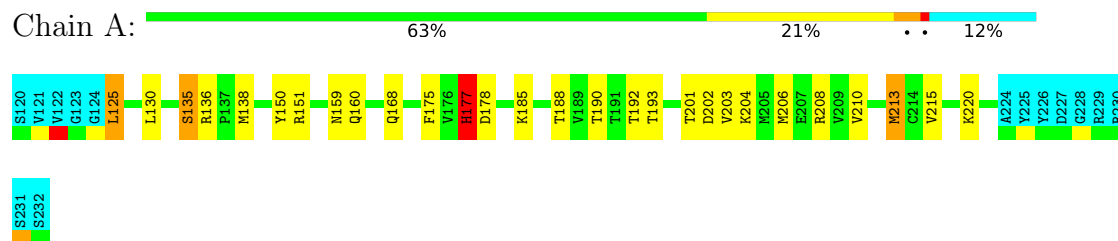
### 4.2.19 Score per residue for model 19

- Molecule 1: Major prion protein



### 4.2.20 Score per residue for model 20

- Molecule 1: Major prion protein



## 5 Refinement protocol and experimental data overview

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

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

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

| Software name | Classification | Version |
|---------------|----------------|---------|
| OPALp         | refinement     |         |

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

|                                              |                |
|----------------------------------------------|----------------|
| Chemical shift file(s)                       | working_cs.cif |
| Number of chemical shift lists               | 1              |
| Total number of shifts                       | 1297           |
| Number of shifts mapped to atoms             | 1297           |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 84%            |

## 6 Model quality i

### 6.1 Standard geometry i

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

| Mol | Chain | Bond lengths |                      | Bond angles |                       |
|-----|-------|--------------|----------------------|-------------|-----------------------|
|     |       | RMSZ         | #Z>5                 | RMSZ        | #Z>5                  |
| 1   | A     | 0.72±0.01    | 0±0/849 ( 0.0± 0.0%) | 1.52±0.04   | 4±3/1147 ( 0.4± 0.2%) |
| All | All   | 0.72         | 0/16980 ( 0.0%)      | 1.52        | 89/22940 ( 0.4%)      |

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   | 2.6±1.3   |
| All | All   | 0         | 53        |

There are no bond-length outliers.

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

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|-----------|-------|-------------|----------|--------|-------|
|     |       |     |      |           |       |             |          | Worst  | Total |
| 1   | A     | 161 | VAL  | CA-CB-CG2 | 10.08 | 127.53      | 110.40   | 10     | 1     |
| 1   | A     | 189 | VAL  | CA-CB-CG2 | 8.71  | 125.21      | 110.40   | 11     | 1     |
| 1   | A     | 178 | ASP  | CA-CB-CG  | 8.36  | 120.96      | 112.60   | 6      | 2     |
| 1   | A     | 174 | ASN  | CA-CB-CG  | 8.32  | 120.92      | 112.60   | 7      | 4     |
| 1   | A     | 192 | THR  | CA-C-N    | 7.75  | 131.00      | 120.38   | 10     | 7     |
| 1   | A     | 192 | THR  | C-N-CA    | 7.75  | 131.00      | 120.38   | 10     | 7     |
| 1   | A     | 208 | ARG  | CD-NE-CZ  | 7.43  | 134.80      | 124.40   | 12     | 1     |
| 1   | A     | 176 | VAL  | CA-CB-CG2 | 7.06  | 122.41      | 110.40   | 12     | 1     |
| 1   | A     | 202 | ASP  | CA-CB-CG  | 6.87  | 119.47      | 112.60   | 20     | 2     |
| 1   | A     | 209 | VAL  | CA-CB-CG1 | 6.51  | 121.46      | 110.40   | 5      | 6     |
| 1   | A     | 175 | PHE  | CA-C-N    | 6.33  | 129.13      | 120.46   | 20     | 2     |
| 1   | A     | 175 | PHE  | C-N-CA    | 6.33  | 129.13      | 120.46   | 20     | 2     |
| 1   | A     | 190 | THR  | CA-CB-CG2 | 6.33  | 121.26      | 110.50   | 15     | 4     |
| 1   | A     | 128 | TYR  | CA-C-N    | 6.26  | 131.35      | 122.09   | 13     | 1     |
| 1   | A     | 128 | TYR  | C-N-CA    | 6.26  | 131.35      | 122.09   | 13     | 1     |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|------------|-------|-------------|----------|--------|-------|
|     |       |     |      |            |       |             |          | Worst  | Total |
| 1   | A     | 187 | HIS  | CB-CA-C    | 6.19  | 118.64      | 109.29   | 15     | 3     |
| 1   | A     | 186 | GLN  | OE1-CD-NE2 | -5.83 | 116.77      | 122.60   | 12     | 1     |
| 1   | A     | 160 | GLN  | OE1-CD-NE2 | 5.75  | 128.35      | 122.60   | 11     | 1     |
| 1   | A     | 187 | HIS  | CB-CG-CD2  | -5.72 | 123.76      | 131.20   | 12     | 6     |
| 1   | A     | 188 | THR  | CA-CB-CG2  | 5.71  | 120.20      | 110.50   | 7      | 5     |
| 1   | A     | 131 | GLY  | CA-C-N     | 5.69  | 132.41      | 121.54   | 3      | 2     |
| 1   | A     | 131 | GLY  | C-N-CA     | 5.69  | 132.41      | 121.54   | 3      | 2     |
| 1   | A     | 164 | ARG  | CD-NE-CZ   | 5.65  | 132.31      | 124.40   | 5      | 1     |
| 1   | A     | 166 | VAL  | CA-CB-CG2  | 5.56  | 119.86      | 110.40   | 1      | 4     |
| 1   | A     | 215 | VAL  | CB-CA-C    | 5.52  | 119.03      | 111.97   | 7      | 2     |
| 1   | A     | 202 | ASP  | CA-C-N     | 5.40  | 127.57      | 120.60   | 12     | 1     |
| 1   | A     | 202 | ASP  | C-N-CA     | 5.40  | 127.57      | 120.60   | 12     | 1     |
| 1   | A     | 200 | GLU  | N-CA-CB    | 5.38  | 118.02      | 110.12   | 18     | 1     |
| 1   | A     | 220 | LYS  | CA-C-N     | 5.33  | 127.86      | 120.29   | 13     | 1     |
| 1   | A     | 220 | LYS  | C-N-CA     | 5.33  | 127.86      | 120.29   | 13     | 1     |
| 1   | A     | 125 | LEU  | CB-CA-C    | 5.25  | 120.18      | 112.09   | 6      | 1     |
| 1   | A     | 174 | ASN  | N-CA-CB    | 5.23  | 118.27      | 110.22   | 18     | 1     |
| 1   | A     | 222 | SER  | N-CA-C     | -5.22 | 105.28      | 110.97   | 6      | 1     |
| 1   | A     | 216 | THR  | CA-C-N     | 5.17  | 127.53      | 120.54   | 7      | 1     |
| 1   | A     | 216 | THR  | C-N-CA     | 5.17  | 127.53      | 120.54   | 7      | 1     |
| 1   | A     | 170 | SER  | N-CA-CB    | -5.17 | 105.59      | 111.79   | 5      | 1     |
| 1   | A     | 140 | HIS  | CB-CG-CD2  | -5.10 | 124.56      | 131.20   | 12     | 1     |
| 1   | A     | 192 | THR  | CA-CB-CG2  | 5.07  | 119.12      | 110.50   | 17     | 1     |
| 1   | A     | 138 | MET  | CB-CA-C    | 5.06  | 118.63      | 109.37   | 7      | 1     |
| 1   | A     | 211 | GLU  | CA-C-O     | -5.03 | 115.53      | 121.07   | 17     | 1     |
| 1   | A     | 203 | VAL  | N-CA-CB    | 5.03  | 116.43      | 110.55   | 20     | 1     |
| 1   | A     | 177 | HIS  | CA-CB-CG   | 5.02  | 118.82      | 113.80   | 20     | 1     |
| 1   | A     | 214 | CYS  | CA-C-N     | 5.01  | 126.87      | 120.56   | 7      | 1     |
| 1   | A     | 214 | CYS  | C-N-CA     | 5.01  | 126.87      | 120.56   | 7      | 1     |
| 1   | A     | 209 | VAL  | CA-CB-CG2  | 5.00  | 118.91      | 110.40   | 3      | 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     | 150 | TYR  | Sidechain | 8              |
| 1   | A     | 151 | ARG  | Sidechain | 8              |
| 1   | A     | 148 | ARG  | Sidechain | 7              |
| 1   | A     | 164 | ARG  | Sidechain | 4              |
| 1   | A     | 128 | TYR  | Sidechain | 4              |

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| Mol | Chain | Res | Type | Group     | Models (Total) |
|-----|-------|-----|------|-----------|----------------|
| 1   | A     | 149 | TYR  | Sidechain | 4              |
| 1   | A     | 156 | ARG  | Sidechain | 4              |
| 1   | A     | 136 | ARG  | Sidechain | 3              |
| 1   | A     | 208 | ARG  | Sidechain | 2              |
| 1   | A     | 157 | TYR  | Sidechain | 2              |
| 1   | A     | 175 | PHE  | Sidechain | 2              |
| 1   | A     | 137 | PRO  | Peptide   | 2              |
| 1   | A     | 163 | TYR  | Sidechain | 1              |
| 1   | A     | 169 | TYR  | Sidechain | 1              |
| 1   | A     | 155 | TYR  | Sidechain | 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     | 829   | 782      | 784      | 8±2     |
| All | All   | 16580 | 15640    | 15680    | 163     |

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 5.

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

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:139:ILE:HD11 | 1:A:209:VAL:HG12 | 0.69     | 1.64        | 15     | 3     |
| 1:A:187:HIS:CE1  | 1:A:206:MET:HE2  | 0.69     | 2.22        | 13     | 2     |
| 1:A:211:GLU:O    | 1:A:215:VAL:HG23 | 0.68     | 1.89        | 12     | 9     |
| 1:A:185:LYS:O    | 1:A:189:VAL:HG22 | 0.68     | 1.88        | 11     | 1     |
| 1:A:177:HIS:CG   | 1:A:178:ASP:H    | 0.65     | 2.09        | 8      | 20    |
| 1:A:177:HIS:CD2  | 1:A:178:ASP:H    | 0.65     | 2.09        | 12     | 15    |
| 1:A:130:LEU:HD11 | 1:A:160:GLN:HB3  | 0.65     | 1.69        | 3      | 12    |
| 1:A:125:LEU:H    | 1:A:125:LEU:HD23 | 0.64     | 1.53        | 9      | 4     |
| 1:A:130:LEU:HD13 | 1:A:162:TYR:CE1  | 0.63     | 2.29        | 10     | 14    |
| 1:A:139:ILE:HD11 | 1:A:209:VAL:CG1  | 0.62     | 2.24        | 5      | 3     |
| 1:A:137:PRO:CG   | 1:A:209:VAL:HG13 | 0.60     | 2.26        | 14     | 6     |
| 1:A:125:LEU:HD22 | 1:A:182:ILE:HG23 | 0.60     | 1.73        | 8      | 1     |
| 1:A:161:VAL:HG13 | 1:A:213:MET:HE2  | 0.59     | 1.72        | 14     | 3     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:125:LEU:HD11 | 1:A:186:GLN:NE2  | 0.59     | 2.12        | 11     | 1     |
| 1:A:125:LEU:HD12 | 1:A:182:ILE:CG2  | 0.57     | 2.29        | 11     | 1     |
| 1:A:176:VAL:HA   | 1:A:179:CYS:SG   | 0.56     | 2.40        | 8      | 5     |
| 1:A:137:PRO:HG3  | 1:A:209:VAL:HG13 | 0.55     | 1.77        | 11     | 5     |
| 1:A:191:THR:CG2  | 1:A:194:LYS:HE3  | 0.55     | 2.32        | 17     | 2     |
| 1:A:125:LEU:HD23 | 1:A:125:LEU:N    | 0.54     | 2.16        | 9      | 3     |
| 1:A:137:PRO:HG2  | 1:A:209:VAL:HG13 | 0.53     | 1.78        | 7      | 1     |
| 1:A:159:ASN:C    | 1:A:213:MET:HE3  | 0.53     | 2.28        | 14     | 3     |
| 1:A:161:VAL:HG11 | 1:A:214:CYS:SG   | 0.50     | 2.47        | 11     | 1     |
| 1:A:157:TYR:HB3  | 1:A:209:VAL:HG11 | 0.50     | 1.82        | 8      | 1     |
| 1:A:141:PHE:CZ   | 1:A:205:MET:SD   | 0.49     | 3.05        | 8      | 1     |
| 1:A:184:ILE:HD11 | 1:A:207:GLU:HA   | 0.49     | 1.85        | 2      | 1     |
| 1:A:130:LEU:HD12 | 1:A:161:VAL:O    | 0.48     | 2.08        | 14     | 5     |
| 1:A:128:TYR:CD1  | 1:A:164:ARG:HG2  | 0.48     | 2.44        | 14     | 5     |
| 1:A:177:HIS:CG   | 1:A:178:ASP:N    | 0.48     | 2.81        | 14     | 9     |
| 1:A:191:THR:HG23 | 1:A:194:LYS:HE3  | 0.48     | 1.85        | 17     | 1     |
| 1:A:125:LEU:H    | 1:A:125:LEU:CD2  | 0.47     | 2.21        | 9      | 1     |
| 1:A:139:ILE:CD1  | 1:A:209:VAL:HG12 | 0.47     | 2.38        | 15     | 1     |
| 1:A:160:GLN:N    | 1:A:213:MET:HE3  | 0.47     | 2.24        | 14     | 1     |
| 1:A:139:ILE:HB   | 1:A:141:PHE:CE2  | 0.47     | 2.44        | 18     | 1     |
| 1:A:187:HIS:CE1  | 1:A:206:MET:HE3  | 0.47     | 2.45        | 1      | 4     |
| 1:A:125:LEU:HD11 | 1:A:186:GLN:HE21 | 0.46     | 1.69        | 11     | 1     |
| 1:A:177:HIS:CD2  | 1:A:178:ASP:N    | 0.46     | 2.82        | 12     | 1     |
| 1:A:130:LEU:HD13 | 1:A:162:TYR:CD1  | 0.46     | 2.46        | 12     | 2     |
| 1:A:188:THR:OG1  | 1:A:206:MET:HE1  | 0.45     | 2.12        | 13     | 1     |
| 1:A:125:LEU:O    | 1:A:125:LEU:HD12 | 0.45     | 2.12        | 6      | 1     |
| 1:A:179:CYS:SG   | 1:A:214:CYS:HB3  | 0.44     | 2.52        | 2      | 1     |
| 1:A:163:TYR:CD2  | 1:A:175:PHE:CZ   | 0.44     | 3.06        | 3      | 1     |
| 1:A:208:ARG:N    | 1:A:208:ARG:CD   | 0.43     | 2.81        | 15     | 2     |
| 1:A:128:TYR:CD1  | 1:A:164:ARG:HG3  | 0.43     | 2.49        | 15     | 3     |
| 1:A:200:GLU:HA   | 1:A:203:VAL:HG22 | 0.43     | 1.89        | 13     | 1     |
| 1:A:172:GLN:HE22 | 1:A:219:GLN:NE2  | 0.43     | 2.12        | 17     | 1     |
| 1:A:149:TYR:CD1  | 1:A:149:TYR:C    | 0.41     | 2.98        | 6      | 1     |
| 1:A:210:VAL:HG22 | 1:A:213:MET:HE1  | 0.40     | 1.94        | 9      | 1     |

## 6.3 Torsion angles ⓘ

### 6.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR

entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

| Mol | Chain | Analysed        | Favoured     | Allowed      | Outliers   | Percentiles |    |
|-----|-------|-----------------|--------------|--------------|------------|-------------|----|
| 1   | A     | 99/113 (88%)    | 84±3 (85±3%) | 12±3 (12±3%) | 2±1 (3±1%) | 6           | 43 |
| All | All   | 1980/2260 (88%) | 1683 (85%)   | 247 (12%)    | 50 (3%)    | 6           | 43 |

All 10 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     | 177 | HIS  | 20             |
| 1   | A     | 132 | SER  | 8              |
| 1   | A     | 125 | LEU  | 6              |
| 1   | A     | 170 | SER  | 5              |
| 1   | A     | 135 | SER  | 5              |
| 1   | A     | 133 | ALA  | 2              |
| 1   | A     | 209 | VAL  | 1              |
| 1   | A     | 126 | GLY  | 1              |
| 1   | A     | 141 | PHE  | 1              |
| 1   | A     | 131 | GLY  | 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     | 93/103 (90%)    | 74±2 (80±2%) | 19±2 (20±2%) | 3           | 32 |
| All | All   | 1860/2060 (90%) | 1479 (80%)   | 381 (20%)    | 3           | 32 |

All 57 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     | 190 | THR  | 20             |
| 1   | A     | 192 | THR  | 20             |
| 1   | A     | 125 | LEU  | 19             |
| 1   | A     | 185 | LYS  | 18             |
| 1   | A     | 220 | LYS  | 18             |
| 1   | A     | 206 | MET  | 17             |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 193 | THR  | 16             |
| 1   | A     | 215 | VAL  | 16             |
| 1   | A     | 138 | MET  | 16             |
| 1   | A     | 168 | GLN  | 14             |
| 1   | A     | 160 | GLN  | 13             |
| 1   | A     | 204 | LYS  | 12             |
| 1   | A     | 203 | VAL  | 12             |
| 1   | A     | 139 | ILE  | 11             |
| 1   | A     | 208 | ARG  | 11             |
| 1   | A     | 134 | MET  | 10             |
| 1   | A     | 178 | ASP  | 10             |
| 1   | A     | 197 | ASN  | 9              |
| 1   | A     | 135 | SER  | 9              |
| 1   | A     | 136 | ARG  | 8              |
| 1   | A     | 156 | ARG  | 8              |
| 1   | A     | 184 | ILE  | 8              |
| 1   | A     | 132 | SER  | 6              |
| 1   | A     | 186 | GLN  | 6              |
| 1   | A     | 213 | MET  | 6              |
| 1   | A     | 154 | MET  | 5              |
| 1   | A     | 174 | ASN  | 5              |
| 1   | A     | 173 | LYS  | 5              |
| 1   | A     | 210 | VAL  | 5              |
| 1   | A     | 205 | MET  | 3              |
| 1   | A     | 170 | SER  | 3              |
| 1   | A     | 164 | ARG  | 3              |
| 1   | A     | 222 | SER  | 3              |
| 1   | A     | 201 | THR  | 3              |
| 1   | A     | 166 | VAL  | 2              |
| 1   | A     | 179 | CYS  | 2              |
| 1   | A     | 144 | ASP  | 2              |
| 1   | A     | 159 | ASN  | 2              |
| 1   | A     | 209 | VAL  | 2              |
| 1   | A     | 128 | TYR  | 2              |
| 1   | A     | 129 | MET  | 2              |
| 1   | A     | 151 | ARG  | 2              |
| 1   | A     | 194 | LYS  | 2              |
| 1   | A     | 196 | GLU  | 2              |
| 1   | A     | 146 | GLU  | 1              |
| 1   | A     | 216 | THR  | 1              |
| 1   | A     | 167 | SER  | 1              |
| 1   | A     | 183 | THR  | 1              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 223 | GLN  | 1              |
| 1   | A     | 152 | GLU  | 1              |
| 1   | A     | 182 | ILE  | 1              |
| 1   | A     | 189 | VAL  | 1              |
| 1   | A     | 191 | THR  | 1              |
| 1   | A     | 211 | GLU  | 1              |
| 1   | A     | 171 | ASN  | 1              |
| 1   | A     | 202 | ASP  | 1              |
| 1   | A     | 188 | THR  | 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](#)

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 84% for the well-defined parts and 83% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

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

#### 7.1.1 Bookkeeping

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                  | 1297 |
| Number of shifts mapped to atoms        | 1297 |
| 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           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 113      | $0.24 \pm 0.17$                 | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}_\beta$  | 105      | $0.63 \pm 0.13$                 | Should be applied          |
| $^{13}\text{C}'$       | 0        | —                               | None (insufficient data)   |
| $^{15}\text{N}$        | 110      | $0.17 \pm 0.17$                 | 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 84%, i.e. 1165 atoms were assigned a chemical shift out of a possible 1384. 0 out of 11 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total         | $^1\text{H}$  | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|---------------|---------------|-----------------|-----------------|
| Backbone  | 390/494 (79%) | 195/200 (98%) | 99/198 (50%)    | 96/96 (100%)    |
| Sidechain | 673/746 (90%) | 455/478 (95%) | 197/230 (86%)   | 21/38 (55%)     |

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|          | Total           | $^1\text{H}$  | $^{13}\text{C}$ | $^{15}\text{N}$ |
|----------|-----------------|---------------|-----------------|-----------------|
| Aromatic | 102/144 (71%)   | 63/69 (91%)   | 38/71 (54%)     | 1/4 (25%)       |
| Overall  | 1165/1384 (84%) | 713/747 (95%) | 334/499 (67%)   | 118/138 (86%)   |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 83%, i.e. 1296 atoms were assigned a chemical shift out of a possible 1554. 0 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total           | $^1\text{H}$  | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|-----------------|---------------|-----------------|-----------------|
| Backbone  | 448/567 (79%)   | 225/231 (97%) | 113/226 (50%)   | 110/110 (100%)  |
| Sidechain | 734/825 (89%)   | 497/529 (94%) | 215/252 (85%)   | 22/44 (50%)     |
| Aromatic  | 114/162 (70%)   | 71/77 (92%)   | 42/81 (52%)     | 1/4 (25%)       |
| Overall   | 1296/1554 (83%) | 793/837 (95%) | 370/559 (66%)   | 133/158 (84%)   |

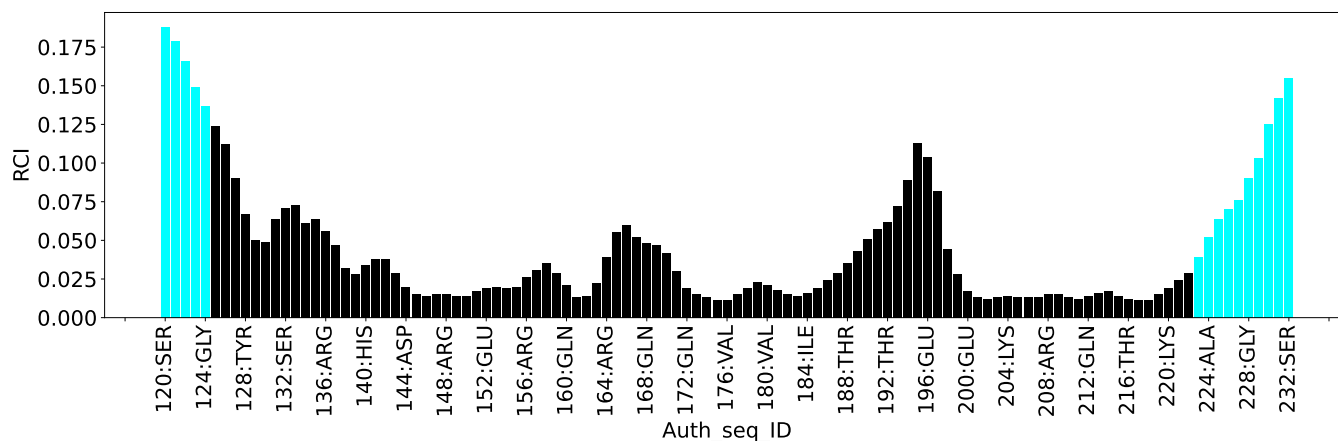
#### 7.1.4 Statistically unusual chemical shifts [i](#)

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                                | 2853  |
| Intra-residue ( $ i-j =0$ )                              | 501   |
| Sequential ( $ i-j =1$ )                                 | 795   |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 834   |
| Long range ( $ i-j \geq 5$ )                             | 723   |
| 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                         | 25.2  |
| Number of long range restraints per residue <sup>1</sup> | 6.4   |

<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)  | 39.4                                   | 0.2     |
| 0.2-0.5 (Medium) | 50.9                                   | 0.5     |
| >0.5 (Large)     | 99.1                                   | 3.83    |

### 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 ⓘ

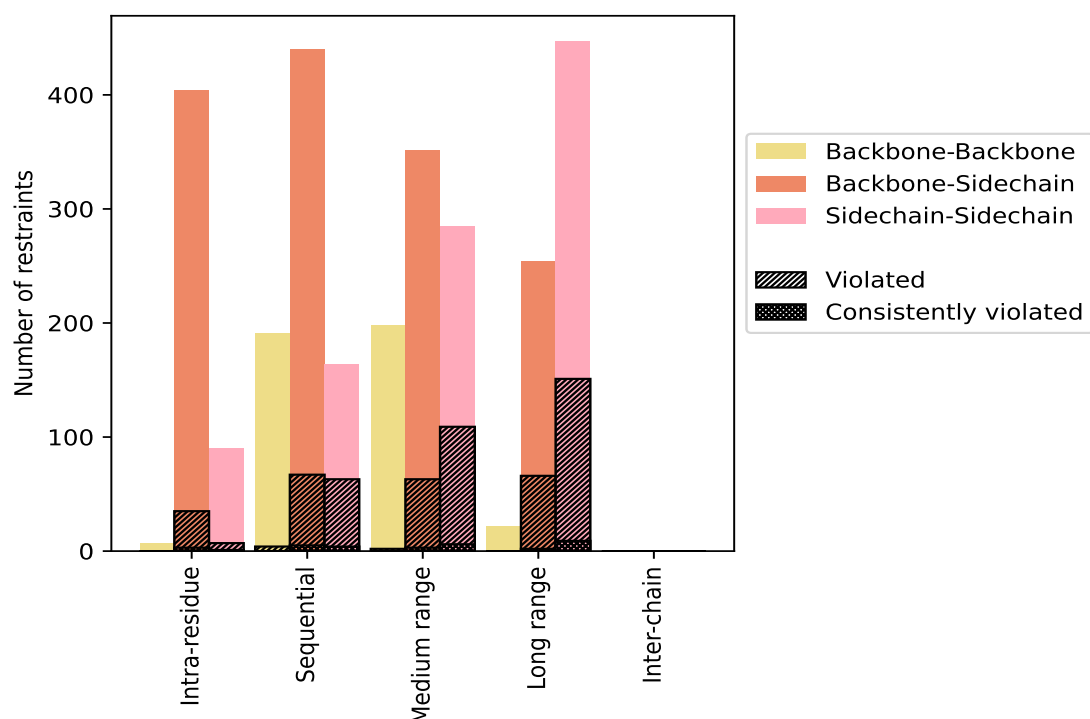
### 9.1 Summary of distance violations ⓘ

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> |
| <b>Intra-residue (<math> i-j =0</math>)</b>                                 | <b>501</b>  | <b>17.6</b>    | <b>42</b>             | <b>8.4</b>     | <b>1.5</b>     | <b>4</b>                           | <b>0.8</b>     | <b>0.1</b>     |
| Backbone-Backbone                                                           | 7           | 0.2            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 404         | 14.2           | 35                    | 8.7            | 1.2            | 3                                  | 0.7            | 0.1            |
| Sidechain-Sidechain                                                         | 90          | 3.2            | 7                     | 7.8            | 0.2            | 1                                  | 1.1            | 0.0            |
| <b>Sequential (<math> i-j =1</math>)</b>                                    | <b>795</b>  | <b>27.9</b>    | <b>134</b>            | <b>16.9</b>    | <b>4.7</b>     | <b>9</b>                           | <b>1.1</b>     | <b>0.3</b>     |
| Backbone-Backbone                                                           | 191         | 6.7            | 4                     | 2.1            | 0.1            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 440         | 15.4           | 67                    | 15.2           | 2.3            | 5                                  | 1.1            | 0.2            |
| Sidechain-Sidechain                                                         | 164         | 5.7            | 63                    | 38.4           | 2.2            | 4                                  | 2.4            | 0.1            |
| <b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b> | <b>834</b>  | <b>29.2</b>    | <b>174</b>            | <b>20.9</b>    | <b>6.1</b>     | <b>9</b>                           | <b>1.1</b>     | <b>0.3</b>     |
| Backbone-Backbone                                                           | 198         | 6.9            | 2                     | 1.0            | 0.1            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 351         | 12.3           | 63                    | 17.9           | 2.2            | 3                                  | 0.9            | 0.1            |
| Sidechain-Sidechain                                                         | 285         | 10.0           | 109                   | 38.2           | 3.8            | 6                                  | 2.1            | 0.2            |
| <b>Long range (<math> i-j \geq 5</math>)</b>                                | <b>723</b>  | <b>25.3</b>    | <b>217</b>            | <b>30.0</b>    | <b>7.6</b>     | <b>11</b>                          | <b>1.5</b>     | <b>0.4</b>     |
| Backbone-Backbone                                                           | 22          | 0.8            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 254         | 8.9            | 66                    | 26.0           | 2.3            | 2                                  | 0.8            | 0.1            |
| Sidechain-Sidechain                                                         | 447         | 15.7           | 151                   | 33.8           | 5.3            | 9                                  | 2.0            | 0.3            |
| <b>Inter-chain</b>                                                          | <b>0</b>    | <b>0.0</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| Backbone-Backbone                                                           | 0           | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 0           | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 0           | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| <b>Hydrogen bond</b>                                                        | <b>0</b>    | <b>0.0</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| <b>Disulfide bond</b>                                                       | <b>0</b>    | <b>0.0</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| <b>Total</b>                                                                | <b>2853</b> | <b>100.0</b>   | <b>567</b>            | <b>19.9</b>    | <b>19.9</b>    | <b>33</b>                          | <b>1.2</b>     | <b>1.2</b>     |
| Backbone-Backbone                                                           | 418         | 14.7           | 6                     | 1.4            | 0.2            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 1449        | 50.8           | 231                   | 15.9           | 8.1            | 13                                 | 0.9            | 0.5            |
| Sidechain-Sidechain                                                         | 986         | 34.6           | 330                   | 33.5           | 11.6           | 20                                 | 2.0            | 0.7            |

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

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



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

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

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

| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 1        | 13                   | 52              | 62              | 73              | 0               | 200   | 0.65     | 3.61    | 0.54                | 0.5        |
| 2        | 19                   | 56              | 67              | 74              | 0               | 216   | 0.72     | 2.33    | 0.57                | 0.57       |
| 3        | 14                   | 46              | 51              | 69              | 0               | 180   | 0.59     | 3.73    | 0.53                | 0.45       |
| 4        | 14                   | 56              | 64              | 72              | 0               | 206   | 0.66     | 2.63    | 0.5                 | 0.55       |
| 5        | 16                   | 48              | 57              | 60              | 0               | 181   | 0.6      | 2.78    | 0.49                | 0.44       |
| 6        | 18                   | 48              | 57              | 62              | 0               | 185   | 0.65     | 2.94    | 0.54                | 0.51       |
| 7        | 20                   | 51              | 57              | 74              | 0               | 202   | 0.64     | 3.74    | 0.58                | 0.48       |
| 8        | 18                   | 57              | 75              | 82              | 0               | 232   | 0.7      | 3.72    | 0.62                | 0.52       |
| 9        | 14                   | 45              | 42              | 59              | 0               | 160   | 0.63     | 3.23    | 0.55                | 0.51       |
| 10       | 17                   | 53              | 45              | 93              | 0               | 208   | 0.69     | 3.69    | 0.61                | 0.5        |

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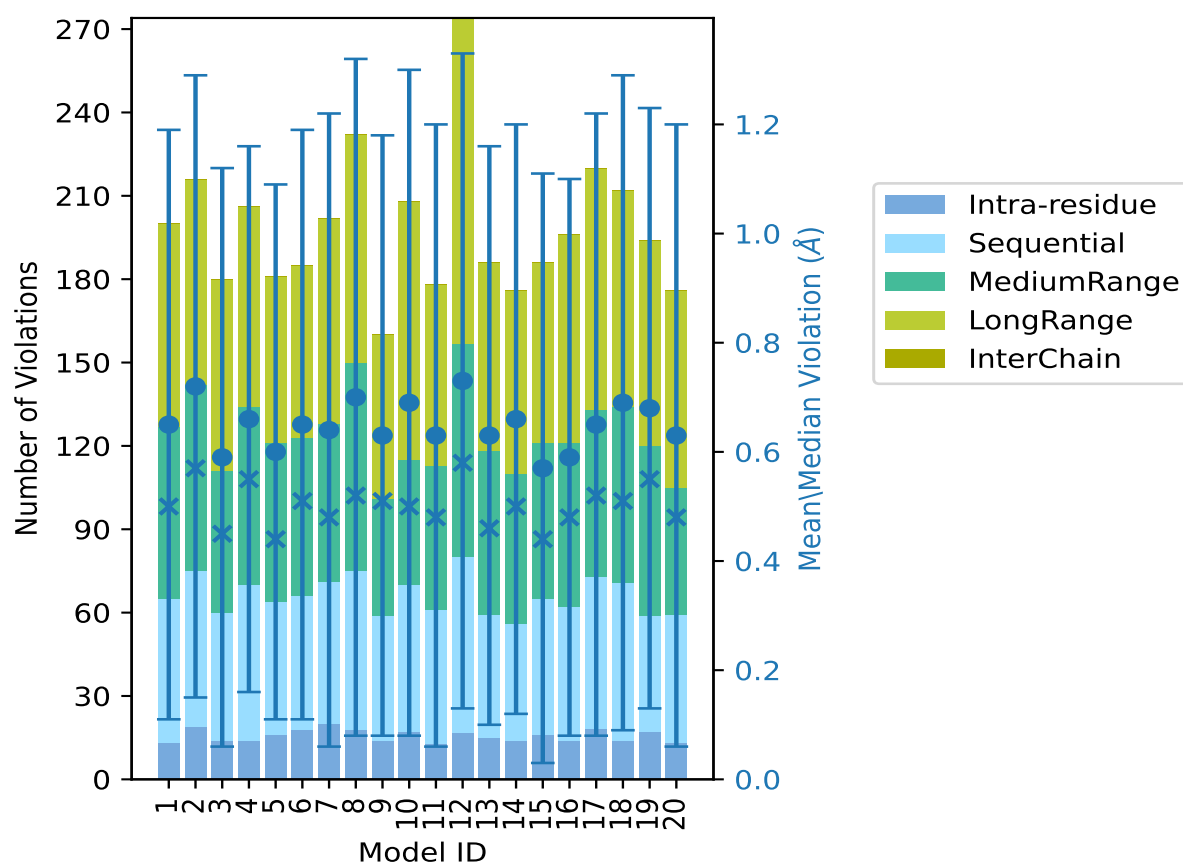
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| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 11       | 13                   | 48              | 52              | 65              | 0               | 178   | 0.63     | 3.26    | 0.57                | 0.48       |
| 12       | 17                   | 63              | 77              | 117             | 0               | 274   | 0.73     | 3.64    | 0.6                 | 0.58       |
| 13       | 15                   | 44              | 59              | 68              | 0               | 186   | 0.63     | 3.34    | 0.53                | 0.46       |
| 14       | 14                   | 42              | 54              | 66              | 0               | 176   | 0.66     | 2.91    | 0.54                | 0.5        |
| 15       | 16                   | 49              | 56              | 65              | 0               | 186   | 0.57     | 2.95    | 0.54                | 0.44       |
| 16       | 14                   | 48              | 59              | 75              | 0               | 196   | 0.59     | 2.79    | 0.51                | 0.48       |
| 17       | 18                   | 55              | 60              | 87              | 0               | 220   | 0.65     | 3.83    | 0.57                | 0.52       |
| 18       | 14                   | 57              | 63              | 78              | 0               | 212   | 0.69     | 3.28    | 0.6                 | 0.51       |
| 19       | 17                   | 42              | 61              | 74              | 0               | 194   | 0.68     | 3.33    | 0.55                | 0.55       |
| 20       | 13                   | 46              | 46              | 71              | 0               | 176   | 0.63     | 3.32    | 0.57                | 0.48       |

<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

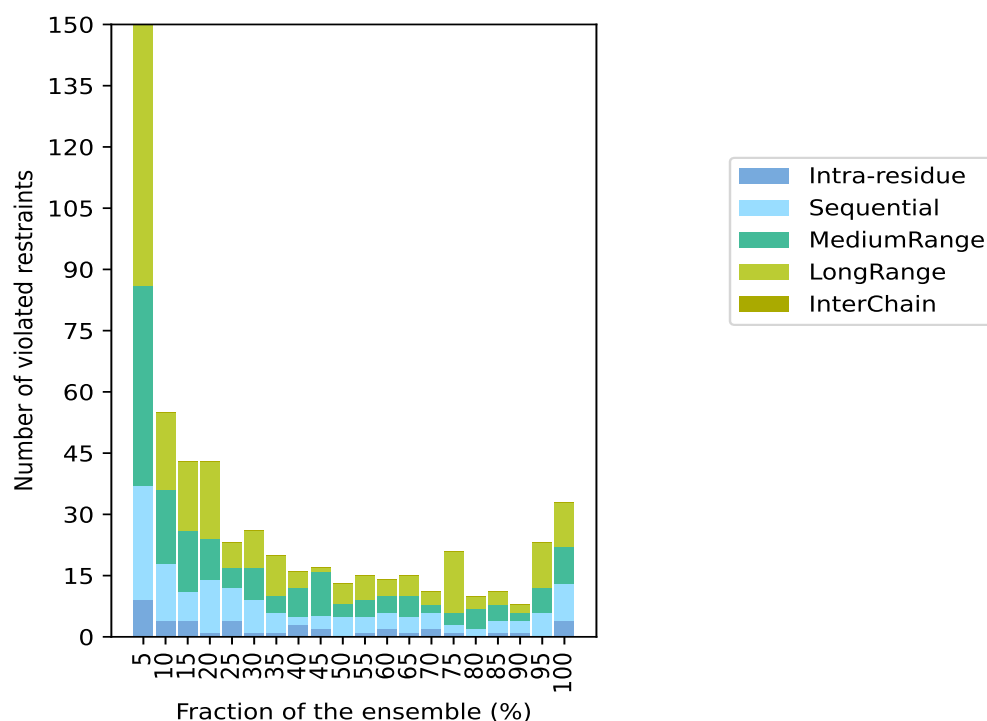
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 2286(IR:459, SQ:661, MR:660, LR:506, IC:0) restraints are 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>       | %     |
| 9                             | 28              | 49              | 64              | 0               | 150   | 1                        | 5.0   |
| 4                             | 14              | 18              | 19              | 0               | 55    | 2                        | 10.0  |
| 4                             | 7               | 15              | 17              | 0               | 43    | 3                        | 15.0  |
| 1                             | 13              | 10              | 19              | 0               | 43    | 4                        | 20.0  |
| 4                             | 8               | 5               | 6               | 0               | 23    | 5                        | 25.0  |
| 1                             | 8               | 8               | 9               | 0               | 26    | 6                        | 30.0  |
| 1                             | 5               | 4               | 10              | 0               | 20    | 7                        | 35.0  |
| 3                             | 2               | 7               | 4               | 0               | 16    | 8                        | 40.0  |
| 2                             | 3               | 11              | 1               | 0               | 17    | 9                        | 45.0  |
| 0                             | 5               | 3               | 5               | 0               | 13    | 10                       | 50.0  |
| 1                             | 4               | 4               | 6               | 0               | 15    | 11                       | 55.0  |
| 2                             | 4               | 4               | 4               | 0               | 14    | 12                       | 60.0  |
| 1                             | 4               | 5               | 5               | 0               | 15    | 13                       | 65.0  |
| 2                             | 4               | 2               | 3               | 0               | 11    | 14                       | 70.0  |
| 1                             | 2               | 3               | 15              | 0               | 21    | 15                       | 75.0  |
| 0                             | 2               | 5               | 3               | 0               | 10    | 16                       | 80.0  |
| 1                             | 3               | 4               | 3               | 0               | 11    | 17                       | 85.0  |
| 1                             | 3               | 2               | 2               | 0               | 8     | 18                       | 90.0  |
| 0                             | 6               | 6               | 11              | 0               | 23    | 19                       | 95.0  |
| 4                             | 9               | 9               | 11              | 0               | 33    | 20                       | 100.0 |

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

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

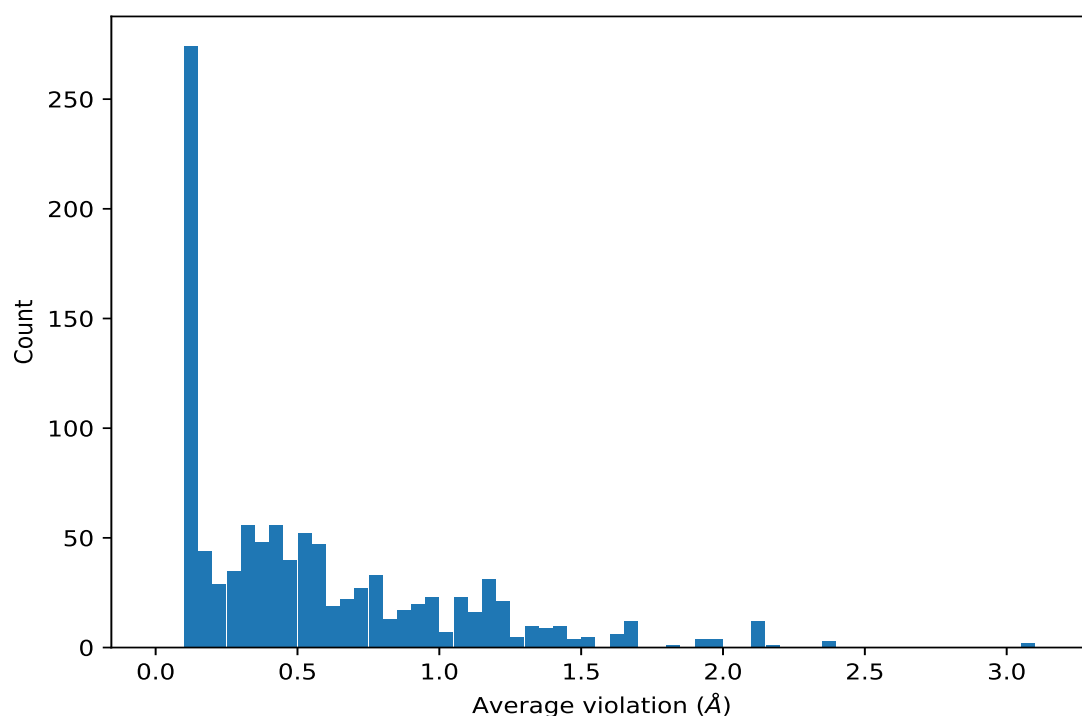
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,2623) | 1:156:A:ARG:HH21 | 1:198:A:PHE:HD1 | 20                  | 3.08     | 0.75                | 3.29       |
| (1,2623) | 1:156:A:ARG:HH21 | 1:198:A:PHE:HD2 | 20                  | 3.08     | 0.75                | 3.29       |
| (1,23)   | 1:220:A:LYS:HG2  | 1:221:A:GLU:HG3 | 20                  | 1.92     | 0.34                | 1.92       |
| (1,1344) | 1:206:A:MET:HB3  | 1:210:A:VAL:HB  | 20                  | 1.49     | 0.26                | 1.62       |
| (1,2315) | 1:160:A:GLN:HE21 | 1:213:A:MET:HB2 | 20                  | 1.25     | 0.18                | 1.27       |
| (1,1235) | 1:205:A:MET:HG3  | 1:206:A:MET:HG2 | 20                  | 1.16     | 0.4                 | 1.23       |
| (1,396)  | 1:210:A:VAL:HA   | 1:213:A:MET:HB3 | 20                  | 1.14     | 0.19                | 1.14       |
| (1,2482) | 1:163:A:TYR:HD1  | 1:221:A:GLU:HG2 | 20                  | 1.14     | 0.28                | 1.21       |
| (1,2482) | 1:163:A:TYR:HD2  | 1:221:A:GLU:HG2 | 20                  | 1.14     | 0.28                | 1.21       |
| (1,2851) | 1:184:A:ILE:HG13 | 1:187:A:HIS:HE1 | 20                  | 1.03     | 0.37                | 1.14       |
| (1,2846) | 1:157:A:TYR:HE1  | 1:206:A:MET:HB2 | 20                  | 1.02     | 0.26                | 0.93       |
| (1,2846) | 1:157:A:TYR:HE2  | 1:206:A:MET:HB2 | 20                  | 1.02     | 0.26                | 0.93       |
| (1,2320) | 1:160:A:GLN:HE22 | 1:213:A:MET:HB2 | 20                  | 0.98     | 0.27                | 1.06       |
| (1,1131) | 1:223:A:GLN:HG2  | 1:226:A:TYR:H   | 20                  | 0.96     | 0.31                | 0.97       |
| (1,2735) | 1:186:A:GLN:HB3  | 1:187:A:HIS:HD2 | 20                  | 0.92     | 0.11                | 0.98       |
| (1,2615) | 1:141:A:PHE:HD1  | 1:147:A:ASP:HB3 | 20                  | 0.82     | 0.21                | 0.84       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2615) | 1:141:A:PHE:HD2  | 1:147:A:ASP:HB3  | 20                  | 0.82     | 0.21                | 0.84       |
| (1,637)  | 1:147:A:ASP:HB2  | 1:148:A:ARG:HG2  | 20                  | 0.74     | 0.24                | 0.76       |
| (1,2650) | 1:139:A:ILE:HG12 | 1:141:A:PHE:HE1  | 20                  | 0.73     | 0.19                | 0.74       |
| (1,2650) | 1:139:A:ILE:HG12 | 1:141:A:PHE:HE2  | 20                  | 0.73     | 0.19                | 0.74       |
| (1,502)  | 1:162:A:TYR:HB3  | 1:183:A:THR:HA   | 20                  | 0.7      | 0.2                 | 0.67       |
| (1,2184) | 1:212:A:GLN:H    | 1:212:A:GLN:HB3  | 20                  | 0.69     | 0.01                | 0.69       |
| (1,323)  | 1:209:A:VAL:HG21 | 1:212:A:GLN:HB3  | 20                  | 0.65     | 0.21                | 0.64       |
| (1,323)  | 1:209:A:VAL:HG22 | 1:212:A:GLN:HB3  | 20                  | 0.65     | 0.21                | 0.64       |
| (1,323)  | 1:209:A:VAL:HG23 | 1:212:A:GLN:HB3  | 20                  | 0.65     | 0.21                | 0.64       |
| (1,1104) | 1:213:A:MET:HB3  | 1:214:A:CYS:HA   | 20                  | 0.65     | 0.15                | 0.62       |
| (1,2774) | 1:128:A:TYR:HE1  | 1:162:A:TYR:HB3  | 20                  | 0.58     | 0.12                | 0.6        |
| (1,2774) | 1:128:A:TYR:HE2  | 1:162:A:TYR:HB3  | 20                  | 0.58     | 0.12                | 0.6        |
| (1,657)  | 1:213:A:MET:HB3  | 1:213:A:MET:HE1  | 20                  | 0.55     | 0.13                | 0.6        |
| (1,657)  | 1:213:A:MET:HB3  | 1:213:A:MET:HE2  | 20                  | 0.55     | 0.13                | 0.6        |
| (1,657)  | 1:213:A:MET:HB3  | 1:213:A:MET:HE3  | 20                  | 0.55     | 0.13                | 0.6        |
| (1,1098) | 1:213:A:MET:HB2  | 1:216:A:THR:HG21 | 20                  | 0.55     | 0.01                | 0.55       |
| (1,1098) | 1:213:A:MET:HB2  | 1:216:A:THR:HG22 | 20                  | 0.55     | 0.01                | 0.55       |
| (1,1098) | 1:213:A:MET:HB2  | 1:216:A:THR:HG23 | 20                  | 0.55     | 0.01                | 0.55       |
| (1,2756) | 1:150:A:TYR:HE1  | 1:205:A:MET:HG2  | 20                  | 0.52     | 0.2                 | 0.48       |
| (1,2756) | 1:150:A:TYR:HE2  | 1:205:A:MET:HG2  | 20                  | 0.52     | 0.2                 | 0.48       |
| (1,2501) | 1:149:A:TYR:HD1  | 1:205:A:MET:HG2  | 20                  | 0.51     | 0.2                 | 0.55       |
| (1,2501) | 1:149:A:TYR:HD2  | 1:205:A:MET:HG2  | 20                  | 0.51     | 0.2                 | 0.55       |
| (1,224)  | 1:127:A:GLY:HA3  | 1:128:A:TYR:HB2  | 20                  | 0.43     | 0.1                 | 0.45       |
| (1,2129) | 1:186:A:GLN:H    | 1:186:A:GLN:HB3  | 20                  | 0.43     | 0.04                | 0.44       |
| (1,1861) | 1:147:A:ASP:HB2  | 1:148:A:ARG:H    | 20                  | 0.42     | 0.08                | 0.4        |
| (1,179)  | 1:201:A:THR:HB   | 1:205:A:MET:HG3  | 20                  | 0.41     | 0.09                | 0.41       |
| (1,1168) | 1:223:A:GLN:H    | 1:223:A:GLN:HG2  | 20                  | 0.4      | 0.07                | 0.4        |
| (1,112)  | 1:214:A:CYS:HA   | 1:215:A:VAL:HG11 | 20                  | 0.36     | 0.26                | 0.13       |
| (1,112)  | 1:214:A:CYS:HA   | 1:215:A:VAL:HG12 | 20                  | 0.36     | 0.26                | 0.13       |
| (1,112)  | 1:214:A:CYS:HA   | 1:215:A:VAL:HG13 | 20                  | 0.36     | 0.26                | 0.13       |
| (1,249)  | 1:203:A:VAL:HA   | 1:206:A:MET:HB2  | 20                  | 0.29     | 0.01                | 0.29       |
| (1,963)  | 1:184:A:ILE:HD11 | 1:185:A:LYS:HA   | 20                  | 0.12     | 0.01                | 0.12       |
| (1,963)  | 1:184:A:ILE:HD12 | 1:185:A:LYS:HA   | 20                  | 0.12     | 0.01                | 0.12       |
| (1,963)  | 1:184:A:ILE:HD13 | 1:185:A:LYS:HA   | 20                  | 0.12     | 0.01                | 0.12       |
| (1,611)  | 1:134:A:MET:HE1  | 1:218:A:TYR:H    | 20                  | 0.12     | 0.01                | 0.12       |
| (1,611)  | 1:134:A:MET:HE2  | 1:218:A:TYR:H    | 20                  | 0.12     | 0.01                | 0.12       |
| (1,611)  | 1:134:A:MET:HE3  | 1:218:A:TYR:H    | 20                  | 0.12     | 0.01                | 0.12       |
| (1,1081) | 1:164:A:ARG:HD2  | 1:168:A:GLN:HG2  | 19                  | 1.96     | 0.75                | 1.99       |
| (1,377)  | 1:209:A:VAL:HG21 | 1:213:A:MET:HG2  | 19                  | 1.69     | 0.71                | 2.03       |
| (1,377)  | 1:209:A:VAL:HG22 | 1:213:A:MET:HG2  | 19                  | 1.69     | 0.71                | 2.03       |
| (1,377)  | 1:209:A:VAL:HG23 | 1:213:A:MET:HG2  | 19                  | 1.69     | 0.71                | 2.03       |
| (1,2374) | 1:168:A:GLN:HE22 | 1:169:A:TYR:HE1  | 19                  | 1.54     | 0.17                | 1.62       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2374) | 1:168:A:GLN:HE22 | 1:169:A:TYR:HE2  | 19                  | 1.54     | 0.17                | 1.62       |
| (1,927)  | 1:212:A:GLN:HA   | 1:213:A:MET:HG2  | 19                  | 1.4      | 0.3                 | 1.47       |
| (1,1459) | 1:136:A:ARG:HB3  | 1:159:A:ASN:HB3  | 19                  | 1.24     | 0.72                | 1.09       |
| (1,2414) | 1:136:A:ARG:HB3  | 1:159:A:ASN:HD21 | 19                  | 1.13     | 0.51                | 1.16       |
| (1,2177) | 1:212:A:GLN:H    | 1:213:A:MET:HG2  | 19                  | 1.09     | 0.19                | 1.1        |
| (1,2347) | 1:139:A:ILE:HG13 | 1:212:A:GLN:HE22 | 19                  | 1.08     | 0.16                | 1.07       |
| (1,2711) | 1:145:A:TRP:HZ3  | 1:146:A:GLU:HG3  | 19                  | 0.98     | 0.25                | 0.99       |
| (1,921)  | 1:167:A:SER:HA   | 1:168:A:GLN:HG3  | 19                  | 0.88     | 0.25                | 0.92       |
| (1,2492) | 1:139:A:ILE:HG12 | 1:150:A:TYR:HD1  | 19                  | 0.77     | 0.16                | 0.73       |
| (1,2492) | 1:139:A:ILE:HG12 | 1:150:A:TYR:HD2  | 19                  | 0.77     | 0.16                | 0.73       |
| (1,89)   | 1:206:A:MET:HB3  | 1:210:A:VAL:HG21 | 19                  | 0.65     | 0.48                | 0.45       |
| (1,89)   | 1:206:A:MET:HB3  | 1:210:A:VAL:HG22 | 19                  | 0.65     | 0.48                | 0.45       |
| (1,89)   | 1:206:A:MET:HB3  | 1:210:A:VAL:HG23 | 19                  | 0.65     | 0.48                | 0.45       |
| (1,1523) | 1:162:A:TYR:HB3  | 1:182:A:ILE:HG12 | 19                  | 0.62     | 0.14                | 0.59       |
| (1,1523) | 1:162:A:TYR:HB3  | 1:182:A:ILE:HG13 | 19                  | 0.62     | 0.14                | 0.59       |
| (1,2657) | 1:141:A:PHE:HE1  | 1:208:A:ARG:HB3  | 19                  | 0.57     | 0.35                | 0.56       |
| (1,2657) | 1:141:A:PHE:HE2  | 1:208:A:ARG:HB3  | 19                  | 0.57     | 0.35                | 0.56       |
| (1,634)  | 1:192:A:THR:HA   | 1:195:A:GLY:HA3  | 19                  | 0.57     | 0.17                | 0.5        |
| (1,893)  | 1:162:A:TYR:HB3  | 1:182:A:ILE:HB   | 19                  | 0.55     | 0.18                | 0.54       |
| (1,2771) | 1:130:A:LEU:HB3  | 1:162:A:TYR:HE1  | 19                  | 0.52     | 0.15                | 0.55       |
| (1,2771) | 1:130:A:LEU:HB3  | 1:162:A:TYR:HE2  | 19                  | 0.52     | 0.15                | 0.55       |
| (1,2699) | 1:141:A:PHE:HZ   | 1:150:A:TYR:HB3  | 19                  | 0.52     | 0.16                | 0.51       |
| (1,2759) | 1:139:A:ILE:HG12 | 1:150:A:TYR:HE1  | 19                  | 0.49     | 0.18                | 0.45       |
| (1,2759) | 1:139:A:ILE:HG12 | 1:150:A:TYR:HE2  | 19                  | 0.49     | 0.18                | 0.45       |
| (1,445)  | 1:180:A:VAL:HA   | 1:184:A:ILE:HG12 | 19                  | 0.46     | 0.29                | 0.4        |
| (1,1212) | 1:184:A:ILE:HD11 | 1:206:A:MET:HB3  | 19                  | 0.39     | 0.12                | 0.4        |
| (1,1212) | 1:184:A:ILE:HD12 | 1:206:A:MET:HB3  | 19                  | 0.39     | 0.12                | 0.4        |
| (1,1212) | 1:184:A:ILE:HD13 | 1:206:A:MET:HB3  | 19                  | 0.39     | 0.12                | 0.4        |
| (1,150)  | 1:126:A:GLY:HA3  | 1:127:A:GLY:H    | 19                  | 0.15     | 0.02                | 0.15       |
| (1,288)  | 1:192:A:THR:HG21 | 1:196:A:GLU:HB2  | 19                  | 0.13     | 0.01                | 0.14       |
| (1,288)  | 1:192:A:THR:HG21 | 1:196:A:GLU:HB3  | 19                  | 0.13     | 0.01                | 0.14       |
| (1,288)  | 1:192:A:THR:HG22 | 1:196:A:GLU:HB2  | 19                  | 0.13     | 0.01                | 0.14       |
| (1,288)  | 1:192:A:THR:HG22 | 1:196:A:GLU:HB3  | 19                  | 0.13     | 0.01                | 0.14       |
| (1,288)  | 1:192:A:THR:HG23 | 1:196:A:GLU:HB2  | 19                  | 0.13     | 0.01                | 0.14       |
| (1,288)  | 1:192:A:THR:HG23 | 1:196:A:GLU:HB3  | 19                  | 0.13     | 0.01                | 0.14       |
| (1,2488) | 1:149:A:TYR:HD1  | 1:153:A:ASN:HB3  | 18                  | 0.6      | 0.23                | 0.64       |
| (1,2488) | 1:149:A:TYR:HD2  | 1:153:A:ASN:HB3  | 18                  | 0.6      | 0.23                | 0.64       |
| (1,752)  | 1:138:A:MET:HE1  | 1:139:A:ILE:HG12 | 18                  | 0.55     | 0.19                | 0.52       |
| (1,752)  | 1:138:A:MET:HE2  | 1:139:A:ILE:HG12 | 18                  | 0.55     | 0.19                | 0.52       |
| (1,752)  | 1:138:A:MET:HE3  | 1:139:A:ILE:HG12 | 18                  | 0.55     | 0.19                | 0.52       |
| (1,1015) | 1:152:A:GLU:HG2  | 1:153:A:ASN:HD22 | 18                  | 0.5      | 0.26                | 0.54       |
| (1,2830) | 1:172:A:GLN:HG2  | 1:218:A:TYR:HE1  | 18                  | 0.41     | 0.12                | 0.4        |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2830) | 1:172:A:GLN:HG2  | 1:218:A:TYR:HE2  | 18                  | 0.41     | 0.12                | 0.4        |
| (1,2553) | 1:126:A:GLY:HA2  | 1:128:A:TYR:HD1  | 18                  | 0.35     | 0.13                | 0.34       |
| (1,2553) | 1:126:A:GLY:HA2  | 1:128:A:TYR:HD2  | 18                  | 0.35     | 0.13                | 0.34       |
| (1,1101) | 1:160:A:GLN:H    | 1:213:A:MET:HB3  | 18                  | 0.34     | 0.09                | 0.37       |
| (1,1070) | 1:152:A:GLU:HA   | 1:152:A:GLU:HG3  | 18                  | 0.22     | 0.05                | 0.2        |
| (1,501)  | 1:161:A:VAL:HA   | 1:162:A:TYR:HB3  | 18                  | 0.19     | 0.05                | 0.2        |
| (1,1)    | 1:138:A:MET:HG3  | 1:139:A:ILE:HG12 | 17                  | 1.81     | 0.7                 | 2.15       |
| (1,2354) | 1:170:A:SER:HB2  | 1:174:A:ASN:HD21 | 17                  | 1.34     | 0.8                 | 1.26       |
| (1,362)  | 1:172:A:GLN:HG3  | 1:215:A:VAL:HG21 | 17                  | 1.21     | 0.72                | 1.55       |
| (1,362)  | 1:172:A:GLN:HG3  | 1:215:A:VAL:HG22 | 17                  | 1.21     | 0.72                | 1.55       |
| (1,362)  | 1:172:A:GLN:HG3  | 1:215:A:VAL:HG23 | 17                  | 1.21     | 0.72                | 1.55       |
| (1,155)  | 1:125:A:LEU:HB3  | 1:126:A:GLY:HA3  | 17                  | 0.79     | 0.17                | 0.78       |
| (1,1303) | 1:137:A:PRO:HB2  | 1:213:A:MET:HG2  | 17                  | 0.72     | 0.28                | 0.74       |
| (1,2681) | 1:141:A:PHE:HZ   | 1:208:A:ARG:HB3  | 17                  | 0.7      | 0.22                | 0.68       |
| (1,1097) | 1:165:A:PRO:HB3  | 1:168:A:GLN:HG2  | 17                  | 0.54     | 0.36                | 0.38       |
| (1,1207) | 1:168:A:GLN:HA   | 1:168:A:GLN:HE22 | 17                  | 0.5      | 0.24                | 0.54       |
| (1,2736) | 1:184:A:ILE:HG13 | 1:187:A:HIS:HD2  | 17                  | 0.47     | 0.26                | 0.48       |
| (1,873)  | 1:146:A:GLU:HA   | 1:150:A:TYR:HB3  | 17                  | 0.37     | 0.17                | 0.35       |
| (1,1220) | 1:195:A:GLY:HA2  | 1:196:A:GLU:HA   | 17                  | 0.22     | 0.03                | 0.23       |
| (1,370)  | 1:158:A:PRO:HG2  | 1:209:A:VAL:HG21 | 16                  | 1.95     | 0.52                | 2.1        |
| (1,370)  | 1:158:A:PRO:HG2  | 1:209:A:VAL:HG22 | 16                  | 1.95     | 0.52                | 2.1        |
| (1,370)  | 1:158:A:PRO:HG2  | 1:209:A:VAL:HG23 | 16                  | 1.95     | 0.52                | 2.1        |
| (1,1283) | 1:206:A:MET:HG2  | 1:207:A:GLU:HG3  | 16                  | 1.31     | 0.35                | 1.33       |
| (1,348)  | 1:122:A:VAL:HG21 | 1:124:A:GLY:HA2  | 16                  | 0.78     | 0.59                | 0.89       |
| (1,348)  | 1:122:A:VAL:HG21 | 1:124:A:GLY:HA3  | 16                  | 0.78     | 0.59                | 0.89       |
| (1,348)  | 1:122:A:VAL:HG22 | 1:124:A:GLY:HA2  | 16                  | 0.78     | 0.59                | 0.89       |
| (1,348)  | 1:122:A:VAL:HG22 | 1:124:A:GLY:HA3  | 16                  | 0.78     | 0.59                | 0.89       |
| (1,348)  | 1:122:A:VAL:HG23 | 1:124:A:GLY:HA2  | 16                  | 0.78     | 0.59                | 0.89       |
| (1,348)  | 1:122:A:VAL:HG23 | 1:124:A:GLY:HA3  | 16                  | 0.78     | 0.59                | 0.89       |
| (1,1256) | 1:184:A:ILE:HG13 | 1:206:A:MET:HG3  | 16                  | 0.78     | 0.41                | 0.74       |
| (1,1937) | 1:220:A:LYS:H    | 1:221:A:GLU:HG3  | 16                  | 0.6      | 0.27                | 0.58       |
| (1,663)  | 1:223:A:GLN:HG2  | 1:227:A:ASP:HB2  | 16                  | 0.5      | 0.04                | 0.51       |
| (1,663)  | 1:223:A:GLN:HG2  | 1:227:A:ASP:HB3  | 16                  | 0.5      | 0.04                | 0.51       |
| (1,862)  | 1:143:A:ASN:HD22 | 1:146:A:GLU:HG2  | 16                  | 0.5      | 0.28                | 0.44       |
| (1,2834) | 1:163:A:TYR:HE1  | 1:221:A:GLU:HG2  | 16                  | 0.36     | 0.19                | 0.37       |
| (1,2834) | 1:163:A:TYR:HE2  | 1:221:A:GLU:HG2  | 16                  | 0.36     | 0.19                | 0.37       |
| (1,216)  | 1:216:A:THR:HG21 | 1:220:A:LYS:HG3  | 16                  | 0.28     | 0.16                | 0.22       |
| (1,216)  | 1:216:A:THR:HG22 | 1:220:A:LYS:HG3  | 16                  | 0.28     | 0.16                | 0.22       |
| (1,216)  | 1:216:A:THR:HG23 | 1:220:A:LYS:HG3  | 16                  | 0.28     | 0.16                | 0.22       |
| (1,807)  | 1:181:A:ASN:HB3  | 1:184:A:ILE:HG21 | 16                  | 0.11     | 0.01                | 0.11       |
| (1,807)  | 1:181:A:ASN:HB3  | 1:184:A:ILE:HG22 | 16                  | 0.11     | 0.01                | 0.11       |
| (1,807)  | 1:181:A:ASN:HB3  | 1:184:A:ILE:HG23 | 16                  | 0.11     | 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) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2682) | 1:141:A:PHE:HZ   | 1:209:A:VAL:HG11 | 15                  | 2.36     | 0.2                 | 2.42       |
| (1,2682) | 1:141:A:PHE:HZ   | 1:209:A:VAL:HG12 | 15                  | 2.36     | 0.2                 | 2.42       |
| (1,2682) | 1:141:A:PHE:HZ   | 1:209:A:VAL:HG13 | 15                  | 2.36     | 0.2                 | 2.42       |
| (1,428)  | 1:127:A:GLY:HA2  | 1:164:A:ARG:HD3  | 15                  | 2.15     | 0.58                | 2.32       |
| (1,2491) | 1:150:A:TYR:HD1  | 1:209:A:VAL:HG11 | 15                  | 1.65     | 0.23                | 1.69       |
| (1,2491) | 1:150:A:TYR:HD1  | 1:209:A:VAL:HG12 | 15                  | 1.65     | 0.23                | 1.69       |
| (1,2491) | 1:150:A:TYR:HD1  | 1:209:A:VAL:HG13 | 15                  | 1.65     | 0.23                | 1.69       |
| (1,2491) | 1:150:A:TYR:HD2  | 1:209:A:VAL:HG11 | 15                  | 1.65     | 0.23                | 1.69       |
| (1,2491) | 1:150:A:TYR:HD2  | 1:209:A:VAL:HG12 | 15                  | 1.65     | 0.23                | 1.69       |
| (1,2491) | 1:150:A:TYR:HD2  | 1:209:A:VAL:HG13 | 15                  | 1.65     | 0.23                | 1.69       |
| (1,78)   | 1:139:A:ILE:HB   | 1:209:A:VAL:HG11 | 15                  | 1.35     | 0.21                | 1.32       |
| (1,78)   | 1:139:A:ILE:HB   | 1:209:A:VAL:HG12 | 15                  | 1.35     | 0.21                | 1.32       |
| (1,78)   | 1:139:A:ILE:HB   | 1:209:A:VAL:HG13 | 15                  | 1.35     | 0.21                | 1.32       |
| (1,704)  | 1:209:A:VAL:HG21 | 1:213:A:MET:HE1  | 15                  | 1.23     | 0.27                | 1.31       |
| (1,704)  | 1:209:A:VAL:HG21 | 1:213:A:MET:HE2  | 15                  | 1.23     | 0.27                | 1.31       |
| (1,704)  | 1:209:A:VAL:HG21 | 1:213:A:MET:HE3  | 15                  | 1.23     | 0.27                | 1.31       |
| (1,704)  | 1:209:A:VAL:HG22 | 1:213:A:MET:HE1  | 15                  | 1.23     | 0.27                | 1.31       |
| (1,704)  | 1:209:A:VAL:HG22 | 1:213:A:MET:HE2  | 15                  | 1.23     | 0.27                | 1.31       |
| (1,704)  | 1:209:A:VAL:HG22 | 1:213:A:MET:HE3  | 15                  | 1.23     | 0.27                | 1.31       |
| (1,704)  | 1:209:A:VAL:HG23 | 1:213:A:MET:HE1  | 15                  | 1.23     | 0.27                | 1.31       |
| (1,704)  | 1:209:A:VAL:HG23 | 1:213:A:MET:HE2  | 15                  | 1.23     | 0.27                | 1.31       |
| (1,704)  | 1:209:A:VAL:HG23 | 1:213:A:MET:HE3  | 15                  | 1.23     | 0.27                | 1.31       |
| (1,2847) | 1:157:A:TYR:HE1  | 1:209:A:VAL:HG11 | 15                  | 1.09     | 0.2                 | 1.11       |
| (1,2847) | 1:157:A:TYR:HE1  | 1:209:A:VAL:HG12 | 15                  | 1.09     | 0.2                 | 1.11       |
| (1,2847) | 1:157:A:TYR:HE1  | 1:209:A:VAL:HG13 | 15                  | 1.09     | 0.2                 | 1.11       |
| (1,2847) | 1:157:A:TYR:HE2  | 1:209:A:VAL:HG11 | 15                  | 1.09     | 0.2                 | 1.11       |
| (1,2847) | 1:157:A:TYR:HE2  | 1:209:A:VAL:HG12 | 15                  | 1.09     | 0.2                 | 1.11       |
| (1,2847) | 1:157:A:TYR:HE2  | 1:209:A:VAL:HG13 | 15                  | 1.09     | 0.2                 | 1.11       |
| (1,322)  | 1:158:A:PRO:HD3  | 1:209:A:VAL:HG21 | 15                  | 0.98     | 0.28                | 0.97       |
| (1,322)  | 1:158:A:PRO:HD3  | 1:209:A:VAL:HG22 | 15                  | 0.98     | 0.28                | 0.97       |
| (1,322)  | 1:158:A:PRO:HD3  | 1:209:A:VAL:HG23 | 15                  | 0.98     | 0.28                | 0.97       |
| (1,1914) | 1:209:A:VAL:HG21 | 1:213:A:MET:H    | 15                  | 0.91     | 0.14                | 0.85       |
| (1,1914) | 1:209:A:VAL:HG22 | 1:213:A:MET:H    | 15                  | 0.91     | 0.14                | 0.85       |
| (1,1914) | 1:209:A:VAL:HG23 | 1:213:A:MET:H    | 15                  | 0.91     | 0.14                | 0.85       |
| (1,98)   | 1:139:A:ILE:HG21 | 1:209:A:VAL:HG11 | 15                  | 0.86     | 0.09                | 0.89       |
| (1,98)   | 1:139:A:ILE:HG21 | 1:209:A:VAL:HG12 | 15                  | 0.86     | 0.09                | 0.89       |
| (1,98)   | 1:139:A:ILE:HG21 | 1:209:A:VAL:HG13 | 15                  | 0.86     | 0.09                | 0.89       |
| (1,98)   | 1:139:A:ILE:HG22 | 1:209:A:VAL:HG11 | 15                  | 0.86     | 0.09                | 0.89       |
| (1,98)   | 1:139:A:ILE:HG22 | 1:209:A:VAL:HG12 | 15                  | 0.86     | 0.09                | 0.89       |
| (1,98)   | 1:139:A:ILE:HG22 | 1:209:A:VAL:HG13 | 15                  | 0.86     | 0.09                | 0.89       |
| (1,98)   | 1:139:A:ILE:HG23 | 1:209:A:VAL:HG11 | 15                  | 0.86     | 0.09                | 0.89       |
| (1,98)   | 1:139:A:ILE:HG23 | 1:209:A:VAL:HG12 | 15                  | 0.86     | 0.09                | 0.89       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,98)   | 1:139:A:ILE:HG23 | 1:209:A:VAL:HG13 | 15                  | 0.86     | 0.09                | 0.89       |
| (1,1231) | 1:209:A:VAL:HG21 | 1:213:A:MET:HG3  | 15                  | 0.84     | 0.34                | 0.93       |
| (1,1231) | 1:209:A:VAL:HG22 | 1:213:A:MET:HG3  | 15                  | 0.84     | 0.34                | 0.93       |
| (1,1231) | 1:209:A:VAL:HG23 | 1:213:A:MET:HG3  | 15                  | 0.84     | 0.34                | 0.93       |
| (1,2758) | 1:150:A:TYR:HE1  | 1:209:A:VAL:HG11 | 15                  | 0.78     | 0.21                | 0.81       |
| (1,2758) | 1:150:A:TYR:HE1  | 1:209:A:VAL:HG12 | 15                  | 0.78     | 0.21                | 0.81       |
| (1,2758) | 1:150:A:TYR:HE1  | 1:209:A:VAL:HG13 | 15                  | 0.78     | 0.21                | 0.81       |
| (1,2758) | 1:150:A:TYR:HE2  | 1:209:A:VAL:HG11 | 15                  | 0.78     | 0.21                | 0.81       |
| (1,2758) | 1:150:A:TYR:HE2  | 1:209:A:VAL:HG12 | 15                  | 0.78     | 0.21                | 0.81       |
| (1,2758) | 1:150:A:TYR:HE2  | 1:209:A:VAL:HG13 | 15                  | 0.78     | 0.21                | 0.81       |
| (1,80)   | 1:208:A:ARG:HA   | 1:209:A:VAL:HG11 | 15                  | 0.64     | 0.06                | 0.63       |
| (1,80)   | 1:208:A:ARG:HA   | 1:209:A:VAL:HG12 | 15                  | 0.64     | 0.06                | 0.63       |
| (1,80)   | 1:208:A:ARG:HA   | 1:209:A:VAL:HG13 | 15                  | 0.64     | 0.06                | 0.63       |
| (1,76)   | 1:139:A:ILE:HG12 | 1:209:A:VAL:HG11 | 15                  | 0.56     | 0.08                | 0.53       |
| (1,76)   | 1:139:A:ILE:HG12 | 1:209:A:VAL:HG12 | 15                  | 0.56     | 0.08                | 0.53       |
| (1,76)   | 1:139:A:ILE:HG12 | 1:209:A:VAL:HG13 | 15                  | 0.56     | 0.08                | 0.53       |
| (1,339)  | 1:209:A:VAL:HG21 | 1:210:A:VAL:HG21 | 15                  | 0.48     | 0.18                | 0.43       |
| (1,339)  | 1:209:A:VAL:HG21 | 1:210:A:VAL:HG22 | 15                  | 0.48     | 0.18                | 0.43       |
| (1,339)  | 1:209:A:VAL:HG21 | 1:210:A:VAL:HG23 | 15                  | 0.48     | 0.18                | 0.43       |
| (1,339)  | 1:209:A:VAL:HG22 | 1:210:A:VAL:HG21 | 15                  | 0.48     | 0.18                | 0.43       |
| (1,339)  | 1:209:A:VAL:HG22 | 1:210:A:VAL:HG22 | 15                  | 0.48     | 0.18                | 0.43       |
| (1,339)  | 1:209:A:VAL:HG22 | 1:210:A:VAL:HG23 | 15                  | 0.48     | 0.18                | 0.43       |
| (1,339)  | 1:209:A:VAL:HG23 | 1:210:A:VAL:HG21 | 15                  | 0.48     | 0.18                | 0.43       |
| (1,339)  | 1:209:A:VAL:HG23 | 1:210:A:VAL:HG22 | 15                  | 0.48     | 0.18                | 0.43       |
| (1,339)  | 1:209:A:VAL:HG23 | 1:210:A:VAL:HG23 | 15                  | 0.48     | 0.18                | 0.43       |
| (1,79)   | 1:138:A:MET:H    | 1:209:A:VAL:HG11 | 15                  | 0.43     | 0.16                | 0.43       |
| (1,79)   | 1:138:A:MET:H    | 1:209:A:VAL:HG12 | 15                  | 0.43     | 0.16                | 0.43       |
| (1,79)   | 1:138:A:MET:H    | 1:209:A:VAL:HG13 | 15                  | 0.43     | 0.16                | 0.43       |
| (1,1678) | 1:125:A:LEU:H    | 1:125:A:LEU:HB2  | 15                  | 0.39     | 0.22                | 0.43       |
| (1,496)  | 1:130:A:LEU:HA   | 1:162:A:TYR:HB2  | 15                  | 0.36     | 0.17                | 0.31       |
| (1,656)  | 1:138:A:MET:HG3  | 1:154:A:MET:HE1  | 15                  | 0.36     | 0.35                | 0.13       |
| (1,656)  | 1:138:A:MET:HG3  | 1:154:A:MET:HE2  | 15                  | 0.36     | 0.35                | 0.13       |
| (1,656)  | 1:138:A:MET:HG3  | 1:154:A:MET:HE3  | 15                  | 0.36     | 0.35                | 0.13       |
| (1,359)  | 1:122:A:VAL:HG21 | 1:182:A:ILE:HG21 | 15                  | 0.32     | 0.2                 | 0.17       |
| (1,359)  | 1:122:A:VAL:HG21 | 1:182:A:ILE:HG22 | 15                  | 0.32     | 0.2                 | 0.17       |
| (1,359)  | 1:122:A:VAL:HG21 | 1:182:A:ILE:HG23 | 15                  | 0.32     | 0.2                 | 0.17       |
| (1,359)  | 1:122:A:VAL:HG22 | 1:182:A:ILE:HG21 | 15                  | 0.32     | 0.2                 | 0.17       |
| (1,359)  | 1:122:A:VAL:HG22 | 1:182:A:ILE:HG22 | 15                  | 0.32     | 0.2                 | 0.17       |
| (1,359)  | 1:122:A:VAL:HG22 | 1:182:A:ILE:HG23 | 15                  | 0.32     | 0.2                 | 0.17       |
| (1,359)  | 1:122:A:VAL:HG23 | 1:182:A:ILE:HG21 | 15                  | 0.32     | 0.2                 | 0.17       |
| (1,359)  | 1:122:A:VAL:HG23 | 1:182:A:ILE:HG22 | 15                  | 0.32     | 0.2                 | 0.17       |
| (1,359)  | 1:122:A:VAL:HG23 | 1:182:A:ILE:HG23 | 15                  | 0.32     | 0.2                 | 0.17       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1155) | 1:130:A:LEU:HB3  | 1:162:A:TYR:HA   | 15                  | 0.22     | 0.05                | 0.24       |
| (1,15)   | 1:130:A:LEU:HD21 | 1:161:A:VAL:HA   | 15                  | 0.11     | 0.0                 | 0.11       |
| (1,15)   | 1:130:A:LEU:HD22 | 1:161:A:VAL:HA   | 15                  | 0.11     | 0.0                 | 0.11       |
| (1,15)   | 1:130:A:LEU:HD23 | 1:161:A:VAL:HA   | 15                  | 0.11     | 0.0                 | 0.11       |
| (1,159)  | 1:228:A:GLY:HA2  | 1:230:A:ARG:HD2  | 14                  | 0.95     | 0.48                | 1.08       |
| (1,159)  | 1:228:A:GLY:HA3  | 1:230:A:ARG:HD2  | 14                  | 0.95     | 0.48                | 1.08       |
| (1,309)  | 1:186:A:GLN:HE21 | 1:189:A:VAL:HG11 | 14                  | 0.77     | 0.61                | 0.78       |
| (1,309)  | 1:186:A:GLN:HE21 | 1:189:A:VAL:HG12 | 14                  | 0.77     | 0.61                | 0.78       |
| (1,309)  | 1:186:A:GLN:HE21 | 1:189:A:VAL:HG13 | 14                  | 0.77     | 0.61                | 0.78       |
| (1,758)  | 1:138:A:MET:HG3  | 1:138:A:MET:HE1  | 14                  | 0.57     | 0.02                | 0.57       |
| (1,758)  | 1:138:A:MET:HG3  | 1:138:A:MET:HE2  | 14                  | 0.57     | 0.02                | 0.57       |
| (1,758)  | 1:138:A:MET:HG3  | 1:138:A:MET:HE3  | 14                  | 0.57     | 0.02                | 0.57       |
| (1,1497) | 1:139:A:ILE:HD11 | 1:212:A:GLN:HB3  | 14                  | 0.57     | 0.23                | 0.68       |
| (1,1497) | 1:139:A:ILE:HD12 | 1:212:A:GLN:HB3  | 14                  | 0.57     | 0.23                | 0.68       |
| (1,1497) | 1:139:A:ILE:HD13 | 1:212:A:GLN:HB3  | 14                  | 0.57     | 0.23                | 0.68       |
| (1,1579) | 1:132:A:SER:HB3  | 1:133:A:ALA:H    | 14                  | 0.53     | 0.11                | 0.54       |
| (1,1294) | 1:138:A:MET:HG3  | 1:139:A:ILE:H    | 14                  | 0.46     | 0.16                | 0.52       |
| (1,2593) | 1:175:A:PHE:HE1  | 1:221:A:GLU:HG2  | 14                  | 0.43     | 0.32                | 0.3        |
| (1,2593) | 1:175:A:PHE:HE2  | 1:221:A:GLU:HG2  | 14                  | 0.43     | 0.32                | 0.3        |
| (1,833)  | 1:207:A:GLU:HA   | 1:207:A:GLU:HG3  | 14                  | 0.43     | 0.04                | 0.44       |
| (1,957)  | 1:184:A:ILE:HD11 | 1:207:A:GLU:HG3  | 14                  | 0.38     | 0.16                | 0.34       |
| (1,957)  | 1:184:A:ILE:HD12 | 1:207:A:GLU:HG3  | 14                  | 0.38     | 0.16                | 0.34       |
| (1,957)  | 1:184:A:ILE:HD13 | 1:207:A:GLU:HG3  | 14                  | 0.38     | 0.16                | 0.34       |
| (1,1893) | 1:208:A:ARG:HB3  | 1:209:A:VAL:H    | 14                  | 0.34     | 0.15                | 0.36       |
| (1,77)   | 1:208:A:ARG:H    | 1:209:A:VAL:HG11 | 14                  | 0.28     | 0.11                | 0.28       |
| (1,77)   | 1:208:A:ARG:H    | 1:209:A:VAL:HG12 | 14                  | 0.28     | 0.11                | 0.28       |
| (1,77)   | 1:208:A:ARG:H    | 1:209:A:VAL:HG13 | 14                  | 0.28     | 0.11                | 0.28       |
| (1,2421) | 1:127:A:GLY:H    | 1:164:A:ARG:HD3  | 13                  | 1.3      | 0.29                | 1.29       |
| (1,158)  | 1:126:A:GLY:HA2  | 1:164:A:ARG:HD3  | 13                  | 1.21     | 0.25                | 1.27       |
| (1,2559) | 1:128:A:TYR:HD1  | 1:164:A:ARG:HD3  | 13                  | 1.16     | 0.14                | 1.19       |
| (1,2559) | 1:128:A:TYR:HD2  | 1:164:A:ARG:HD3  | 13                  | 1.16     | 0.14                | 1.19       |
| (1,565)  | 1:129:A:MET:HE1  | 1:132:A:SER:HB2  | 13                  | 0.99     | 0.12                | 1.02       |
| (1,565)  | 1:129:A:MET:HE2  | 1:132:A:SER:HB2  | 13                  | 0.99     | 0.12                | 1.02       |
| (1,565)  | 1:129:A:MET:HE3  | 1:132:A:SER:HB2  | 13                  | 0.99     | 0.12                | 1.02       |
| (1,2548) | 1:162:A:TYR:HD1  | 1:186:A:GLN:HB3  | 13                  | 0.56     | 0.13                | 0.57       |
| (1,2548) | 1:162:A:TYR:HD2  | 1:186:A:GLN:HB3  | 13                  | 0.56     | 0.13                | 0.57       |
| (1,1197) | 1:160:A:GLN:HB2  | 1:183:A:THR:HG21 | 13                  | 0.45     | 0.25                | 0.46       |
| (1,1197) | 1:160:A:GLN:HB2  | 1:183:A:THR:HG22 | 13                  | 0.45     | 0.25                | 0.46       |
| (1,1197) | 1:160:A:GLN:HB2  | 1:183:A:THR:HG23 | 13                  | 0.45     | 0.25                | 0.46       |
| (1,1060) | 1:207:A:GLU:HG3  | 1:208:A:ARG:H    | 13                  | 0.45     | 0.12                | 0.45       |
| (1,740)  | 1:197:A:ASN:HB2  | 1:198:A:PHE:H    | 13                  | 0.43     | 0.06                | 0.42       |
| (1,2807) | 1:149:A:TYR:HE1  | 1:153:A:ASN:HB3  | 13                  | 0.4      | 0.18                | 0.42       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2807) | 1:149:A:TYR:HE2  | 1:153:A:ASN:HB3  | 13                  | 0.4      | 0.18                | 0.42       |
| (1,2270) | 1:132:A:SER:H    | 1:132:A:SER:HB2  | 13                  | 0.39     | 0.1                 | 0.39       |
| (1,162)  | 1:226:A:TYR:HB2  | 1:228:A:GLY:HA2  | 13                  | 0.24     | 0.05                | 0.27       |
| (1,162)  | 1:226:A:TYR:HB2  | 1:228:A:GLY:HA3  | 13                  | 0.24     | 0.05                | 0.27       |
| (1,32)   | 1:219:A:GLN:HB3  | 1:220:A:LYS:HG3  | 13                  | 0.13     | 0.02                | 0.14       |
| (1,2520) | 1:154:A:MET:HE1  | 1:155:A:TYR:HD1  | 13                  | 0.13     | 0.01                | 0.13       |
| (1,2520) | 1:154:A:MET:HE1  | 1:155:A:TYR:HD2  | 13                  | 0.13     | 0.01                | 0.13       |
| (1,2520) | 1:154:A:MET:HE2  | 1:155:A:TYR:HD1  | 13                  | 0.13     | 0.01                | 0.13       |
| (1,2520) | 1:154:A:MET:HE2  | 1:155:A:TYR:HD2  | 13                  | 0.13     | 0.01                | 0.13       |
| (1,2520) | 1:154:A:MET:HE3  | 1:155:A:TYR:HD1  | 13                  | 0.13     | 0.01                | 0.13       |
| (1,2520) | 1:154:A:MET:HE3  | 1:155:A:TYR:HD2  | 13                  | 0.13     | 0.01                | 0.13       |
| (1,296)  | 1:187:A:HIS:HB3  | 1:190:A:THR:HG21 | 13                  | 0.12     | 0.01                | 0.12       |
| (1,296)  | 1:187:A:HIS:HB3  | 1:190:A:THR:HG22 | 13                  | 0.12     | 0.01                | 0.12       |
| (1,296)  | 1:187:A:HIS:HB3  | 1:190:A:THR:HG23 | 13                  | 0.12     | 0.01                | 0.12       |
| (1,261)  | 1:185:A:LYS:HD2  | 1:188:A:THR:HG21 | 13                  | 0.12     | 0.01                | 0.12       |
| (1,261)  | 1:185:A:LYS:HD2  | 1:188:A:THR:HG22 | 13                  | 0.12     | 0.01                | 0.12       |
| (1,261)  | 1:185:A:LYS:HD2  | 1:188:A:THR:HG23 | 13                  | 0.12     | 0.01                | 0.12       |
| (1,261)  | 1:185:A:LYS:HD3  | 1:188:A:THR:HG21 | 13                  | 0.12     | 0.01                | 0.12       |
| (1,261)  | 1:185:A:LYS:HD3  | 1:188:A:THR:HG22 | 13                  | 0.12     | 0.01                | 0.12       |
| (1,261)  | 1:185:A:LYS:HD3  | 1:188:A:THR:HG23 | 13                  | 0.12     | 0.01                | 0.12       |
| (1,751)  | 1:222:A:SER:HB2  | 1:223:A:GLN:HA   | 12                  | 1.12     | 0.13                | 1.14       |
| (1,312)  | 1:166:A:VAL:HG21 | 1:170:A:SER:HB3  | 12                  | 1.1      | 1.05                | 0.44       |
| (1,312)  | 1:166:A:VAL:HG22 | 1:170:A:SER:HB3  | 12                  | 1.1      | 1.05                | 0.44       |
| (1,312)  | 1:166:A:VAL:HG23 | 1:170:A:SER:HB3  | 12                  | 1.1      | 1.05                | 0.44       |
| (1,2356) | 1:169:A:TYR:HB2  | 1:174:A:ASN:HD21 | 12                  | 1.1      | 0.52                | 1.14       |
| (1,380)  | 1:122:A:VAL:HG21 | 1:123:A:GLY:HA2  | 12                  | 1.07     | 0.3                 | 1.17       |
| (1,380)  | 1:122:A:VAL:HG21 | 1:123:A:GLY:HA3  | 12                  | 1.07     | 0.3                 | 1.17       |
| (1,380)  | 1:122:A:VAL:HG22 | 1:123:A:GLY:HA2  | 12                  | 1.07     | 0.3                 | 1.17       |
| (1,380)  | 1:122:A:VAL:HG22 | 1:123:A:GLY:HA3  | 12                  | 1.07     | 0.3                 | 1.17       |
| (1,380)  | 1:122:A:VAL:HG23 | 1:123:A:GLY:HA2  | 12                  | 1.07     | 0.3                 | 1.17       |
| (1,380)  | 1:122:A:VAL:HG23 | 1:123:A:GLY:HA3  | 12                  | 1.07     | 0.3                 | 1.17       |
| (1,220)  | 1:127:A:GLY:HA2  | 1:164:A:ARG:HE   | 12                  | 1.06     | 0.58                | 1.29       |
| (1,357)  | 1:122:A:VAL:HG21 | 1:125:A:LEU:HG   | 12                  | 0.97     | 0.63                | 0.86       |
| (1,357)  | 1:122:A:VAL:HG22 | 1:125:A:LEU:HG   | 12                  | 0.97     | 0.63                | 0.86       |
| (1,357)  | 1:122:A:VAL:HG23 | 1:125:A:LEU:HG   | 12                  | 0.97     | 0.63                | 0.86       |
| (1,506)  | 1:179:A:CYS:HB2  | 1:214:A:CYS:HB2  | 12                  | 0.77     | 0.33                | 0.86       |
| (1,733)  | 1:222:A:SER:HB2  | 1:226:A:TYR:HD1  | 12                  | 0.61     | 0.27                | 0.64       |
| (1,733)  | 1:222:A:SER:HB2  | 1:226:A:TYR:HD2  | 12                  | 0.61     | 0.27                | 0.64       |
| (1,1701) | 1:129:A:MET:H    | 1:129:A:MET:HG3  | 12                  | 0.5      | 0.09                | 0.5        |
| (1,1095) | 1:165:A:PRO:HA   | 1:168:A:GLN:HG2  | 12                  | 0.48     | 0.28                | 0.47       |
| (1,563)  | 1:132:A:SER:HB3  | 1:133:A:ALA:HB1  | 12                  | 0.43     | 0.06                | 0.44       |
| (1,563)  | 1:132:A:SER:HB3  | 1:133:A:ALA:HB2  | 12                  | 0.43     | 0.06                | 0.44       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,563)  | 1:132:A:SER:HB3  | 1:133:A:ALA:HB3  | 12                  | 0.43     | 0.06                | 0.44       |
| (1,569)  | 1:128:A:TYR:HE1  | 1:179:A:CYS:HB3  | 12                  | 0.35     | 0.19                | 0.36       |
| (1,569)  | 1:128:A:TYR:HE2  | 1:179:A:CYS:HB3  | 12                  | 0.35     | 0.19                | 0.36       |
| (1,1746) | 1:184:A:ILE:H    | 1:184:A:ILE:HG12 | 12                  | 0.25     | 0.13                | 0.22       |
| (1,350)  | 1:122:A:VAL:HG21 | 1:123:A:GLY:H    | 12                  | 0.19     | 0.07                | 0.2        |
| (1,350)  | 1:122:A:VAL:HG22 | 1:123:A:GLY:H    | 12                  | 0.19     | 0.07                | 0.2        |
| (1,350)  | 1:122:A:VAL:HG23 | 1:123:A:GLY:H    | 12                  | 0.19     | 0.07                | 0.2        |
| (1,470)  | 1:122:A:VAL:HG21 | 1:125:A:LEU:HB2  | 11                  | 1.54     | 0.61                | 1.38       |
| (1,470)  | 1:122:A:VAL:HG22 | 1:125:A:LEU:HB2  | 11                  | 1.54     | 0.61                | 1.38       |
| (1,470)  | 1:122:A:VAL:HG23 | 1:125:A:LEU:HB2  | 11                  | 1.54     | 0.61                | 1.38       |
| (1,258)  | 1:122:A:VAL:HG11 | 1:190:A:THR:HG21 | 11                  | 1.4      | 0.66                | 1.48       |
| (1,258)  | 1:122:A:VAL:HG11 | 1:190:A:THR:HG22 | 11                  | 1.4      | 0.66                | 1.48       |
| (1,258)  | 1:122:A:VAL:HG11 | 1:190:A:THR:HG23 | 11                  | 1.4      | 0.66                | 1.48       |
| (1,258)  | 1:122:A:VAL:HG12 | 1:190:A:THR:HG21 | 11                  | 1.4      | 0.66                | 1.48       |
| (1,258)  | 1:122:A:VAL:HG12 | 1:190:A:THR:HG22 | 11                  | 1.4      | 0.66                | 1.48       |
| (1,258)  | 1:122:A:VAL:HG12 | 1:190:A:THR:HG23 | 11                  | 1.4      | 0.66                | 1.48       |
| (1,258)  | 1:122:A:VAL:HG13 | 1:190:A:THR:HG21 | 11                  | 1.4      | 0.66                | 1.48       |
| (1,258)  | 1:122:A:VAL:HG13 | 1:190:A:THR:HG22 | 11                  | 1.4      | 0.66                | 1.48       |
| (1,258)  | 1:122:A:VAL:HG13 | 1:190:A:THR:HG23 | 11                  | 1.4      | 0.66                | 1.48       |
| (1,160)  | 1:223:A:GLN:HE21 | 1:228:A:GLY:HA2  | 11                  | 1.08     | 0.44                | 1.28       |
| (1,160)  | 1:223:A:GLN:HE21 | 1:228:A:GLY:HA3  | 11                  | 1.08     | 0.44                | 1.28       |
| (1,423)  | 1:151:A:ARG:HD3  | 1:152:A:GLU:H    | 11                  | 0.93     | 0.19                | 0.97       |
| (1,177)  | 1:195:A:GLY:HA3  | 1:197:A:ASN:HD21 | 11                  | 0.76     | 0.46                | 0.64       |
| (1,2792) | 1:128:A:TYR:HE1  | 1:164:A:ARG:HD3  | 11                  | 0.59     | 0.21                | 0.57       |
| (1,2792) | 1:128:A:TYR:HE2  | 1:164:A:ARG:HD3  | 11                  | 0.59     | 0.21                | 0.57       |
| (1,1584) | 1:122:A:VAL:H    | 1:122:A:VAL:HG11 | 11                  | 0.47     | 0.11                | 0.51       |
| (1,1584) | 1:122:A:VAL:H    | 1:122:A:VAL:HG12 | 11                  | 0.47     | 0.11                | 0.51       |
| (1,1584) | 1:122:A:VAL:H    | 1:122:A:VAL:HG13 | 11                  | 0.47     | 0.11                | 0.51       |
| (1,389)  | 1:121:A:VAL:HA   | 1:122:A:VAL:HG11 | 11                  | 0.45     | 0.17                | 0.45       |
| (1,389)  | 1:121:A:VAL:HA   | 1:122:A:VAL:HG12 | 11                  | 0.45     | 0.17                | 0.45       |
| (1,389)  | 1:121:A:VAL:HA   | 1:122:A:VAL:HG13 | 11                  | 0.45     | 0.17                | 0.45       |
| (1,864)  | 1:134:A:MET:HB3  | 1:135:A:SER:HB2  | 11                  | 0.43     | 0.22                | 0.46       |
| (1,574)  | 1:153:A:ASN:HB2  | 1:155:A:TYR:HE1  | 11                  | 0.25     | 0.1                 | 0.24       |
| (1,574)  | 1:153:A:ASN:HB2  | 1:155:A:TYR:HE2  | 11                  | 0.25     | 0.1                 | 0.24       |
| (1,1309) | 1:129:A:MET:HG2  | 1:164:A:ARG:HA   | 11                  | 0.22     | 0.04                | 0.24       |
| (1,1495) | 1:212:A:GLN:HB2  | 1:216:A:THR:H    | 11                  | 0.21     | 0.08                | 0.19       |
| (1,735)  | 1:222:A:SER:HB2  | 1:223:A:GLN:HB2  | 11                  | 0.18     | 0.02                | 0.19       |
| (1,735)  | 1:222:A:SER:HB2  | 1:223:A:GLN:HB3  | 11                  | 0.18     | 0.02                | 0.19       |
| (1,612)  | 1:134:A:MET:HE1  | 1:213:A:MET:H    | 11                  | 0.11     | 0.01                | 0.11       |
| (1,612)  | 1:134:A:MET:HE2  | 1:213:A:MET:H    | 11                  | 0.11     | 0.01                | 0.11       |
| (1,612)  | 1:134:A:MET:HE3  | 1:213:A:MET:H    | 11                  | 0.11     | 0.01                | 0.11       |
| (1,667)  | 1:138:A:MET:HE1  | 1:154:A:MET:HE1  | 11                  | 0.11     | 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) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,667)  | 1:138:A:MET:HE1  | 1:154:A:MET:HE2  | 11                  | 0.11     | 0.01                | 0.11       |
| (1,667)  | 1:138:A:MET:HE1  | 1:154:A:MET:HE3  | 11                  | 0.11     | 0.01                | 0.11       |
| (1,667)  | 1:138:A:MET:HE2  | 1:154:A:MET:HE1  | 11                  | 0.11     | 0.01                | 0.11       |
| (1,667)  | 1:138:A:MET:HE2  | 1:154:A:MET:HE2  | 11                  | 0.11     | 0.01                | 0.11       |
| (1,667)  | 1:138:A:MET:HE2  | 1:154:A:MET:HE3  | 11                  | 0.11     | 0.01                | 0.11       |
| (1,667)  | 1:138:A:MET:HE3  | 1:154:A:MET:HE1  | 11                  | 0.11     | 0.01                | 0.11       |
| (1,667)  | 1:138:A:MET:HE3  | 1:154:A:MET:HE2  | 11                  | 0.11     | 0.01                | 0.11       |
| (1,667)  | 1:138:A:MET:HE3  | 1:154:A:MET:HE3  | 11                  | 0.11     | 0.01                | 0.11       |
| (1,677)  | 1:135:A:SER:HB2  | 1:213:A:MET:HA   | 10                  | 1.12     | 0.51                | 1.34       |
| (1,567)  | 1:230:A:ARG:HB2  | 1:231:A:SER:HB3  | 10                  | 1.04     | 0.43                | 1.04       |
| (1,2338) | 1:212:A:GLN:HE21 | 1:215:A:VAL:HG11 | 10                  | 0.93     | 0.29                | 1.01       |
| (1,2338) | 1:212:A:GLN:HE21 | 1:215:A:VAL:HG12 | 10                  | 0.93     | 0.29                | 1.01       |
| (1,2338) | 1:212:A:GLN:HE21 | 1:215:A:VAL:HG13 | 10                  | 0.93     | 0.29                | 1.01       |
| (1,2721) | 1:177:A:HIS:HD2  | 1:178:A:ASP:HB3  | 10                  | 0.68     | 0.21                | 0.66       |
| (1,983)  | 1:149:A:TYR:H    | 1:152:A:GLU:HG2  | 10                  | 0.54     | 0.53                | 0.3        |
| (1,525)  | 1:132:A:SER:HB2  | 1:160:A:GLN:HE21 | 10                  | 0.4      | 0.25                | 0.29       |
| (1,2474) | 1:168:A:GLN:HG2  | 1:169:A:TYR:HD1  | 10                  | 0.29     | 0.15                | 0.29       |
| (1,2474) | 1:168:A:GLN:HG2  | 1:169:A:TYR:HD2  | 10                  | 0.29     | 0.15                | 0.29       |
| (1,1050) | 1:128:A:TYR:HA   | 1:129:A:MET:HG3  | 10                  | 0.28     | 0.08                | 0.26       |
| (1,1340) | 1:160:A:GLN:HA   | 1:213:A:MET:HB2  | 10                  | 0.18     | 0.04                | 0.17       |
| (1,902)  | 1:147:A:ASP:HB2  | 1:148:A:ARG:HA   | 10                  | 0.13     | 0.02                | 0.12       |
| (1,1926) | 1:134:A:MET:HE1  | 1:214:A:CYS:H    | 10                  | 0.11     | 0.01                | 0.11       |
| (1,1926) | 1:134:A:MET:HE2  | 1:214:A:CYS:H    | 10                  | 0.11     | 0.01                | 0.11       |
| (1,1926) | 1:134:A:MET:HE3  | 1:214:A:CYS:H    | 10                  | 0.11     | 0.01                | 0.11       |
| (1,2631) | 1:198:A:PHE:HD1  | 1:203:A:VAL:HA   | 10                  | 0.11     | 0.01                | 0.11       |
| (1,2631) | 1:198:A:PHE:HD2  | 1:203:A:VAL:HA   | 10                  | 0.11     | 0.01                | 0.11       |
| (1,421)  | 1:121:A:VAL:HG11 | 1:123:A:GLY:HA2  | 10                  | 0.11     | 0.01                | 0.11       |
| (1,421)  | 1:121:A:VAL:HG11 | 1:123:A:GLY:HA3  | 10                  | 0.11     | 0.01                | 0.11       |
| (1,421)  | 1:121:A:VAL:HG12 | 1:123:A:GLY:HA2  | 10                  | 0.11     | 0.01                | 0.11       |
| (1,421)  | 1:121:A:VAL:HG12 | 1:123:A:GLY:HA3  | 10                  | 0.11     | 0.01                | 0.11       |
| (1,421)  | 1:121:A:VAL:HG13 | 1:123:A:GLY:HA2  | 10                  | 0.11     | 0.01                | 0.11       |
| (1,421)  | 1:121:A:VAL:HG13 | 1:123:A:GLY:HA3  | 10                  | 0.11     | 0.01                | 0.11       |
| (1,1912) | 1:213:A:MET:H    | 1:215:A:VAL:HG11 | 9                   | 1.26     | 0.18                | 1.32       |
| (1,1912) | 1:213:A:MET:H    | 1:215:A:VAL:HG12 | 9                   | 1.26     | 0.18                | 1.32       |
| (1,1912) | 1:213:A:MET:H    | 1:215:A:VAL:HG13 | 9                   | 1.26     | 0.18                | 1.32       |
| (1,104)  | 1:213:A:MET:HA   | 1:215:A:VAL:HG11 | 9                   | 1.19     | 0.2                 | 1.31       |
| (1,104)  | 1:213:A:MET:HA   | 1:215:A:VAL:HG12 | 9                   | 1.19     | 0.2                 | 1.31       |
| (1,104)  | 1:213:A:MET:HA   | 1:215:A:VAL:HG13 | 9                   | 1.19     | 0.2                 | 1.31       |
| (1,2571) | 1:215:A:VAL:HG21 | 1:218:A:TYR:HD1  | 9                   | 1.16     | 0.14                | 1.15       |
| (1,2571) | 1:215:A:VAL:HG21 | 1:218:A:TYR:HD2  | 9                   | 1.16     | 0.14                | 1.15       |
| (1,2571) | 1:215:A:VAL:HG22 | 1:218:A:TYR:HD1  | 9                   | 1.16     | 0.14                | 1.15       |
| (1,2571) | 1:215:A:VAL:HG22 | 1:218:A:TYR:HD2  | 9                   | 1.16     | 0.14                | 1.15       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2571) | 1:215:A:VAL:HG23 | 1:218:A:TYR:HD1  | 9                   | 1.16     | 0.14                | 1.15       |
| (1,2571) | 1:215:A:VAL:HG23 | 1:218:A:TYR:HD2  | 9                   | 1.16     | 0.14                | 1.15       |
| (1,1164) | 1:215:A:VAL:HG21 | 1:219:A:GLN:HG2  | 9                   | 1.01     | 0.34                | 0.87       |
| (1,1164) | 1:215:A:VAL:HG22 | 1:219:A:GLN:HG2  | 9                   | 1.01     | 0.34                | 0.87       |
| (1,1164) | 1:215:A:VAL:HG23 | 1:219:A:GLN:HG2  | 9                   | 1.01     | 0.34                | 0.87       |
| (1,467)  | 1:122:A:VAL:HG21 | 1:125:A:LEU:HB3  | 9                   | 0.79     | 0.41                | 0.79       |
| (1,467)  | 1:122:A:VAL:HG22 | 1:125:A:LEU:HB3  | 9                   | 0.79     | 0.41                | 0.79       |
| (1,467)  | 1:122:A:VAL:HG23 | 1:125:A:LEU:HB3  | 9                   | 0.79     | 0.41                | 0.79       |
| (1,189)  | 1:123:A:GLY:HA2  | 1:125:A:LEU:HD21 | 9                   | 0.76     | 0.66                | 0.75       |
| (1,189)  | 1:123:A:GLY:HA2  | 1:125:A:LEU:HD22 | 9                   | 0.76     | 0.66                | 0.75       |
| (1,189)  | 1:123:A:GLY:HA2  | 1:125:A:LEU:HD23 | 9                   | 0.76     | 0.66                | 0.75       |
| (1,189)  | 1:123:A:GLY:HA3  | 1:125:A:LEU:HD21 | 9                   | 0.76     | 0.66                | 0.75       |
| (1,189)  | 1:123:A:GLY:HA3  | 1:125:A:LEU:HD22 | 9                   | 0.76     | 0.66                | 0.75       |
| (1,189)  | 1:123:A:GLY:HA3  | 1:125:A:LEU:HD23 | 9                   | 0.76     | 0.66                | 0.75       |
| (1,1166) | 1:215:A:VAL:HG21 | 1:219:A:GLN:HG3  | 9                   | 0.66     | 0.26                | 0.65       |
| (1,1166) | 1:215:A:VAL:HG22 | 1:219:A:GLN:HG3  | 9                   | 0.66     | 0.26                | 0.65       |
| (1,1166) | 1:215:A:VAL:HG23 | 1:219:A:GLN:HG3  | 9                   | 0.66     | 0.26                | 0.65       |
| (1,101)  | 1:138:A:MET:HA   | 1:209:A:VAL:HG11 | 9                   | 0.65     | 0.24                | 0.69       |
| (1,101)  | 1:138:A:MET:HA   | 1:209:A:VAL:HG12 | 9                   | 0.65     | 0.24                | 0.69       |
| (1,101)  | 1:138:A:MET:HA   | 1:209:A:VAL:HG13 | 9                   | 0.65     | 0.24                | 0.69       |
| (1,1679) | 1:122:A:VAL:HG21 | 1:125:A:LEU:H    | 9                   | 0.65     | 0.49                | 0.48       |
| (1,1679) | 1:122:A:VAL:HG22 | 1:125:A:LEU:H    | 9                   | 0.65     | 0.49                | 0.48       |
| (1,1679) | 1:122:A:VAL:HG23 | 1:125:A:LEU:H    | 9                   | 0.65     | 0.49                | 0.48       |
| (1,1894) | 1:215:A:VAL:HG21 | 1:219:A:GLN:H    | 9                   | 0.55     | 0.06                | 0.54       |
| (1,1894) | 1:215:A:VAL:HG22 | 1:219:A:GLN:H    | 9                   | 0.55     | 0.06                | 0.54       |
| (1,1894) | 1:215:A:VAL:HG23 | 1:219:A:GLN:H    | 9                   | 0.55     | 0.06                | 0.54       |
| (1,658)  | 1:154:A:MET:HG3  | 1:154:A:MET:HE1  | 9                   | 0.48     | 0.25                | 0.65       |
| (1,658)  | 1:154:A:MET:HG3  | 1:154:A:MET:HE2  | 9                   | 0.48     | 0.25                | 0.65       |
| (1,658)  | 1:154:A:MET:HG3  | 1:154:A:MET:HE3  | 9                   | 0.48     | 0.25                | 0.65       |
| (1,1213) | 1:230:A:ARG:HA   | 1:230:A:ARG:HG3  | 9                   | 0.37     | 0.03                | 0.36       |
| (1,881)  | 1:145:A:TRP:HE3  | 1:146:A:GLU:HG3  | 9                   | 0.35     | 0.14                | 0.35       |
| (1,828)  | 1:222:A:SER:HA   | 1:226:A:TYR:HB3  | 9                   | 0.27     | 0.12                | 0.21       |
| (1,31)   | 1:219:A:GLN:HA   | 1:220:A:LYS:HG3  | 9                   | 0.15     | 0.05                | 0.15       |
| (1,393)  | 1:120:A:SER:HB2  | 1:121:A:VAL:HG11 | 9                   | 0.11     | 0.01                | 0.11       |
| (1,393)  | 1:120:A:SER:HB2  | 1:121:A:VAL:HG12 | 9                   | 0.11     | 0.01                | 0.11       |
| (1,393)  | 1:120:A:SER:HB2  | 1:121:A:VAL:HG13 | 9                   | 0.11     | 0.01                | 0.11       |
| (1,393)  | 1:120:A:SER:HB3  | 1:121:A:VAL:HG11 | 9                   | 0.11     | 0.01                | 0.11       |
| (1,393)  | 1:120:A:SER:HB3  | 1:121:A:VAL:HG12 | 9                   | 0.11     | 0.01                | 0.11       |
| (1,393)  | 1:120:A:SER:HB3  | 1:121:A:VAL:HG13 | 9                   | 0.11     | 0.01                | 0.11       |
| (1,2703) | 1:143:A:ASN:HB2  | 1:145:A:TRP:HD1  | 9                   | 0.1      | 0.0                 | 0.1        |
| (1,2703) | 1:143:A:ASN:HB3  | 1:145:A:TRP:HD1  | 9                   | 0.1      | 0.0                 | 0.1        |
| (1,392)  | 1:122:A:VAL:HG11 | 1:190:A:THR:HB   | 8                   | 1.31     | 0.67                | 1.5        |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,392)  | 1:122:A:VAL:HG12 | 1:190:A:THR:HB   | 8                   | 1.31     | 0.67                | 1.5        |
| (1,392)  | 1:122:A:VAL:HG13 | 1:190:A:THR:HB   | 8                   | 1.31     | 0.67                | 1.5        |
| (1,429)  | 1:122:A:VAL:HG11 | 1:186:A:GLN:HA   | 8                   | 1.21     | 0.49                | 1.31       |
| (1,429)  | 1:122:A:VAL:HG12 | 1:186:A:GLN:HA   | 8                   | 1.21     | 0.49                | 1.31       |
| (1,429)  | 1:122:A:VAL:HG13 | 1:186:A:GLN:HA   | 8                   | 1.21     | 0.49                | 1.31       |
| (1,1375) | 1:136:A:ARG:HD2  | 1:154:A:MET:HG3  | 8                   | 0.88     | 0.4                 | 0.82       |
| (1,1089) | 1:182:A:ILE:HD11 | 1:186:A:GLN:HE21 | 8                   | 0.74     | 0.32                | 0.82       |
| (1,1089) | 1:182:A:ILE:HD12 | 1:186:A:GLN:HE21 | 8                   | 0.74     | 0.32                | 0.82       |
| (1,1089) | 1:182:A:ILE:HD13 | 1:186:A:GLN:HE21 | 8                   | 0.74     | 0.32                | 0.82       |
| (1,107)  | 1:211:A:GLU:HG3  | 1:215:A:VAL:HG11 | 8                   | 0.69     | 0.34                | 0.73       |
| (1,107)  | 1:211:A:GLU:HG3  | 1:215:A:VAL:HG12 | 8                   | 0.69     | 0.34                | 0.73       |
| (1,107)  | 1:211:A:GLU:HG3  | 1:215:A:VAL:HG13 | 8                   | 0.69     | 0.34                | 0.73       |
| (1,1575) | 1:136:A:ARG:H    | 1:136:A:ARG:HD3  | 8                   | 0.64     | 0.24                | 0.72       |
| (1,105)  | 1:212:A:GLN:HA   | 1:215:A:VAL:HG11 | 8                   | 0.56     | 0.18                | 0.61       |
| (1,105)  | 1:212:A:GLN:HA   | 1:215:A:VAL:HG12 | 8                   | 0.56     | 0.18                | 0.61       |
| (1,105)  | 1:212:A:GLN:HA   | 1:215:A:VAL:HG13 | 8                   | 0.56     | 0.18                | 0.61       |
| (1,318)  | 1:153:A:ASN:HB2  | 1:156:A:ARG:HD3  | 8                   | 0.56     | 0.33                | 0.36       |
| (1,2045) | 1:230:A:ARG:HG3  | 1:231:A:SER:H    | 8                   | 0.51     | 0.22                | 0.5        |
| (1,260)  | 1:186:A:GLN:HB2  | 1:190:A:THR:HG21 | 8                   | 0.37     | 0.26                | 0.25       |
| (1,260)  | 1:186:A:GLN:HB2  | 1:190:A:THR:HG22 | 8                   | 0.37     | 0.26                | 0.25       |
| (1,260)  | 1:186:A:GLN:HB2  | 1:190:A:THR:HG23 | 8                   | 0.37     | 0.26                | 0.25       |
| (1,1227) | 1:210:A:VAL:HA   | 1:213:A:MET:HG2  | 8                   | 0.28     | 0.18                | 0.18       |
| (1,1847) | 1:197:A:ASN:H    | 1:197:A:ASN:HB3  | 8                   | 0.24     | 0.08                | 0.24       |
| (1,2322) | 1:130:A:LEU:HG   | 1:160:A:GLN:HE22 | 8                   | 0.18     | 0.04                | 0.19       |
| (1,814)  | 1:226:A:TYR:HB2  | 1:227:A:ASP:HA   | 8                   | 0.17     | 0.06                | 0.14       |
| (1,1152) | 1:205:A:MET:HA   | 1:205:A:MET:HG3  | 8                   | 0.13     | 0.02                | 0.12       |
| (1,1007) | 1:137:A:PRO:HA   | 1:139:A:ILE:HD11 | 8                   | 0.12     | 0.01                | 0.12       |
| (1,1007) | 1:137:A:PRO:HA   | 1:139:A:ILE:HD12 | 8                   | 0.12     | 0.01                | 0.12       |
| (1,1007) | 1:137:A:PRO:HA   | 1:139:A:ILE:HD13 | 8                   | 0.12     | 0.01                | 0.12       |
| (1,2794) | 1:128:A:TYR:HE1  | 1:164:A:ARG:HG2  | 7                   | 1.15     | 0.27                | 1.31       |
| (1,2794) | 1:128:A:TYR:HE2  | 1:164:A:ARG:HG2  | 7                   | 1.15     | 0.27                | 1.31       |
| (1,602)  | 1:230:A:ARG:H    | 1:231:A:SER:HB3  | 7                   | 0.95     | 0.45                | 0.99       |
| (1,2821) | 1:129:A:MET:HB3  | 1:163:A:TYR:HE1  | 7                   | 0.87     | 0.04                | 0.88       |
| (1,2821) | 1:129:A:MET:HB3  | 1:163:A:TYR:HE2  | 7                   | 0.87     | 0.04                | 0.88       |
| (1,1085) | 1:129:A:MET:HB2  | 1:164:A:ARG:HA   | 7                   | 0.85     | 0.16                | 0.75       |
| (1,2674) | 1:175:A:PHE:HZ   | 1:221:A:GLU:HG2  | 7                   | 0.65     | 0.38                | 0.67       |
| (1,2824) | 1:218:A:TYR:HE1  | 1:222:A:SER:HB3  | 7                   | 0.52     | 0.24                | 0.39       |
| (1,2824) | 1:218:A:TYR:HE2  | 1:222:A:SER:HB3  | 7                   | 0.52     | 0.24                | 0.39       |
| (1,2326) | 1:223:A:GLN:HE21 | 1:228:A:GLY:H    | 7                   | 0.51     | 0.06                | 0.5        |
| (1,739)  | 1:166:A:VAL:HG11 | 1:222:A:SER:HB3  | 7                   | 0.44     | 0.22                | 0.37       |
| (1,739)  | 1:166:A:VAL:HG12 | 1:222:A:SER:HB3  | 7                   | 0.44     | 0.22                | 0.37       |
| (1,739)  | 1:166:A:VAL:HG13 | 1:222:A:SER:HB3  | 7                   | 0.44     | 0.22                | 0.37       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,528)  | 1:143:A:ASN:HB2  | 1:147:A:ASP:HB3  | 7                   | 0.4      | 0.19                | 0.34       |
| (1,528)  | 1:143:A:ASN:HB3  | 1:147:A:ASP:HB3  | 7                   | 0.4      | 0.19                | 0.34       |
| (1,521)  | 1:223:A:GLN:HG3  | 1:224:A:ALA:HB1  | 7                   | 0.37     | 0.13                | 0.32       |
| (1,521)  | 1:223:A:GLN:HG3  | 1:224:A:ALA:HB2  | 7                   | 0.37     | 0.13                | 0.32       |
| (1,521)  | 1:223:A:GLN:HG3  | 1:224:A:ALA:HB3  | 7                   | 0.37     | 0.13                | 0.32       |
| (1,2445) | 1:122:A:VAL:HG21 | 1:124:A:GLY:H    | 7                   | 0.35     | 0.21                | 0.25       |
| (1,2445) | 1:122:A:VAL:HG22 | 1:124:A:GLY:H    | 7                   | 0.35     | 0.21                | 0.25       |
| (1,2445) | 1:122:A:VAL:HG23 | 1:124:A:GLY:H    | 7                   | 0.35     | 0.21                | 0.25       |
| (1,196)  | 1:161:A:VAL:HG21 | 1:216:A:THR:HG21 | 7                   | 0.34     | 0.55                | 0.12       |
| (1,196)  | 1:161:A:VAL:HG21 | 1:216:A:THR:HG22 | 7                   | 0.34     | 0.55                | 0.12       |
| (1,196)  | 1:161:A:VAL:HG21 | 1:216:A:THR:HG23 | 7                   | 0.34     | 0.55                | 0.12       |
| (1,196)  | 1:161:A:VAL:HG22 | 1:216:A:THR:HG21 | 7                   | 0.34     | 0.55                | 0.12       |
| (1,196)  | 1:161:A:VAL:HG22 | 1:216:A:THR:HG22 | 7                   | 0.34     | 0.55                | 0.12       |
| (1,196)  | 1:161:A:VAL:HG22 | 1:216:A:THR:HG23 | 7                   | 0.34     | 0.55                | 0.12       |
| (1,196)  | 1:161:A:VAL:HG23 | 1:216:A:THR:HG21 | 7                   | 0.34     | 0.55                | 0.12       |
| (1,196)  | 1:161:A:VAL:HG23 | 1:216:A:THR:HG22 | 7                   | 0.34     | 0.55                | 0.12       |
| (1,196)  | 1:161:A:VAL:HG23 | 1:216:A:THR:HG23 | 7                   | 0.34     | 0.55                | 0.12       |
| (1,151)  | 1:126:A:GLY:HA3  | 1:164:A:ARG:HD3  | 7                   | 0.33     | 0.09                | 0.32       |
| (1,1466) | 1:210:A:VAL:H    | 1:211:A:GLU:HB3  | 7                   | 0.25     | 0.12                | 0.19       |
| (1,333)  | 1:172:A:GLN:HE22 | 1:215:A:VAL:HG21 | 7                   | 0.22     | 0.07                | 0.26       |
| (1,333)  | 1:172:A:GLN:HE22 | 1:215:A:VAL:HG22 | 7                   | 0.22     | 0.07                | 0.26       |
| (1,333)  | 1:172:A:GLN:HE22 | 1:215:A:VAL:HG23 | 7                   | 0.22     | 0.07                | 0.26       |
| (1,1535) | 1:165:A:PRO:HD2  | 1:166:A:VAL:H    | 7                   | 0.15     | 0.04                | 0.13       |
| (1,1968) | 1:205:A:MET:H    | 1:205:A:MET:HG3  | 7                   | 0.13     | 0.03                | 0.13       |
| (1,217)  | 1:193:A:THR:HG21 | 1:196:A:GLU:HB2  | 7                   | 0.12     | 0.01                | 0.12       |
| (1,217)  | 1:193:A:THR:HG21 | 1:196:A:GLU:HB3  | 7                   | 0.12     | 0.01                | 0.12       |
| (1,217)  | 1:193:A:THR:HG22 | 1:196:A:GLU:HB2  | 7                   | 0.12     | 0.01                | 0.12       |
| (1,217)  | 1:193:A:THR:HG22 | 1:196:A:GLU:HB3  | 7                   | 0.12     | 0.01                | 0.12       |
| (1,217)  | 1:193:A:THR:HG23 | 1:196:A:GLU:HB2  | 7                   | 0.12     | 0.01                | 0.12       |
| (1,217)  | 1:193:A:THR:HG23 | 1:196:A:GLU:HB3  | 7                   | 0.12     | 0.01                | 0.12       |
| (1,2843) | 1:157:A:TYR:HE1  | 1:206:A:MET:HE1  | 7                   | 0.12     | 0.01                | 0.12       |
| (1,2843) | 1:157:A:TYR:HE1  | 1:206:A:MET:HE2  | 7                   | 0.12     | 0.01                | 0.12       |
| (1,2843) | 1:157:A:TYR:HE1  | 1:206:A:MET:HE3  | 7                   | 0.12     | 0.01                | 0.12       |
| (1,2843) | 1:157:A:TYR:HE2  | 1:206:A:MET:HE1  | 7                   | 0.12     | 0.01                | 0.12       |
| (1,2843) | 1:157:A:TYR:HE2  | 1:206:A:MET:HE2  | 7                   | 0.12     | 0.01                | 0.12       |
| (1,2843) | 1:157:A:TYR:HE2  | 1:206:A:MET:HE3  | 7                   | 0.12     | 0.01                | 0.12       |
| (1,1234) | 1:122:A:VAL:HB   | 1:123:A:GLY:HA2  | 7                   | 0.12     | 0.0                 | 0.12       |
| (1,1234) | 1:122:A:VAL:HB   | 1:123:A:GLY:HA3  | 7                   | 0.12     | 0.0                 | 0.12       |
| (1,2634) | 1:198:A:PHE:HD1  | 1:203:A:VAL:HG11 | 6                   | 2.13     | 0.05                | 2.14       |
| (1,2634) | 1:198:A:PHE:HD1  | 1:203:A:VAL:HG12 | 6                   | 2.13     | 0.05                | 2.14       |
| (1,2634) | 1:198:A:PHE:HD1  | 1:203:A:VAL:HG13 | 6                   | 2.13     | 0.05                | 2.14       |
| (1,2634) | 1:198:A:PHE:HD2  | 1:203:A:VAL:HG11 | 6                   | 2.13     | 0.05                | 2.14       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2634) | 1:198:A:PHE:HD2  | 1:203:A:VAL:HG12 | 6                   | 2.13     | 0.05                | 2.14       |
| (1,2634) | 1:198:A:PHE:HD2  | 1:203:A:VAL:HG13 | 6                   | 2.13     | 0.05                | 2.14       |
| (1,355)  | 1:203:A:VAL:HG21 | 1:204:A:LYS:HD2  | 6                   | 2.1      | 0.09                | 2.1        |
| (1,355)  | 1:203:A:VAL:HG21 | 1:204:A:LYS:HD3  | 6                   | 2.1      | 0.09                | 2.1        |
| (1,355)  | 1:203:A:VAL:HG22 | 1:204:A:LYS:HD2  | 6                   | 2.1      | 0.09                | 2.1        |
| (1,355)  | 1:203:A:VAL:HG22 | 1:204:A:LYS:HD3  | 6                   | 2.1      | 0.09                | 2.1        |
| (1,355)  | 1:203:A:VAL:HG23 | 1:204:A:LYS:HD2  | 6                   | 2.1      | 0.09                | 2.1        |
| (1,355)  | 1:203:A:VAL:HG23 | 1:204:A:LYS:HD3  | 6                   | 2.1      | 0.09                | 2.1        |
| (1,1662) | 1:198:A:PHE:H    | 1:203:A:VAL:HG11 | 6                   | 1.93     | 0.27                | 2.01       |
| (1,1662) | 1:198:A:PHE:H    | 1:203:A:VAL:HG12 | 6                   | 1.93     | 0.27                | 2.01       |
| (1,1662) | 1:198:A:PHE:H    | 1:203:A:VAL:HG13 | 6                   | 1.93     | 0.27                | 2.01       |
| (1,356)  | 1:203:A:VAL:HG21 | 1:204:A:LYS:HG2  | 6                   | 1.66     | 0.3                 | 1.74       |
| (1,356)  | 1:203:A:VAL:HG22 | 1:204:A:LYS:HG2  | 6                   | 1.66     | 0.3                 | 1.74       |
| (1,356)  | 1:203:A:VAL:HG23 | 1:204:A:LYS:HG2  | 6                   | 1.66     | 0.3                 | 1.74       |
| (1,358)  | 1:203:A:VAL:HG21 | 1:204:A:LYS:HG3  | 6                   | 1.61     | 0.39                | 1.4        |
| (1,358)  | 1:203:A:VAL:HG22 | 1:204:A:LYS:HG3  | 6                   | 1.61     | 0.39                | 1.4        |
| (1,358)  | 1:203:A:VAL:HG23 | 1:204:A:LYS:HG3  | 6                   | 1.61     | 0.39                | 1.4        |
| (1,1125) | 1:198:A:PHE:HA   | 1:203:A:VAL:HG11 | 6                   | 1.45     | 0.12                | 1.47       |
| (1,1125) | 1:198:A:PHE:HA   | 1:203:A:VAL:HG12 | 6                   | 1.45     | 0.12                | 1.47       |
| (1,1125) | 1:198:A:PHE:HA   | 1:203:A:VAL:HG13 | 6                   | 1.45     | 0.12                | 1.47       |
| (1,601)  | 1:166:A:VAL:HG21 | 1:170:A:SER:HB2  | 6                   | 1.36     | 0.99                | 1.45       |
| (1,601)  | 1:166:A:VAL:HG22 | 1:170:A:SER:HB2  | 6                   | 1.36     | 0.99                | 1.45       |
| (1,601)  | 1:166:A:VAL:HG23 | 1:170:A:SER:HB2  | 6                   | 1.36     | 0.99                | 1.45       |
| (1,311)  | 1:201:A:THR:HA   | 1:203:A:VAL:HG21 | 6                   | 1.32     | 0.06                | 1.34       |
| (1,311)  | 1:201:A:THR:HA   | 1:203:A:VAL:HG22 | 6                   | 1.32     | 0.06                | 1.34       |
| (1,311)  | 1:201:A:THR:HA   | 1:203:A:VAL:HG23 | 6                   | 1.32     | 0.06                | 1.34       |
| (1,2352) | 1:171:A:ASN:HA   | 1:174:A:ASN:HD21 | 6                   | 1.24     | 0.26                | 1.18       |
| (1,173)  | 1:198:A:PHE:HB2  | 1:203:A:VAL:HG11 | 6                   | 1.23     | 0.2                 | 1.23       |
| (1,173)  | 1:198:A:PHE:HB2  | 1:203:A:VAL:HG12 | 6                   | 1.23     | 0.2                 | 1.23       |
| (1,173)  | 1:198:A:PHE:HB2  | 1:203:A:VAL:HG13 | 6                   | 1.23     | 0.2                 | 1.23       |
| (1,169)  | 1:198:A:PHE:HB3  | 1:203:A:VAL:HG11 | 6                   | 1.17     | 0.09                | 1.18       |
| (1,169)  | 1:198:A:PHE:HB3  | 1:203:A:VAL:HG12 | 6                   | 1.17     | 0.09                | 1.18       |
| (1,169)  | 1:198:A:PHE:HB3  | 1:203:A:VAL:HG13 | 6                   | 1.17     | 0.09                | 1.18       |
| (1,58)   | 1:122:A:VAL:HG21 | 1:125:A:LEU:HD11 | 6                   | 1.16     | 0.61                | 1.08       |
| (1,58)   | 1:122:A:VAL:HG21 | 1:125:A:LEU:HD12 | 6                   | 1.16     | 0.61                | 1.08       |
| (1,58)   | 1:122:A:VAL:HG21 | 1:125:A:LEU:HD13 | 6                   | 1.16     | 0.61                | 1.08       |
| (1,58)   | 1:122:A:VAL:HG22 | 1:125:A:LEU:HD11 | 6                   | 1.16     | 0.61                | 1.08       |
| (1,58)   | 1:122:A:VAL:HG22 | 1:125:A:LEU:HD12 | 6                   | 1.16     | 0.61                | 1.08       |
| (1,58)   | 1:122:A:VAL:HG22 | 1:125:A:LEU:HD13 | 6                   | 1.16     | 0.61                | 1.08       |
| (1,58)   | 1:122:A:VAL:HG23 | 1:125:A:LEU:HD11 | 6                   | 1.16     | 0.61                | 1.08       |
| (1,58)   | 1:122:A:VAL:HG23 | 1:125:A:LEU:HD12 | 6                   | 1.16     | 0.61                | 1.08       |
| (1,58)   | 1:122:A:VAL:HG23 | 1:125:A:LEU:HD13 | 6                   | 1.16     | 0.61                | 1.08       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2123) | 1:199:A:THR:H    | 1:203:A:VAL:HG11 | 6                   | 1.06     | 0.14                | 1.02       |
| (1,2123) | 1:199:A:THR:H    | 1:203:A:VAL:HG12 | 6                   | 1.06     | 0.14                | 1.02       |
| (1,2123) | 1:199:A:THR:H    | 1:203:A:VAL:HG13 | 6                   | 1.06     | 0.14                | 1.02       |
| (1,476)  | 1:203:A:VAL:HG21 | 1:204:A:LYS:HE2  | 6                   | 0.93     | 0.37                | 0.79       |
| (1,476)  | 1:203:A:VAL:HG21 | 1:204:A:LYS:HE3  | 6                   | 0.93     | 0.37                | 0.79       |
| (1,476)  | 1:203:A:VAL:HG22 | 1:204:A:LYS:HE2  | 6                   | 0.93     | 0.37                | 0.79       |
| (1,476)  | 1:203:A:VAL:HG22 | 1:204:A:LYS:HE3  | 6                   | 0.93     | 0.37                | 0.79       |
| (1,476)  | 1:203:A:VAL:HG23 | 1:204:A:LYS:HE2  | 6                   | 0.93     | 0.37                | 0.79       |
| (1,476)  | 1:203:A:VAL:HG23 | 1:204:A:LYS:HE3  | 6                   | 0.93     | 0.37                | 0.79       |
| (1,2782) | 1:150:A:TYR:HE1  | 1:154:A:MET:HG3  | 6                   | 0.74     | 0.27                | 0.76       |
| (1,2782) | 1:150:A:TYR:HE2  | 1:154:A:MET:HG3  | 6                   | 0.74     | 0.27                | 0.76       |
| (1,1480) | 1:203:A:VAL:HG21 | 1:207:A:GLU:HB2  | 6                   | 0.73     | 0.41                | 0.62       |
| (1,1480) | 1:203:A:VAL:HG22 | 1:207:A:GLU:HB2  | 6                   | 0.73     | 0.41                | 0.62       |
| (1,1480) | 1:203:A:VAL:HG23 | 1:207:A:GLU:HB2  | 6                   | 0.73     | 0.41                | 0.62       |
| (1,901)  | 1:203:A:VAL:HG21 | 1:204:A:LYS:HA   | 6                   | 0.58     | 0.08                | 0.57       |
| (1,901)  | 1:203:A:VAL:HG22 | 1:204:A:LYS:HA   | 6                   | 0.58     | 0.08                | 0.57       |
| (1,901)  | 1:203:A:VAL:HG23 | 1:204:A:LYS:HA   | 6                   | 0.58     | 0.08                | 0.57       |
| (1,2313) | 1:159:A:ASN:HD22 | 1:160:A:GLN:HE21 | 6                   | 0.5      | 0.2                 | 0.54       |
| (1,174)  | 1:202:A:ASP:HB3  | 1:203:A:VAL:HG11 | 6                   | 0.38     | 0.11                | 0.4        |
| (1,174)  | 1:202:A:ASP:HB3  | 1:203:A:VAL:HG12 | 6                   | 0.38     | 0.11                | 0.4        |
| (1,174)  | 1:202:A:ASP:HB3  | 1:203:A:VAL:HG13 | 6                   | 0.38     | 0.11                | 0.4        |
| (1,167)  | 1:203:A:VAL:H    | 1:203:A:VAL:HG11 | 6                   | 0.3      | 0.06                | 0.29       |
| (1,167)  | 1:203:A:VAL:H    | 1:203:A:VAL:HG12 | 6                   | 0.3      | 0.06                | 0.29       |
| (1,167)  | 1:203:A:VAL:H    | 1:203:A:VAL:HG13 | 6                   | 0.3      | 0.06                | 0.29       |
| (1,944)  | 1:171:A:ASN:HB3  | 1:172:A:GLN:HA   | 6                   | 0.29     | 0.15                | 0.29       |
| (1,1501) | 1:137:A:PRO:HD3  | 1:209:A:VAL:HG21 | 6                   | 0.23     | 0.07                | 0.24       |
| (1,1501) | 1:137:A:PRO:HD3  | 1:209:A:VAL:HG22 | 6                   | 0.23     | 0.07                | 0.24       |
| (1,1501) | 1:137:A:PRO:HD3  | 1:209:A:VAL:HG23 | 6                   | 0.23     | 0.07                | 0.24       |
| (1,497)  | 1:128:A:TYR:HB2  | 1:162:A:TYR:HB2  | 6                   | 0.17     | 0.07                | 0.14       |
| (1,307)  | 1:176:A:VAL:HG11 | 1:215:A:VAL:HG21 | 6                   | 0.13     | 0.02                | 0.13       |
| (1,307)  | 1:176:A:VAL:HG11 | 1:215:A:VAL:HG22 | 6                   | 0.13     | 0.02                | 0.13       |
| (1,307)  | 1:176:A:VAL:HG11 | 1:215:A:VAL:HG23 | 6                   | 0.13     | 0.02                | 0.13       |
| (1,307)  | 1:176:A:VAL:HG12 | 1:215:A:VAL:HG21 | 6                   | 0.13     | 0.02                | 0.13       |
| (1,307)  | 1:176:A:VAL:HG12 | 1:215:A:VAL:HG22 | 6                   | 0.13     | 0.02                | 0.13       |
| (1,307)  | 1:176:A:VAL:HG12 | 1:215:A:VAL:HG23 | 6                   | 0.13     | 0.02                | 0.13       |
| (1,307)  | 1:176:A:VAL:HG13 | 1:215:A:VAL:HG21 | 6                   | 0.13     | 0.02                | 0.13       |
| (1,307)  | 1:176:A:VAL:HG13 | 1:215:A:VAL:HG22 | 6                   | 0.13     | 0.02                | 0.13       |
| (1,307)  | 1:176:A:VAL:HG13 | 1:215:A:VAL:HG23 | 6                   | 0.13     | 0.02                | 0.13       |
| (1,1215) | 1:227:A:ASP:HB2  | 1:229:A:ARG:HA   | 6                   | 0.11     | 0.0                 | 0.11       |
| (1,1215) | 1:227:A:ASP:HB3  | 1:229:A:ARG:HA   | 6                   | 0.11     | 0.0                 | 0.11       |
| (1,1975) | 1:184:A:ILE:HD11 | 1:206:A:MET:H    | 6                   | 0.1      | 0.0                 | 0.11       |
| (1,1975) | 1:184:A:ILE:HD12 | 1:206:A:MET:H    | 6                   | 0.1      | 0.0                 | 0.11       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1975) | 1:184:A:ILE:HD13 | 1:206:A:MET:H    | 6                   | 0.1      | 0.0                 | 0.11       |
| (1,2407) | 1:136:A:ARG:HE   | 1:159:A:ASN:HB3  | 5                   | 1.34     | 0.42                | 1.49       |
| (1,1689) | 1:134:A:MET:H    | 1:159:A:ASN:HB2  | 5                   | 1.27     | 0.16                | 1.34       |
| (1,2250) | 1:217:A:GLN:HE21 | 1:218:A:TYR:HA   | 5                   | 0.87     | 0.2                 | 0.89       |
| (1,2510) | 1:226:A:TYR:HD1  | 1:229:A:ARG:HB2  | 5                   | 0.87     | 0.4                 | 0.92       |
| (1,2510) | 1:226:A:TYR:HD2  | 1:229:A:ARG:HB2  | 5                   | 0.87     | 0.4                 | 0.92       |
| (1,2518) | 1:155:A:TYR:HD1  | 1:156:A:ARG:HD2  | 5                   | 0.8      | 0.21                | 0.84       |
| (1,2518) | 1:155:A:TYR:HD2  | 1:156:A:ARG:HD2  | 5                   | 0.8      | 0.21                | 0.84       |
| (1,974)  | 1:148:A:ARG:HE   | 1:152:A:GLU:HG2  | 5                   | 0.62     | 0.17                | 0.69       |
| (1,138)  | 1:125:A:LEU:HA   | 1:125:A:LEU:HD21 | 5                   | 0.57     | 0.14                | 0.64       |
| (1,138)  | 1:125:A:LEU:HA   | 1:125:A:LEU:HD22 | 5                   | 0.57     | 0.14                | 0.64       |
| (1,138)  | 1:125:A:LEU:HA   | 1:125:A:LEU:HD23 | 5                   | 0.57     | 0.14                | 0.64       |
| (1,1407) | 1:134:A:MET:HB3  | 1:220:A:LYS:HD2  | 5                   | 0.52     | 0.28                | 0.32       |
| (1,1407) | 1:134:A:MET:HB3  | 1:220:A:LYS:HD3  | 5                   | 0.52     | 0.28                | 0.32       |
| (1,436)  | 1:229:A:ARG:HA   | 1:230:A:ARG:HD3  | 5                   | 0.49     | 0.13                | 0.47       |
| (1,1285) | 1:205:A:MET:H    | 1:206:A:MET:HG2  | 5                   | 0.48     | 0.18                | 0.48       |
| (1,1538) | 1:164:A:ARG:HD2  | 1:165:A:PRO:HD3  | 5                   | 0.42     | 0.13                | 0.42       |
| (1,435)  | 1:230:A:ARG:HA   | 1:230:A:ARG:HD2  | 5                   | 0.35     | 0.12                | 0.28       |
| (1,2791) | 1:126:A:GLY:HA2  | 1:128:A:TYR:HE1  | 5                   | 0.34     | 0.18                | 0.27       |
| (1,2791) | 1:126:A:GLY:HA2  | 1:128:A:TYR:HE2  | 5                   | 0.34     | 0.18                | 0.27       |
| (1,2279) | 1:186:A:GLN:HB3  | 1:188:A:THR:H    | 5                   | 0.33     | 0.07                | 0.33       |
| (1,1655) | 1:230:A:ARG:H    | 1:230:A:ARG:HG3  | 5                   | 0.32     | 0.04                | 0.31       |
| (1,1392) | 1:133:A:ALA:HA   | 1:159:A:ASN:HB2  | 5                   | 0.23     | 0.06                | 0.25       |
| (1,774)  | 1:206:A:MET:HB2  | 1:206:A:MET:HE1  | 5                   | 0.17     | 0.05                | 0.16       |
| (1,774)  | 1:206:A:MET:HB2  | 1:206:A:MET:HE2  | 5                   | 0.17     | 0.05                | 0.16       |
| (1,774)  | 1:206:A:MET:HB2  | 1:206:A:MET:HE3  | 5                   | 0.17     | 0.05                | 0.16       |
| (1,1479) | 1:145:A:TRP:HB2  | 1:146:A:GLU:HG2  | 5                   | 0.17     | 0.07                | 0.13       |
| (1,1479) | 1:145:A:TRP:HB3  | 1:146:A:GLU:HG2  | 5                   | 0.17     | 0.07                | 0.13       |
| (1,659)  | 1:136:A:ARG:HG2  | 1:154:A:MET:HE1  | 5                   | 0.12     | 0.01                | 0.12       |
| (1,659)  | 1:136:A:ARG:HG2  | 1:154:A:MET:HE2  | 5                   | 0.12     | 0.01                | 0.12       |
| (1,659)  | 1:136:A:ARG:HG2  | 1:154:A:MET:HE3  | 5                   | 0.12     | 0.01                | 0.12       |
| (1,659)  | 1:136:A:ARG:HG3  | 1:154:A:MET:HE1  | 5                   | 0.12     | 0.01                | 0.12       |
| (1,659)  | 1:136:A:ARG:HG3  | 1:154:A:MET:HE2  | 5                   | 0.12     | 0.01                | 0.12       |
| (1,659)  | 1:136:A:ARG:HG3  | 1:154:A:MET:HE3  | 5                   | 0.12     | 0.01                | 0.12       |
| (1,1253) | 1:203:A:VAL:HA   | 1:204:A:LYS:HB2  | 5                   | 0.11     | 0.01                | 0.1        |
| (1,1253) | 1:203:A:VAL:HA   | 1:204:A:LYS:HB3  | 5                   | 0.11     | 0.01                | 0.1        |
| (1,1385) | 1:183:A:THR:HG21 | 1:187:A:HIS:HB2  | 5                   | 0.11     | 0.01                | 0.1        |
| (1,1385) | 1:183:A:THR:HG22 | 1:187:A:HIS:HB2  | 5                   | 0.11     | 0.01                | 0.1        |
| (1,1385) | 1:183:A:THR:HG23 | 1:187:A:HIS:HB2  | 5                   | 0.11     | 0.01                | 0.1        |
| (1,2323) | 1:133:A:ALA:HB1  | 1:160:A:GLN:HE22 | 5                   | 0.11     | 0.0                 | 0.11       |
| (1,2323) | 1:133:A:ALA:HB2  | 1:160:A:GLN:HE22 | 5                   | 0.11     | 0.0                 | 0.11       |
| (1,2323) | 1:133:A:ALA:HB3  | 1:160:A:GLN:HE22 | 5                   | 0.11     | 0.0                 | 0.11       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1422) | 1:194:A:LYS:HD2  | 1:195:A:GLY:H    | 5                   | 0.1      | 0.0                 | 0.1        |
| (1,1422) | 1:194:A:LYS:HD3  | 1:195:A:GLY:H    | 5                   | 0.1      | 0.0                 | 0.1        |
| (1,934)  | 1:166:A:VAL:HG11 | 1:221:A:GLU:HG2  | 4                   | 1.63     | 0.45                | 1.72       |
| (1,934)  | 1:166:A:VAL:HG12 | 1:221:A:GLU:HG2  | 4                   | 1.63     | 0.45                | 1.72       |
| (1,934)  | 1:166:A:VAL:HG13 | 1:221:A:GLU:HG2  | 4                   | 1.63     | 0.45                | 1.72       |
| (1,269)  | 1:165:A:PRO:HB3  | 1:166:A:VAL:HG11 | 4                   | 1.36     | 0.17                | 1.4        |
| (1,269)  | 1:165:A:PRO:HB3  | 1:166:A:VAL:HG12 | 4                   | 1.36     | 0.17                | 1.4        |
| (1,269)  | 1:165:A:PRO:HB3  | 1:166:A:VAL:HG13 | 4                   | 1.36     | 0.17                | 1.4        |
| (1,437)  | 1:229:A:ARG:HB3  | 1:230:A:ARG:HD3  | 4                   | 1.19     | 0.32                | 1.34       |
| (1,437)  | 1:229:A:ARG:HB2  | 1:230:A:ARG:HD3  | 4                   | 1.19     | 0.32                | 1.34       |
| (1,314)  | 1:166:A:VAL:HG21 | 1:169:A:TYR:HB3  | 4                   | 1.14     | 0.4                 | 1.17       |
| (1,314)  | 1:166:A:VAL:HG22 | 1:169:A:TYR:HB3  | 4                   | 1.14     | 0.4                 | 1.17       |
| (1,314)  | 1:166:A:VAL:HG23 | 1:169:A:TYR:HB3  | 4                   | 1.14     | 0.4                 | 1.17       |
| (1,1073) | 1:166:A:VAL:HG11 | 1:221:A:GLU:HA   | 4                   | 1.06     | 0.31                | 1.16       |
| (1,1073) | 1:166:A:VAL:HG12 | 1:221:A:GLU:HA   | 4                   | 1.06     | 0.31                | 1.16       |
| (1,1073) | 1:166:A:VAL:HG13 | 1:221:A:GLU:HA   | 4                   | 1.06     | 0.31                | 1.16       |
| (1,2254) | 1:217:A:GLN:HE22 | 1:220:A:LYS:HE2  | 4                   | 0.99     | 0.09                | 0.95       |
| (1,2254) | 1:217:A:GLN:HE22 | 1:220:A:LYS:HE3  | 4                   | 0.99     | 0.09                | 0.95       |
| (1,1752) | 1:166:A:VAL:HG11 | 1:223:A:GLN:H    | 4                   | 0.97     | 0.23                | 0.92       |
| (1,1752) | 1:166:A:VAL:HG12 | 1:223:A:GLN:H    | 4                   | 0.97     | 0.23                | 0.92       |
| (1,1752) | 1:166:A:VAL:HG13 | 1:223:A:GLN:H    | 4                   | 0.97     | 0.23                | 0.92       |
| (1,273)  | 1:166:A:VAL:HG11 | 1:225:A:TYR:HB2  | 4                   | 0.96     | 0.24                | 1.09       |
| (1,273)  | 1:166:A:VAL:HG12 | 1:225:A:TYR:HB2  | 4                   | 0.96     | 0.24                | 1.09       |
| (1,273)  | 1:166:A:VAL:HG13 | 1:225:A:TYR:HB2  | 4                   | 0.96     | 0.24                | 1.09       |
| (1,188)  | 1:124:A:GLY:HA2  | 1:125:A:LEU:HD21 | 4                   | 0.9      | 0.32                | 1.0        |
| (1,188)  | 1:124:A:GLY:HA2  | 1:125:A:LEU:HD22 | 4                   | 0.9      | 0.32                | 1.0        |
| (1,188)  | 1:124:A:GLY:HA2  | 1:125:A:LEU:HD23 | 4                   | 0.9      | 0.32                | 1.0        |
| (1,188)  | 1:124:A:GLY:HA3  | 1:125:A:LEU:HD21 | 4                   | 0.9      | 0.32                | 1.0        |
| (1,188)  | 1:124:A:GLY:HA3  | 1:125:A:LEU:HD22 | 4                   | 0.9      | 0.32                | 1.0        |
| (1,188)  | 1:124:A:GLY:HA3  | 1:125:A:LEU:HD23 | 4                   | 0.9      | 0.32                | 1.0        |
| (1,2054) | 1:166:A:VAL:HG11 | 1:221:A:GLU:H    | 4                   | 0.83     | 0.35                | 1.0        |
| (1,2054) | 1:166:A:VAL:HG12 | 1:221:A:GLU:H    | 4                   | 0.83     | 0.35                | 1.0        |
| (1,2054) | 1:166:A:VAL:HG13 | 1:221:A:GLU:H    | 4                   | 0.83     | 0.35                | 1.0        |
| (1,996)  | 1:176:A:VAL:HA   | 1:211:A:GLU:HG3  | 4                   | 0.72     | 0.37                | 0.54       |
| (1,55)   | 1:125:A:LEU:HD11 | 1:162:A:TYR:HB2  | 4                   | 0.7      | 0.1                 | 0.72       |
| (1,55)   | 1:125:A:LEU:HD12 | 1:162:A:TYR:HB2  | 4                   | 0.7      | 0.1                 | 0.72       |
| (1,55)   | 1:125:A:LEU:HD13 | 1:162:A:TYR:HB2  | 4                   | 0.7      | 0.1                 | 0.72       |
| (1,2469) | 1:166:A:VAL:HG21 | 1:169:A:TYR:HD1  | 4                   | 0.57     | 0.14                | 0.54       |
| (1,2469) | 1:166:A:VAL:HG21 | 1:169:A:TYR:HD2  | 4                   | 0.57     | 0.14                | 0.54       |
| (1,2469) | 1:166:A:VAL:HG22 | 1:169:A:TYR:HD1  | 4                   | 0.57     | 0.14                | 0.54       |
| (1,2469) | 1:166:A:VAL:HG22 | 1:169:A:TYR:HD2  | 4                   | 0.57     | 0.14                | 0.54       |
| (1,2469) | 1:166:A:VAL:HG23 | 1:169:A:TYR:HD1  | 4                   | 0.57     | 0.14                | 0.54       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2469) | 1:166:A:VAL:HG23 | 1:169:A:TYR:HD2  | 4                   | 0.57     | 0.14                | 0.54       |
| (1,630)  | 1:165:A:PRO:HA   | 1:166:A:VAL:HG11 | 4                   | 0.54     | 0.21                | 0.62       |
| (1,630)  | 1:165:A:PRO:HA   | 1:166:A:VAL:HG12 | 4                   | 0.54     | 0.21                | 0.62       |
| (1,630)  | 1:165:A:PRO:HA   | 1:166:A:VAL:HG13 | 4                   | 0.54     | 0.21                | 0.62       |
| (1,166)  | 1:203:A:VAL:HG11 | 1:206:A:MET:HG2  | 4                   | 0.53     | 0.14                | 0.55       |
| (1,166)  | 1:203:A:VAL:HG12 | 1:206:A:MET:HG2  | 4                   | 0.53     | 0.14                | 0.55       |
| (1,166)  | 1:203:A:VAL:HG13 | 1:206:A:MET:HG2  | 4                   | 0.53     | 0.14                | 0.55       |
| (1,1055) | 1:203:A:VAL:HG21 | 1:207:A:GLU:HG2  | 4                   | 0.51     | 0.34                | 0.55       |
| (1,1055) | 1:203:A:VAL:HG22 | 1:207:A:GLU:HG2  | 4                   | 0.51     | 0.34                | 0.55       |
| (1,1055) | 1:203:A:VAL:HG23 | 1:207:A:GLU:HG2  | 4                   | 0.51     | 0.34                | 0.55       |
| (1,2483) | 1:161:A:VAL:HG21 | 1:163:A:TYR:HD1  | 4                   | 0.49     | 0.65                | 0.11       |
| (1,2483) | 1:161:A:VAL:HG21 | 1:163:A:TYR:HD2  | 4                   | 0.49     | 0.65                | 0.11       |
| (1,2483) | 1:161:A:VAL:HG22 | 1:163:A:TYR:HD1  | 4                   | 0.49     | 0.65                | 0.11       |
| (1,2483) | 1:161:A:VAL:HG22 | 1:163:A:TYR:HD2  | 4                   | 0.49     | 0.65                | 0.11       |
| (1,2483) | 1:161:A:VAL:HG23 | 1:163:A:TYR:HD1  | 4                   | 0.49     | 0.65                | 0.11       |
| (1,2483) | 1:161:A:VAL:HG23 | 1:163:A:TYR:HD2  | 4                   | 0.49     | 0.65                | 0.11       |
| (1,907)  | 1:226:A:TYR:HA   | 1:229:A:ARG:HB2  | 4                   | 0.49     | 0.13                | 0.53       |
| (1,507)  | 1:211:A:GLU:HG3  | 1:214:A:CYS:HB2  | 4                   | 0.44     | 0.32                | 0.36       |
| (1,1250) | 1:205:A:MET:HB2  | 1:206:A:MET:HG2  | 4                   | 0.42     | 0.32                | 0.31       |
| (1,388)  | 1:122:A:VAL:HG11 | 1:186:A:GLN:HE21 | 4                   | 0.42     | 0.08                | 0.43       |
| (1,388)  | 1:122:A:VAL:HG12 | 1:186:A:GLN:HE21 | 4                   | 0.42     | 0.08                | 0.43       |
| (1,388)  | 1:122:A:VAL:HG13 | 1:186:A:GLN:HE21 | 4                   | 0.42     | 0.08                | 0.43       |
| (1,775)  | 1:203:A:VAL:HG11 | 1:206:A:MET:HE1  | 4                   | 0.39     | 0.13                | 0.44       |
| (1,775)  | 1:203:A:VAL:HG11 | 1:206:A:MET:HE2  | 4                   | 0.39     | 0.13                | 0.44       |
| (1,775)  | 1:203:A:VAL:HG11 | 1:206:A:MET:HE3  | 4                   | 0.39     | 0.13                | 0.44       |
| (1,775)  | 1:203:A:VAL:HG12 | 1:206:A:MET:HE1  | 4                   | 0.39     | 0.13                | 0.44       |
| (1,775)  | 1:203:A:VAL:HG12 | 1:206:A:MET:HE2  | 4                   | 0.39     | 0.13                | 0.44       |
| (1,775)  | 1:203:A:VAL:HG12 | 1:206:A:MET:HE3  | 4                   | 0.39     | 0.13                | 0.44       |
| (1,775)  | 1:203:A:VAL:HG13 | 1:206:A:MET:HE1  | 4                   | 0.39     | 0.13                | 0.44       |
| (1,775)  | 1:203:A:VAL:HG13 | 1:206:A:MET:HE2  | 4                   | 0.39     | 0.13                | 0.44       |
| (1,775)  | 1:203:A:VAL:HG13 | 1:206:A:MET:HE3  | 4                   | 0.39     | 0.13                | 0.44       |
| (1,2763) | 1:155:A:TYR:HE1  | 1:156:A:ARG:HD2  | 4                   | 0.39     | 0.13                | 0.38       |
| (1,2763) | 1:155:A:TYR:HE2  | 1:156:A:ARG:HD2  | 4                   | 0.39     | 0.13                | 0.38       |
| (1,730)  | 1:166:A:VAL:HG11 | 1:167:A:SER:HB3  | 4                   | 0.33     | 0.1                 | 0.33       |
| (1,730)  | 1:166:A:VAL:HG12 | 1:167:A:SER:HB3  | 4                   | 0.33     | 0.1                 | 0.33       |
| (1,730)  | 1:166:A:VAL:HG13 | 1:167:A:SER:HB3  | 4                   | 0.33     | 0.1                 | 0.33       |
| (1,202)  | 1:183:A:THR:HG21 | 1:184:A:ILE:HG12 | 4                   | 0.28     | 0.09                | 0.3        |
| (1,202)  | 1:183:A:THR:HG22 | 1:184:A:ILE:HG12 | 4                   | 0.28     | 0.09                | 0.3        |
| (1,202)  | 1:183:A:THR:HG23 | 1:184:A:ILE:HG12 | 4                   | 0.28     | 0.09                | 0.3        |
| (1,1558) | 1:208:A:ARG:HG3  | 1:209:A:VAL:H    | 4                   | 0.26     | 0.08                | 0.29       |
| (1,2043) | 1:231:A:SER:H    | 1:231:A:SER:HB3  | 4                   | 0.23     | 0.08                | 0.28       |
| (1,1135) | 1:137:A:PRO:HB3  | 1:212:A:GLN:HG2  | 4                   | 0.23     | 0.04                | 0.24       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2234) | 1:221:A:GLU:HG3  | 1:222:A:SER:H    | 4                   | 0.22     | 0.09                | 0.2        |
| (1,111)  | 1:215:A:VAL:HG11 | 1:216:A:THR:HB   | 4                   | 0.16     | 0.04                | 0.16       |
| (1,111)  | 1:215:A:VAL:HG12 | 1:216:A:THR:HB   | 4                   | 0.16     | 0.04                | 0.16       |
| (1,111)  | 1:215:A:VAL:HG13 | 1:216:A:THR:HB   | 4                   | 0.16     | 0.04                | 0.16       |
| (1,745)  | 1:122:A:VAL:HA   | 1:190:A:THR:HG21 | 4                   | 0.13     | 0.02                | 0.14       |
| (1,745)  | 1:122:A:VAL:HA   | 1:190:A:THR:HG22 | 4                   | 0.13     | 0.02                | 0.14       |
| (1,745)  | 1:122:A:VAL:HA   | 1:190:A:THR:HG23 | 4                   | 0.13     | 0.02                | 0.14       |
| (1,1026) | 1:186:A:GLN:HB2  | 1:187:A:HIS:HA   | 4                   | 0.13     | 0.01                | 0.14       |
| (1,2466) | 1:169:A:TYR:HD1  | 1:174:A:ASN:HB3  | 4                   | 0.12     | 0.03                | 0.11       |
| (1,2466) | 1:169:A:TYR:HD2  | 1:174:A:ASN:HB3  | 4                   | 0.12     | 0.03                | 0.11       |
| (1,960)  | 1:180:A:VAL:HG21 | 1:184:A:ILE:HD11 | 4                   | 0.12     | 0.01                | 0.12       |
| (1,960)  | 1:180:A:VAL:HG21 | 1:184:A:ILE:HD12 | 4                   | 0.12     | 0.01                | 0.12       |
| (1,960)  | 1:180:A:VAL:HG21 | 1:184:A:ILE:HD13 | 4                   | 0.12     | 0.01                | 0.12       |
| (1,960)  | 1:180:A:VAL:HG22 | 1:184:A:ILE:HD11 | 4                   | 0.12     | 0.01                | 0.12       |
| (1,960)  | 1:180:A:VAL:HG22 | 1:184:A:ILE:HD12 | 4                   | 0.12     | 0.01                | 0.12       |
| (1,960)  | 1:180:A:VAL:HG22 | 1:184:A:ILE:HD13 | 4                   | 0.12     | 0.01                | 0.12       |
| (1,960)  | 1:180:A:VAL:HG23 | 1:184:A:ILE:HD11 | 4                   | 0.12     | 0.01                | 0.12       |
| (1,960)  | 1:180:A:VAL:HG23 | 1:184:A:ILE:HD12 | 4                   | 0.12     | 0.01                | 0.12       |
| (1,960)  | 1:180:A:VAL:HG23 | 1:184:A:ILE:HD13 | 4                   | 0.12     | 0.01                | 0.12       |
| (1,760)  | 1:184:A:ILE:HB   | 1:206:A:MET:HE1  | 4                   | 0.12     | 0.01                | 0.12       |
| (1,760)  | 1:184:A:ILE:HB   | 1:206:A:MET:HE2  | 4                   | 0.12     | 0.01                | 0.12       |
| (1,760)  | 1:184:A:ILE:HB   | 1:206:A:MET:HE3  | 4                   | 0.12     | 0.01                | 0.12       |
| (1,591)  | 1:139:A:ILE:HD11 | 1:205:A:MET:HE1  | 4                   | 0.12     | 0.02                | 0.11       |
| (1,591)  | 1:139:A:ILE:HD11 | 1:205:A:MET:HE2  | 4                   | 0.12     | 0.02                | 0.11       |
| (1,591)  | 1:139:A:ILE:HD11 | 1:205:A:MET:HE3  | 4                   | 0.12     | 0.02                | 0.11       |
| (1,591)  | 1:139:A:ILE:HD12 | 1:205:A:MET:HE1  | 4                   | 0.12     | 0.02                | 0.11       |
| (1,591)  | 1:139:A:ILE:HD12 | 1:205:A:MET:HE2  | 4                   | 0.12     | 0.02                | 0.11       |
| (1,591)  | 1:139:A:ILE:HD12 | 1:205:A:MET:HE3  | 4                   | 0.12     | 0.02                | 0.11       |
| (1,591)  | 1:139:A:ILE:HD13 | 1:205:A:MET:HE1  | 4                   | 0.12     | 0.02                | 0.11       |
| (1,591)  | 1:139:A:ILE:HD13 | 1:205:A:MET:HE2  | 4                   | 0.12     | 0.02                | 0.11       |
| (1,591)  | 1:139:A:ILE:HD13 | 1:205:A:MET:HE3  | 4                   | 0.12     | 0.02                | 0.11       |
| (1,2397) | 1:185:A:LYS:HB2  | 1:186:A:GLN:HE22 | 4                   | 0.11     | 0.0                 | 0.11       |
| (1,2397) | 1:185:A:LYS:HB3  | 1:186:A:GLN:HE22 | 4                   | 0.11     | 0.0                 | 0.11       |
| (1,582)  | 1:139:A:ILE:HG21 | 1:205:A:MET:HE1  | 4                   | 0.11     | 0.0                 | 0.11       |
| (1,582)  | 1:139:A:ILE:HG21 | 1:205:A:MET:HE2  | 4                   | 0.11     | 0.0                 | 0.11       |
| (1,582)  | 1:139:A:ILE:HG21 | 1:205:A:MET:HE3  | 4                   | 0.11     | 0.0                 | 0.11       |
| (1,582)  | 1:139:A:ILE:HG22 | 1:205:A:MET:HE1  | 4                   | 0.11     | 0.0                 | 0.11       |
| (1,582)  | 1:139:A:ILE:HG22 | 1:205:A:MET:HE2  | 4                   | 0.11     | 0.0                 | 0.11       |
| (1,582)  | 1:139:A:ILE:HG22 | 1:205:A:MET:HE3  | 4                   | 0.11     | 0.0                 | 0.11       |
| (1,582)  | 1:139:A:ILE:HG23 | 1:205:A:MET:HE1  | 4                   | 0.11     | 0.0                 | 0.11       |
| (1,582)  | 1:139:A:ILE:HG23 | 1:205:A:MET:HE2  | 4                   | 0.11     | 0.0                 | 0.11       |
| (1,582)  | 1:139:A:ILE:HG23 | 1:205:A:MET:HE3  | 4                   | 0.11     | 0.0                 | 0.11       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2829) | 1:166:A:VAL:HB   | 1:218:A:TYR:HE1  | 4                   | 0.11     | 0.0                 | 0.11       |
| (1,2829) | 1:166:A:VAL:HB   | 1:218:A:TYR:HE2  | 4                   | 0.11     | 0.0                 | 0.11       |
| (1,2751) | 1:164:A:ARG:HG2  | 1:169:A:TYR:HE1  | 4                   | 0.11     | 0.0                 | 0.11       |
| (1,2751) | 1:164:A:ARG:HG2  | 1:169:A:TYR:HE2  | 4                   | 0.11     | 0.0                 | 0.11       |
| (1,2636) | 1:157:A:TYR:HD1  | 1:209:A:VAL:H    | 4                   | 0.11     | 0.0                 | 0.11       |
| (1,2636) | 1:157:A:TYR:HD2  | 1:209:A:VAL:H    | 4                   | 0.11     | 0.0                 | 0.11       |
| (1,1505) | 1:137:A:PRO:HD2  | 1:209:A:VAL:HG11 | 4                   | 0.1      | 0.0                 | 0.11       |
| (1,1505) | 1:137:A:PRO:HD2  | 1:209:A:VAL:HG12 | 4                   | 0.1      | 0.0                 | 0.11       |
| (1,1505) | 1:137:A:PRO:HD2  | 1:209:A:VAL:HG13 | 4                   | 0.1      | 0.0                 | 0.11       |
| (1,2600) | 1:166:A:VAL:HG21 | 1:175:A:PHE:HE1  | 4                   | 0.1      | 0.0                 | 0.1        |
| (1,2600) | 1:166:A:VAL:HG21 | 1:175:A:PHE:HE2  | 4                   | 0.1      | 0.0                 | 0.1        |
| (1,2600) | 1:166:A:VAL:HG22 | 1:175:A:PHE:HE1  | 4                   | 0.1      | 0.0                 | 0.1        |
| (1,2600) | 1:166:A:VAL:HG22 | 1:175:A:PHE:HE2  | 4                   | 0.1      | 0.0                 | 0.1        |
| (1,2600) | 1:166:A:VAL:HG23 | 1:175:A:PHE:HE1  | 4                   | 0.1      | 0.0                 | 0.1        |
| (1,2600) | 1:166:A:VAL:HG23 | 1:175:A:PHE:HE2  | 4                   | 0.1      | 0.0                 | 0.1        |
| (1,315)  | 1:166:A:VAL:HG11 | 1:221:A:GLU:HB2  | 3                   | 1.13     | 0.22                | 1.02       |
| (1,315)  | 1:166:A:VAL:HG12 | 1:221:A:GLU:HB2  | 3                   | 1.13     | 0.22                | 1.02       |
| (1,315)  | 1:166:A:VAL:HG13 | 1:221:A:GLU:HB2  | 3                   | 1.13     | 0.22                | 1.02       |
| (1,931)  | 1:166:A:VAL:HG11 | 1:221:A:GLU:HG3  | 3                   | 0.83     | 0.31                | 0.82       |
| (1,931)  | 1:166:A:VAL:HG12 | 1:221:A:GLU:HG3  | 3                   | 0.83     | 0.31                | 0.82       |
| (1,931)  | 1:166:A:VAL:HG13 | 1:221:A:GLU:HG3  | 3                   | 0.83     | 0.31                | 0.82       |
| (1,2825) | 1:176:A:VAL:HG21 | 1:218:A:TYR:HE1  | 3                   | 0.74     | 0.89                | 0.12       |
| (1,2825) | 1:176:A:VAL:HG21 | 1:218:A:TYR:HE2  | 3                   | 0.74     | 0.89                | 0.12       |
| (1,2825) | 1:176:A:VAL:HG22 | 1:218:A:TYR:HE1  | 3                   | 0.74     | 0.89                | 0.12       |
| (1,2825) | 1:176:A:VAL:HG22 | 1:218:A:TYR:HE2  | 3                   | 0.74     | 0.89                | 0.12       |
| (1,2825) | 1:176:A:VAL:HG23 | 1:218:A:TYR:HE1  | 3                   | 0.74     | 0.89                | 0.12       |
| (1,2825) | 1:176:A:VAL:HG23 | 1:218:A:TYR:HE2  | 3                   | 0.74     | 0.89                | 0.12       |
| (1,52)   | 1:176:A:VAL:HG21 | 1:217:A:GLN:HB3  | 3                   | 0.71     | 0.85                | 0.11       |
| (1,52)   | 1:176:A:VAL:HG22 | 1:217:A:GLN:HB3  | 3                   | 0.71     | 0.85                | 0.11       |
| (1,52)   | 1:176:A:VAL:HG23 | 1:217:A:GLN:HB3  | 3                   | 0.71     | 0.85                | 0.11       |
| (1,2579) | 1:218:A:TYR:HD1  | 1:219:A:GLN:HG3  | 3                   | 0.64     | 0.1                 | 0.63       |
| (1,2579) | 1:218:A:TYR:HD2  | 1:219:A:GLN:HG3  | 3                   | 0.64     | 0.1                 | 0.63       |
| (1,1096) | 1:165:A:PRO:HD3  | 1:168:A:GLN:HG2  | 3                   | 0.63     | 0.4                 | 0.58       |
| (1,240)  | 1:166:A:VAL:HG21 | 1:169:A:TYR:HB2  | 3                   | 0.6      | 0.27                | 0.72       |
| (1,240)  | 1:166:A:VAL:HG22 | 1:169:A:TYR:HB2  | 3                   | 0.6      | 0.27                | 0.72       |
| (1,240)  | 1:166:A:VAL:HG23 | 1:169:A:TYR:HB2  | 3                   | 0.6      | 0.27                | 0.72       |
| (1,2536) | 1:167:A:SER:HB3  | 1:225:A:TYR:HD1  | 3                   | 0.54     | 0.02                | 0.55       |
| (1,2536) | 1:167:A:SER:HB3  | 1:225:A:TYR:HD2  | 3                   | 0.54     | 0.02                | 0.55       |
| (1,272)  | 1:166:A:VAL:HG11 | 1:221:A:GLU:HB3  | 3                   | 0.52     | 0.16                | 0.43       |
| (1,272)  | 1:166:A:VAL:HG12 | 1:221:A:GLU:HB3  | 3                   | 0.52     | 0.16                | 0.43       |
| (1,272)  | 1:166:A:VAL:HG13 | 1:221:A:GLU:HB3  | 3                   | 0.52     | 0.16                | 0.43       |
| (1,336)  | 1:163:A:TYR:HD1  | 1:166:A:VAL:HG11 | 3                   | 0.5      | 0.04                | 0.49       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,336)  | 1:163:A:TYR:HD1  | 1:166:A:VAL:HG12 | 3                   | 0.5      | 0.04                | 0.49       |
| (1,336)  | 1:163:A:TYR:HD1  | 1:166:A:VAL:HG13 | 3                   | 0.5      | 0.04                | 0.49       |
| (1,336)  | 1:163:A:TYR:HD2  | 1:166:A:VAL:HG11 | 3                   | 0.5      | 0.04                | 0.49       |
| (1,336)  | 1:163:A:TYR:HD2  | 1:166:A:VAL:HG12 | 3                   | 0.5      | 0.04                | 0.49       |
| (1,336)  | 1:163:A:TYR:HD2  | 1:166:A:VAL:HG13 | 3                   | 0.5      | 0.04                | 0.49       |
| (1,1058) | 1:203:A:VAL:HG21 | 1:207:A:GLU:HG3  | 3                   | 0.49     | 0.25                | 0.33       |
| (1,1058) | 1:203:A:VAL:HG22 | 1:207:A:GLU:HG3  | 3                   | 0.49     | 0.25                | 0.33       |
| (1,1058) | 1:203:A:VAL:HG23 | 1:207:A:GLU:HG3  | 3                   | 0.49     | 0.25                | 0.33       |
| (1,2364) | 1:171:A:ASN:HD22 | 1:174:A:ASN:HD22 | 3                   | 0.43     | 0.19                | 0.38       |
| (1,2237) | 1:166:A:VAL:HG11 | 1:222:A:SER:H    | 3                   | 0.43     | 0.18                | 0.37       |
| (1,2237) | 1:166:A:VAL:HG12 | 1:222:A:SER:H    | 3                   | 0.43     | 0.18                | 0.37       |
| (1,2237) | 1:166:A:VAL:HG13 | 1:222:A:SER:H    | 3                   | 0.43     | 0.18                | 0.37       |
| (1,1023) | 1:206:A:MET:HG3  | 1:207:A:GLU:HG3  | 3                   | 0.34     | 0.09                | 0.32       |
| (1,2309) | 1:171:A:ASN:HD22 | 1:174:A:ASN:HD21 | 3                   | 0.33     | 0.01                | 0.33       |
| (1,2076) | 1:208:A:ARG:H    | 1:208:A:ARG:HG3  | 3                   | 0.33     | 0.06                | 0.29       |
| (1,559)  | 1:162:A:TYR:HB3  | 1:182:A:ILE:HG21 | 3                   | 0.32     | 0.19                | 0.25       |
| (1,559)  | 1:162:A:TYR:HB3  | 1:182:A:ILE:HG22 | 3                   | 0.32     | 0.19                | 0.25       |
| (1,559)  | 1:162:A:TYR:HB3  | 1:182:A:ILE:HG23 | 3                   | 0.32     | 0.19                | 0.25       |
| (1,1048) | 1:125:A:LEU:HB3  | 1:128:A:TYR:HA   | 3                   | 0.31     | 0.2                 | 0.25       |
| (1,289)  | 1:189:A:VAL:HG21 | 1:192:A:THR:HG21 | 3                   | 0.3      | 0.25                | 0.13       |
| (1,289)  | 1:189:A:VAL:HG21 | 1:192:A:THR:HG22 | 3                   | 0.3      | 0.25                | 0.13       |
| (1,289)  | 1:189:A:VAL:HG21 | 1:192:A:THR:HG23 | 3                   | 0.3      | 0.25                | 0.13       |
| (1,289)  | 1:189:A:VAL:HG22 | 1:192:A:THR:HG21 | 3                   | 0.3      | 0.25                | 0.13       |
| (1,289)  | 1:189:A:VAL:HG22 | 1:192:A:THR:HG22 | 3                   | 0.3      | 0.25                | 0.13       |
| (1,289)  | 1:189:A:VAL:HG22 | 1:192:A:THR:HG23 | 3                   | 0.3      | 0.25                | 0.13       |
| (1,289)  | 1:189:A:VAL:HG23 | 1:192:A:THR:HG21 | 3                   | 0.3      | 0.25                | 0.13       |
| (1,289)  | 1:189:A:VAL:HG23 | 1:192:A:THR:HG22 | 3                   | 0.3      | 0.25                | 0.13       |
| (1,289)  | 1:189:A:VAL:HG23 | 1:192:A:THR:HG23 | 3                   | 0.3      | 0.25                | 0.13       |
| (1,349)  | 1:122:A:VAL:HG21 | 1:186:A:GLN:HE21 | 3                   | 0.26     | 0.12                | 0.27       |
| (1,349)  | 1:122:A:VAL:HG22 | 1:186:A:GLN:HE21 | 3                   | 0.26     | 0.12                | 0.27       |
| (1,349)  | 1:122:A:VAL:HG23 | 1:186:A:GLN:HE21 | 3                   | 0.26     | 0.12                | 0.27       |
| (1,2537) | 1:166:A:VAL:HG11 | 1:225:A:TYR:HD1  | 3                   | 0.26     | 0.12                | 0.19       |
| (1,2537) | 1:166:A:VAL:HG11 | 1:225:A:TYR:HD2  | 3                   | 0.26     | 0.12                | 0.19       |
| (1,2537) | 1:166:A:VAL:HG12 | 1:225:A:TYR:HD1  | 3                   | 0.26     | 0.12                | 0.19       |
| (1,2537) | 1:166:A:VAL:HG12 | 1:225:A:TYR:HD2  | 3                   | 0.26     | 0.12                | 0.19       |
| (1,2537) | 1:166:A:VAL:HG13 | 1:225:A:TYR:HD1  | 3                   | 0.26     | 0.12                | 0.19       |
| (1,2537) | 1:166:A:VAL:HG13 | 1:225:A:TYR:HD2  | 3                   | 0.26     | 0.12                | 0.19       |
| (1,1304) | 1:153:A:ASN:HA   | 1:156:A:ARG:HD3  | 3                   | 0.24     | 0.02                | 0.24       |
| (1,448)  | 1:226:A:TYR:HE1  | 1:230:A:ARG:HD2  | 3                   | 0.24     | 0.08                | 0.29       |
| (1,448)  | 1:226:A:TYR:HE2  | 1:230:A:ARG:HD2  | 3                   | 0.24     | 0.08                | 0.29       |
| (1,1799) | 1:166:A:VAL:H    | 1:166:A:VAL:HG11 | 3                   | 0.23     | 0.02                | 0.23       |
| (1,1799) | 1:166:A:VAL:H    | 1:166:A:VAL:HG12 | 3                   | 0.23     | 0.02                | 0.23       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1799) | 1:166:A:VAL:H    | 1:166:A:VAL:HG13 | 3                   | 0.23     | 0.02                | 0.23       |
| (1,2314) | 1:133:A:ALA:HA   | 1:160:A:GLN:HE21 | 3                   | 0.23     | 0.01                | 0.24       |
| (1,2328) | 1:223:A:GLN:HE21 | 1:227:A:ASP:HB2  | 3                   | 0.22     | 0.07                | 0.18       |
| (1,2328) | 1:223:A:GLN:HE21 | 1:227:A:ASP:HB3  | 3                   | 0.22     | 0.07                | 0.18       |
| (1,527)  | 1:202:A:ASP:HB2  | 1:203:A:VAL:HG11 | 3                   | 0.18     | 0.04                | 0.18       |
| (1,527)  | 1:202:A:ASP:HB2  | 1:203:A:VAL:HG12 | 3                   | 0.18     | 0.04                | 0.18       |
| (1,527)  | 1:202:A:ASP:HB2  | 1:203:A:VAL:HG13 | 3                   | 0.18     | 0.04                | 0.18       |
| (1,1632) | 1:231:A:SER:HB3  | 1:232:A:SER:H    | 3                   | 0.18     | 0.05                | 0.21       |
| (1,2092) | 1:169:A:TYR:H    | 1:169:A:TYR:HB3  | 3                   | 0.15     | 0.04                | 0.12       |
| (1,784)  | 1:166:A:VAL:HG11 | 1:218:A:TYR:HA   | 3                   | 0.12     | 0.01                | 0.12       |
| (1,784)  | 1:166:A:VAL:HG12 | 1:218:A:TYR:HA   | 3                   | 0.12     | 0.01                | 0.12       |
| (1,784)  | 1:166:A:VAL:HG13 | 1:218:A:TYR:HA   | 3                   | 0.12     | 0.01                | 0.12       |
| (1,2464) | 1:169:A:TYR:HD1  | 1:218:A:TYR:HE1  | 3                   | 0.12     | 0.0                 | 0.12       |
| (1,2464) | 1:169:A:TYR:HD1  | 1:218:A:TYR:HE2  | 3                   | 0.12     | 0.0                 | 0.12       |
| (1,2464) | 1:169:A:TYR:HD2  | 1:218:A:TYR:HE1  | 3                   | 0.12     | 0.0                 | 0.12       |
| (1,2464) | 1:169:A:TYR:HD2  | 1:218:A:TYR:HE2  | 3                   | 0.12     | 0.0                 | 0.12       |
| (1,2500) | 1:149:A:TYR:HD1  | 1:201:A:THR:HG21 | 3                   | 0.11     | 0.01                | 0.11       |
| (1,2500) | 1:149:A:TYR:HD1  | 1:201:A:THR:HG22 | 3                   | 0.11     | 0.01                | 0.11       |
| (1,2500) | 1:149:A:TYR:HD1  | 1:201:A:THR:HG23 | 3                   | 0.11     | 0.01                | 0.11       |
| (1,2500) | 1:149:A:TYR:HD2  | 1:201:A:THR:HG21 | 3                   | 0.11     | 0.01                | 0.11       |
| (1,2500) | 1:149:A:TYR:HD2  | 1:201:A:THR:HG22 | 3                   | 0.11     | 0.01                | 0.11       |
| (1,2500) | 1:149:A:TYR:HD2  | 1:201:A:THR:HG23 | 3                   | 0.11     | 0.01                | 0.11       |
| (1,2667) | 1:191:A:THR:HG21 | 1:198:A:PHE:HE1  | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,2667) | 1:191:A:THR:HG21 | 1:198:A:PHE:HE2  | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,2667) | 1:191:A:THR:HG22 | 1:198:A:PHE:HE1  | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,2667) | 1:191:A:THR:HG22 | 1:198:A:PHE:HE2  | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,2667) | 1:191:A:THR:HG23 | 1:198:A:PHE:HE1  | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,2667) | 1:191:A:THR:HG23 | 1:198:A:PHE:HE2  | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,332)  | 1:185:A:LYS:HD2  | 1:189:A:VAL:HG11 | 3                   | 0.11     | 0.01                | 0.1        |
| (1,332)  | 1:185:A:LYS:HD2  | 1:189:A:VAL:HG12 | 3                   | 0.11     | 0.01                | 0.1        |
| (1,332)  | 1:185:A:LYS:HD2  | 1:189:A:VAL:HG13 | 3                   | 0.11     | 0.01                | 0.1        |
| (1,332)  | 1:185:A:LYS:HD3  | 1:189:A:VAL:HG11 | 3                   | 0.11     | 0.01                | 0.1        |
| (1,332)  | 1:185:A:LYS:HD3  | 1:189:A:VAL:HG12 | 3                   | 0.11     | 0.01                | 0.1        |
| (1,332)  | 1:185:A:LYS:HD3  | 1:189:A:VAL:HG13 | 3                   | 0.11     | 0.01                | 0.1        |
| (1,1278) | 1:137:A:PRO:HB2  | 1:139:A:ILE:HG21 | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,1278) | 1:137:A:PRO:HB2  | 1:139:A:ILE:HG22 | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,1278) | 1:137:A:PRO:HB2  | 1:139:A:ILE:HG23 | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,2752) | 1:169:A:TYR:HE1  | 1:174:A:ASN:HA   | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,2752) | 1:169:A:TYR:HE2  | 1:174:A:ASN:HA   | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,660)  | 1:154:A:MET:HB2  | 1:154:A:MET:HE1  | 3                   | 0.1      | 0.0                 | 0.1        |
| (1,660)  | 1:154:A:MET:HB2  | 1:154:A:MET:HE2  | 3                   | 0.1      | 0.0                 | 0.1        |
| (1,660)  | 1:154:A:MET:HB2  | 1:154:A:MET:HE3  | 3                   | 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) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1562) | 1:228:A:GLY:HA2  | 1:229:A:ARG:HG2  | 3                   | 0.1      | 0.0                 | 0.1        |
| (1,1562) | 1:228:A:GLY:HA2  | 1:229:A:ARG:HG3  | 3                   | 0.1      | 0.0                 | 0.1        |
| (1,1562) | 1:228:A:GLY:HA3  | 1:229:A:ARG:HG2  | 3                   | 0.1      | 0.0                 | 0.1        |
| (1,1562) | 1:228:A:GLY:HA3  | 1:229:A:ARG:HG3  | 3                   | 0.1      | 0.0                 | 0.1        |
| (1,2557) | 1:128:A:TYR:HD1  | 1:164:A:ARG:HA   | 3                   | 0.1      | 0.0                 | 0.1        |
| (1,2557) | 1:128:A:TYR:HD2  | 1:164:A:ARG:HA   | 3                   | 0.1      | 0.0                 | 0.1        |
| (1,394)  | 1:216:A:THR:HA   | 1:220:A:LYS:HE2  | 3                   | 0.1      | 0.0                 | 0.1        |
| (1,394)  | 1:216:A:THR:HA   | 1:220:A:LYS:HE3  | 3                   | 0.1      | 0.0                 | 0.1        |
| (1,2719) | 1:173:A:LYS:HD2  | 1:177:A:HIS:HD2  | 3                   | 0.1      | 0.0                 | 0.1        |
| (1,2719) | 1:173:A:LYS:HD3  | 1:177:A:HIS:HD2  | 3                   | 0.1      | 0.0                 | 0.1        |
| (1,970)  | 1:161:A:VAL:HG21 | 1:217:A:GLN:HA   | 2                   | 1.18     | 1.08                | 1.18       |
| (1,970)  | 1:161:A:VAL:HG22 | 1:217:A:GLN:HA   | 2                   | 1.18     | 1.08                | 1.18       |
| (1,970)  | 1:161:A:VAL:HG23 | 1:217:A:GLN:HA   | 2                   | 1.18     | 1.08                | 1.18       |
| (1,430)  | 1:122:A:VAL:HG11 | 1:186:A:GLN:HG3  | 2                   | 0.75     | 0.04                | 0.75       |
| (1,430)  | 1:122:A:VAL:HG12 | 1:186:A:GLN:HG3  | 2                   | 0.75     | 0.04                | 0.75       |
| (1,430)  | 1:122:A:VAL:HG13 | 1:186:A:GLN:HG3  | 2                   | 0.75     | 0.04                | 0.75       |
| (1,851)  | 1:151:A:ARG:HA   | 1:151:A:ARG:HG2  | 2                   | 0.62     | 0.07                | 0.62       |
| (1,1169) | 1:216:A:THR:HB   | 1:219:A:GLN:HG3  | 2                   | 0.53     | 0.04                | 0.53       |
| (1,993)  | 1:211:A:GLU:HG3  | 1:215:A:VAL:H    | 2                   | 0.52     | 0.29                | 0.52       |
| (1,2439) | 1:229:A:ARG:HE   | 1:230:A:ARG:HB3  | 2                   | 0.5      | 0.08                | 0.5        |
| (1,2831) | 1:166:A:VAL:HG21 | 1:218:A:TYR:HE1  | 2                   | 0.5      | 0.34                | 0.5        |
| (1,2831) | 1:166:A:VAL:HG21 | 1:218:A:TYR:HE2  | 2                   | 0.5      | 0.34                | 0.5        |
| (1,2831) | 1:166:A:VAL:HG22 | 1:218:A:TYR:HE1  | 2                   | 0.5      | 0.34                | 0.5        |
| (1,2831) | 1:166:A:VAL:HG22 | 1:218:A:TYR:HE2  | 2                   | 0.5      | 0.34                | 0.5        |
| (1,2831) | 1:166:A:VAL:HG23 | 1:218:A:TYR:HE1  | 2                   | 0.5      | 0.34                | 0.5        |
| (1,2831) | 1:166:A:VAL:HG23 | 1:218:A:TYR:HE2  | 2                   | 0.5      | 0.34                | 0.5        |
| (1,391)  | 1:122:A:VAL:HG21 | 1:125:A:LEU:HD21 | 2                   | 0.44     | 0.32                | 0.44       |
| (1,391)  | 1:122:A:VAL:HG21 | 1:125:A:LEU:HD22 | 2                   | 0.44     | 0.32                | 0.44       |
| (1,391)  | 1:122:A:VAL:HG21 | 1:125:A:LEU:HD23 | 2                   | 0.44     | 0.32                | 0.44       |
| (1,391)  | 1:122:A:VAL:HG22 | 1:125:A:LEU:HD21 | 2                   | 0.44     | 0.32                | 0.44       |
| (1,391)  | 1:122:A:VAL:HG22 | 1:125:A:LEU:HD22 | 2                   | 0.44     | 0.32                | 0.44       |
| (1,391)  | 1:122:A:VAL:HG22 | 1:125:A:LEU:HD23 | 2                   | 0.44     | 0.32                | 0.44       |
| (1,391)  | 1:122:A:VAL:HG23 | 1:125:A:LEU:HD21 | 2                   | 0.44     | 0.32                | 0.44       |
| (1,391)  | 1:122:A:VAL:HG23 | 1:125:A:LEU:HD22 | 2                   | 0.44     | 0.32                | 0.44       |
| (1,391)  | 1:122:A:VAL:HG23 | 1:125:A:LEU:HD23 | 2                   | 0.44     | 0.32                | 0.44       |
| (1,2040) | 1:128:A:TYR:H    | 1:164:A:ARG:HG3  | 2                   | 0.43     | 0.14                | 0.43       |
| (1,128)  | 1:161:A:VAL:HG11 | 1:213:A:MET:HB3  | 2                   | 0.42     | 0.05                | 0.42       |
| (1,128)  | 1:161:A:VAL:HG12 | 1:213:A:MET:HB3  | 2                   | 0.42     | 0.05                | 0.42       |
| (1,128)  | 1:161:A:VAL:HG13 | 1:213:A:MET:HB3  | 2                   | 0.42     | 0.05                | 0.42       |
| (1,2562) | 1:125:A:LEU:HD21 | 1:128:A:TYR:HD1  | 2                   | 0.42     | 0.32                | 0.42       |
| (1,2562) | 1:125:A:LEU:HD21 | 1:128:A:TYR:HD2  | 2                   | 0.42     | 0.32                | 0.42       |
| (1,2562) | 1:125:A:LEU:HD22 | 1:128:A:TYR:HD1  | 2                   | 0.42     | 0.32                | 0.42       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2562) | 1:125:A:LEU:HD22 | 1:128:A:TYR:HD2  | 2                   | 0.42     | 0.32                | 0.42       |
| (1,2562) | 1:125:A:LEU:HD23 | 1:128:A:TYR:HD1  | 2                   | 0.42     | 0.32                | 0.42       |
| (1,2562) | 1:125:A:LEU:HD23 | 1:128:A:TYR:HD2  | 2                   | 0.42     | 0.32                | 0.42       |
| (1,987)  | 1:149:A:TYR:HA   | 1:152:A:GLU:HG2  | 2                   | 0.42     | 0.1                 | 0.42       |
| (1,2507) | 1:150:A:TYR:HD1  | 1:151:A:ARG:HG3  | 2                   | 0.34     | 0.12                | 0.34       |
| (1,2507) | 1:150:A:TYR:HD2  | 1:151:A:ARG:HG3  | 2                   | 0.34     | 0.12                | 0.34       |
| (1,1257) | 1:206:A:MET:HG3  | 1:210:A:VAL:HG21 | 2                   | 0.34     | 0.24                | 0.34       |
| (1,1257) | 1:206:A:MET:HG3  | 1:210:A:VAL:HG22 | 2                   | 0.34     | 0.24                | 0.34       |
| (1,1257) | 1:206:A:MET:HG3  | 1:210:A:VAL:HG23 | 2                   | 0.34     | 0.24                | 0.34       |
| (1,268)  | 1:166:A:VAL:HG11 | 1:225:A:TYR:HB3  | 2                   | 0.33     | 0.03                | 0.33       |
| (1,268)  | 1:166:A:VAL:HG12 | 1:225:A:TYR:HB3  | 2                   | 0.33     | 0.03                | 0.33       |
| (1,268)  | 1:166:A:VAL:HG13 | 1:225:A:TYR:HB3  | 2                   | 0.33     | 0.03                | 0.33       |
| (1,1396) | 1:148:A:ARG:HA   | 1:151:A:ARG:HB2  | 2                   | 0.3      | 0.03                | 0.3        |
| (1,1907) | 1:178:A:ASP:HB2  | 1:179:A:CYS:H    | 2                   | 0.29     | 0.15                | 0.29       |
| (1,510)  | 1:211:A:GLU:HG3  | 1:214:A:CYS:HB3  | 2                   | 0.28     | 0.06                | 0.28       |
| (1,579)  | 1:152:A:GLU:HB2  | 1:153:A:ASN:HB3  | 2                   | 0.27     | 0.12                | 0.27       |
| (1,579)  | 1:152:A:GLU:HB3  | 1:153:A:ASN:HB3  | 2                   | 0.27     | 0.12                | 0.27       |
| (1,1033) | 1:205:A:MET:H    | 1:207:A:GLU:HG3  | 2                   | 0.26     | 0.08                | 0.26       |
| (1,976)  | 1:148:A:ARG:HG3  | 1:152:A:GLU:HG2  | 2                   | 0.24     | 0.0                 | 0.24       |
| (1,552)  | 1:153:A:ASN:HB2  | 1:156:A:ARG:HD2  | 2                   | 0.22     | 0.05                | 0.22       |
| (1,182)  | 1:216:A:THR:HB   | 1:220:A:LYS:HG3  | 2                   | 0.18     | 0.02                | 0.18       |
| (1,1011) | 1:208:A:ARG:HA   | 1:208:A:ARG:HG3  | 2                   | 0.18     | 0.08                | 0.18       |
| (1,1400) | 1:183:A:THR:HB   | 1:184:A:ILE:HG12 | 2                   | 0.18     | 0.06                | 0.18       |
| (1,2050) | 1:221:A:GLU:H    | 1:221:A:GLU:HG3  | 2                   | 0.18     | 0.0                 | 0.18       |
| (1,967)  | 1:135:A:SER:HA   | 1:136:A:ARG:HB2  | 2                   | 0.17     | 0.05                | 0.17       |
| (1,374)  | 1:209:A:VAL:HG21 | 1:210:A:VAL:H    | 2                   | 0.16     | 0.01                | 0.16       |
| (1,374)  | 1:209:A:VAL:HG22 | 1:210:A:VAL:H    | 2                   | 0.16     | 0.01                | 0.16       |
| (1,374)  | 1:209:A:VAL:HG23 | 1:210:A:VAL:H    | 2                   | 0.16     | 0.01                | 0.16       |
| (1,1546) | 1:158:A:PRO:HD2  | 1:209:A:VAL:HG21 | 2                   | 0.16     | 0.04                | 0.16       |
| (1,1546) | 1:158:A:PRO:HD2  | 1:209:A:VAL:HG22 | 2                   | 0.16     | 0.04                | 0.16       |
| (1,1546) | 1:158:A:PRO:HD2  | 1:209:A:VAL:HG23 | 2                   | 0.16     | 0.04                | 0.16       |
| (1,538)  | 1:146:A:GLU:HG3  | 1:205:A:MET:HE1  | 2                   | 0.16     | 0.04                | 0.16       |
| (1,538)  | 1:146:A:GLU:HG3  | 1:205:A:MET:HE2  | 2                   | 0.16     | 0.04                | 0.16       |
| (1,538)  | 1:146:A:GLU:HG3  | 1:205:A:MET:HE3  | 2                   | 0.16     | 0.04                | 0.16       |
| (1,2095) | 1:166:A:VAL:HG21 | 1:169:A:TYR:H    | 2                   | 0.16     | 0.02                | 0.16       |
| (1,2095) | 1:166:A:VAL:HG22 | 1:169:A:TYR:H    | 2                   | 0.16     | 0.02                | 0.16       |
| (1,2095) | 1:166:A:VAL:HG23 | 1:169:A:TYR:H    | 2                   | 0.16     | 0.02                | 0.16       |
| (1,2683) | 1:139:A:ILE:HG12 | 1:141:A:PHE:HZ   | 2                   | 0.16     | 0.02                | 0.16       |
| (1,300)  | 1:191:A:THR:HG21 | 1:194:A:LYS:HB2  | 2                   | 0.13     | 0.0                 | 0.13       |
| (1,300)  | 1:191:A:THR:HG22 | 1:194:A:LYS:HB2  | 2                   | 0.13     | 0.0                 | 0.13       |
| (1,300)  | 1:191:A:THR:HG23 | 1:194:A:LYS:HB2  | 2                   | 0.13     | 0.0                 | 0.13       |
| (1,2152) | 1:134:A:MET:HB3  | 1:135:A:SER:H    | 2                   | 0.12     | 0.02                | 0.12       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,472)  | 1:194:A:LYS:HE2  | 1:195:A:GLY:HA3  | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,472)  | 1:194:A:LYS:HE3  | 1:195:A:GLY:HA3  | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,653)  | 1:139:A:ILE:H    | 1:154:A:MET:HE1  | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,653)  | 1:139:A:ILE:H    | 1:154:A:MET:HE2  | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,653)  | 1:139:A:ILE:H    | 1:154:A:MET:HE3  | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,939)  | 1:169:A:TYR:HA   | 1:170:A:SER:HA   | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,2575) | 1:166:A:VAL:HG21 | 1:218:A:TYR:HD1  | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,2575) | 1:166:A:VAL:HG21 | 1:218:A:TYR:HD2  | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,2575) | 1:166:A:VAL:HG22 | 1:218:A:TYR:HD1  | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,2575) | 1:166:A:VAL:HG22 | 1:218:A:TYR:HD2  | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,2575) | 1:166:A:VAL:HG23 | 1:218:A:TYR:HD1  | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,2575) | 1:166:A:VAL:HG23 | 1:218:A:TYR:HD2  | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,185)  | 1:194:A:LYS:HE2  | 1:195:A:GLY:HA2  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,185)  | 1:194:A:LYS:HE3  | 1:195:A:GLY:HA2  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1230) | 1:137:A:PRO:HD2  | 1:213:A:MET:HG3  | 2                   | 0.11     | 0.01                | 0.11       |
| (1,2580) | 1:166:A:VAL:HB   | 1:218:A:TYR:HD1  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,2580) | 1:166:A:VAL:HB   | 1:218:A:TYR:HD2  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1272) | 1:137:A:PRO:HB3  | 1:213:A:MET:HE1  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1272) | 1:137:A:PRO:HB3  | 1:213:A:MET:HE2  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1272) | 1:137:A:PRO:HB3  | 1:213:A:MET:HE3  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1425) | 1:193:A:THR:HG21 | 1:194:A:LYS:HD2  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1425) | 1:193:A:THR:HG21 | 1:194:A:LYS:HD3  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1425) | 1:193:A:THR:HG22 | 1:194:A:LYS:HD2  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1425) | 1:193:A:THR:HG22 | 1:194:A:LYS:HD3  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1425) | 1:193:A:THR:HG23 | 1:194:A:LYS:HD2  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1425) | 1:193:A:THR:HG23 | 1:194:A:LYS:HD3  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,2166) | 1:133:A:ALA:HB1  | 1:159:A:ASN:H    | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,2166) | 1:133:A:ALA:HB2  | 1:159:A:ASN:H    | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,2166) | 1:133:A:ALA:HB3  | 1:159:A:ASN:H    | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,2526) | 1:155:A:TYR:HD1  | 1:156:A:ARG:HG3  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,2526) | 1:155:A:TYR:HD2  | 1:156:A:ARG:HG3  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,2709) | 1:145:A:TRP:HZ3  | 1:205:A:MET:HE1  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,2709) | 1:145:A:TRP:HZ3  | 1:205:A:MET:HE2  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,2709) | 1:145:A:TRP:HZ3  | 1:205:A:MET:HE3  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,2806) | 1:149:A:TYR:HE1  | 1:205:A:MET:HB2  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,2806) | 1:149:A:TYR:HE2  | 1:205:A:MET:HB2  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,39)   | 1:201:A:THR:HG21 | 1:204:A:LYS:HG3  | 2                   | 0.1      | 0.0                 | 0.1        |
| (1,39)   | 1:201:A:THR:HG22 | 1:204:A:LYS:HG3  | 2                   | 0.1      | 0.0                 | 0.1        |
| (1,39)   | 1:201:A:THR:HG23 | 1:204:A:LYS:HG3  | 2                   | 0.1      | 0.0                 | 0.1        |
| (1,298)  | 1:184:A:ILE:HB   | 1:188:A:THR:HG21 | 2                   | 0.1      | 0.0                 | 0.1        |
| (1,298)  | 1:184:A:ILE:HB   | 1:188:A:THR:HG22 | 2                   | 0.1      | 0.0                 | 0.1        |
| (1,298)  | 1:184:A:ILE:HB   | 1:188:A:THR:HG23 | 2                   | 0.1      | 0.0                 | 0.1        |

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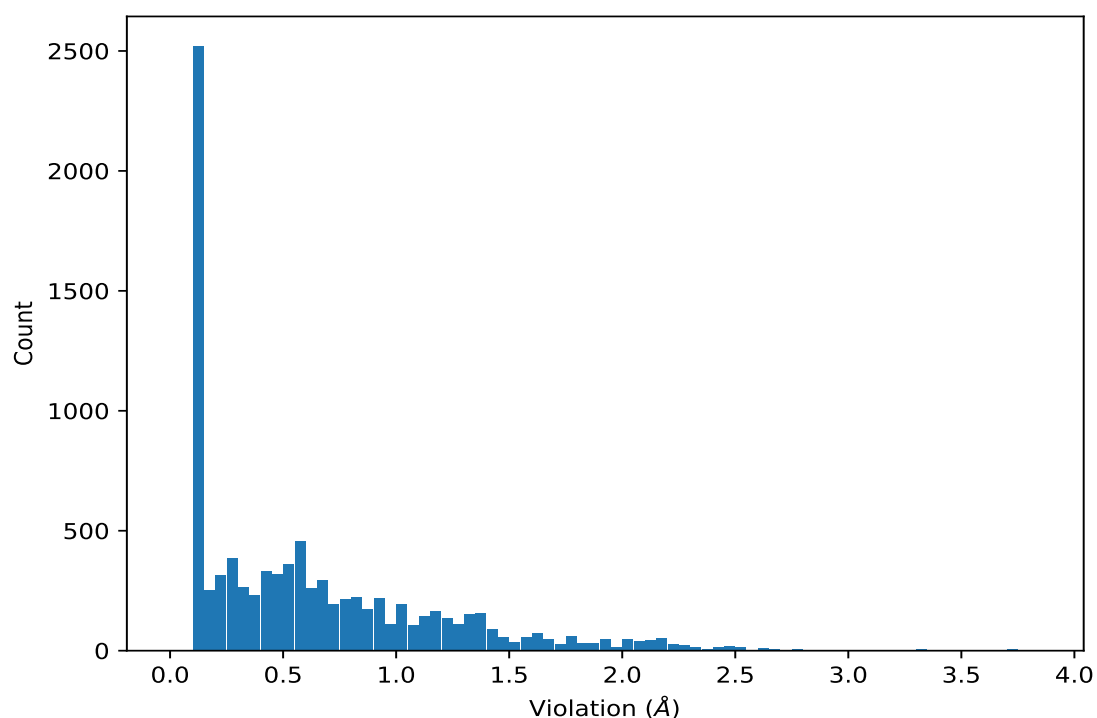
| Key      | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,344)  | 1:189:A:VAL:H   | 1:189:A:VAL:HG11 | 2                   | 0.1      | 0.0                 | 0.1        |
| (1,344)  | 1:189:A:VAL:H   | 1:189:A:VAL:HG12 | 2                   | 0.1      | 0.0                 | 0.1        |
| (1,344)  | 1:189:A:VAL:H   | 1:189:A:VAL:HG13 | 2                   | 0.1      | 0.0                 | 0.1        |
| (1,825)  | 1:133:A:ALA:HB1 | 1:159:A:ASN:HB3  | 2                   | 0.1      | 0.0                 | 0.1        |
| (1,825)  | 1:133:A:ALA:HB2 | 1:159:A:ASN:HB3  | 2                   | 0.1      | 0.0                 | 0.1        |
| (1,825)  | 1:133:A:ALA:HB3 | 1:159:A:ASN:HB3  | 2                   | 0.1      | 0.0                 | 0.1        |
| (1,1322) | 1:133:A:ALA:HB1 | 1:134:A:MET:HG2  | 2                   | 0.1      | 0.0                 | 0.1        |
| (1,1322) | 1:133:A:ALA:HB2 | 1:134:A:MET:HG2  | 2                   | 0.1      | 0.0                 | 0.1        |
| (1,1322) | 1:133:A:ALA:HB3 | 1:134:A:MET:HG2  | 2                   | 0.1      | 0.0                 | 0.1        |
| (1,2496) | 1:149:A:TYR:HD1 | 1:152:A:GLU:HB2  | 2                   | 0.1      | 0.0                 | 0.1        |
| (1,2496) | 1:149:A:TYR:HD1 | 1:152:A:GLU:HB3  | 2                   | 0.1      | 0.0                 | 0.1        |
| (1,2496) | 1:149:A:TYR:HD2 | 1:152:A:GLU:HB2  | 2                   | 0.1      | 0.0                 | 0.1        |
| (1,2496) | 1:149:A:TYR:HD2 | 1:152:A:GLU:HB3  | 2                   | 0.1      | 0.0                 | 0.1        |
| (1,2666) | 1:156:A:ARG:HG2 | 1:198:A:PHE:HE1  | 2                   | 0.1      | 0.0                 | 0.1        |
| (1,2666) | 1:156:A:ARG:HG2 | 1:198:A:PHE:HE2  | 2                   | 0.1      | 0.0                 | 0.1        |
| (1,2776) | 1:150:A:TYR:HE1 | 1:209:A:VAL:H    | 2                   | 0.1      | 0.0                 | 0.1        |
| (1,2776) | 1:150:A:TYR:HE2 | 1:209:A:VAL:H    | 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) |
|----------|------------------|-----------------|----------|---------------|
| (1,2623) | 1:156:A:ARG:HH21 | 1:198:A:PHE:HD1 | 17       | 3.83          |
| (1,2623) | 1:156:A:ARG:HH21 | 1:198:A:PHE:HD2 | 17       | 3.83          |
| (1,2623) | 1:156:A:ARG:HH21 | 1:198:A:PHE:HD1 | 7        | 3.74          |
| (1,2623) | 1:156:A:ARG:HH21 | 1:198:A:PHE:HD2 | 7        | 3.74          |
| (1,2623) | 1:156:A:ARG:HH21 | 1:198:A:PHE:HD1 | 3        | 3.73          |
| (1,2623) | 1:156:A:ARG:HH21 | 1:198:A:PHE:HD2 | 3        | 3.73          |
| (1,2623) | 1:156:A:ARG:HH21 | 1:198:A:PHE:HD1 | 8        | 3.72          |
| (1,2623) | 1:156:A:ARG:HH21 | 1:198:A:PHE:HD2 | 8        | 3.72          |
| (1,2623) | 1:156:A:ARG:HH21 | 1:198:A:PHE:HD1 | 10       | 3.69          |
| (1,2623) | 1:156:A:ARG:HH21 | 1:198:A:PHE:HD2 | 10       | 3.69          |
| (1,2623) | 1:156:A:ARG:HH21 | 1:198:A:PHE:HD1 | 12       | 3.64          |
| (1,2623) | 1:156:A:ARG:HH21 | 1:198:A:PHE:HD2 | 12       | 3.64          |
| (1,2623) | 1:156:A:ARG:HH21 | 1:198:A:PHE:HD1 | 1        | 3.61          |
| (1,2623) | 1:156:A:ARG:HH21 | 1:198:A:PHE:HD2 | 1        | 3.61          |
| (1,2623) | 1:156:A:ARG:HH21 | 1:198:A:PHE:HD1 | 13       | 3.34          |
| (1,2623) | 1:156:A:ARG:HH21 | 1:198:A:PHE:HD2 | 13       | 3.34          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2623) | 1:156:A:ARG:HH21 | 1:198:A:PHE:HD1  | 19       | 3.33          |
| (1,2623) | 1:156:A:ARG:HH21 | 1:198:A:PHE:HD2  | 19       | 3.33          |
| (1,2623) | 1:156:A:ARG:HH21 | 1:198:A:PHE:HD1  | 20       | 3.32          |
| (1,2623) | 1:156:A:ARG:HH21 | 1:198:A:PHE:HD2  | 20       | 3.32          |
| (1,1081) | 1:164:A:ARG:HD2  | 1:168:A:GLN:HG2  | 18       | 3.28          |
| (1,2623) | 1:156:A:ARG:HH21 | 1:198:A:PHE:HD1  | 11       | 3.26          |
| (1,2623) | 1:156:A:ARG:HH21 | 1:198:A:PHE:HD2  | 11       | 3.26          |
| (1,2623) | 1:156:A:ARG:HH21 | 1:198:A:PHE:HD1  | 9        | 3.23          |
| (1,2623) | 1:156:A:ARG:HH21 | 1:198:A:PHE:HD2  | 9        | 3.23          |
| (1,2354) | 1:170:A:SER:HB2  | 1:174:A:ASN:HD21 | 7        | 3.17          |
| (1,2623) | 1:156:A:ARG:HH21 | 1:198:A:PHE:HD1  | 15       | 2.95          |
| (1,2623) | 1:156:A:ARG:HH21 | 1:198:A:PHE:HD2  | 15       | 2.95          |
| (1,2354) | 1:170:A:SER:HB2  | 1:174:A:ASN:HD21 | 6        | 2.94          |
| (1,2623) | 1:156:A:ARG:HH21 | 1:198:A:PHE:HD1  | 14       | 2.91          |
| (1,2623) | 1:156:A:ARG:HH21 | 1:198:A:PHE:HD2  | 14       | 2.91          |
| (1,1081) | 1:164:A:ARG:HD2  | 1:168:A:GLN:HG2  | 8        | 2.91          |
| (1,1081) | 1:164:A:ARG:HD2  | 1:168:A:GLN:HG2  | 15       | 2.86          |
| (1,312)  | 1:166:A:VAL:HG21 | 1:170:A:SER:HB3  | 12       | 2.85          |
| (1,312)  | 1:166:A:VAL:HG22 | 1:170:A:SER:HB3  | 12       | 2.85          |
| (1,312)  | 1:166:A:VAL:HG23 | 1:170:A:SER:HB3  | 12       | 2.85          |
| (1,428)  | 1:127:A:GLY:HA2  | 1:164:A:ARG:HD3  | 15       | 2.82          |
| (1,2623) | 1:156:A:ARG:HH21 | 1:198:A:PHE:HD1  | 16       | 2.79          |
| (1,2623) | 1:156:A:ARG:HH21 | 1:198:A:PHE:HD2  | 16       | 2.79          |
| (1,2623) | 1:156:A:ARG:HH21 | 1:198:A:PHE:HD1  | 5        | 2.78          |
| (1,2623) | 1:156:A:ARG:HH21 | 1:198:A:PHE:HD2  | 5        | 2.78          |
| (1,2623) | 1:156:A:ARG:HH21 | 1:198:A:PHE:HD1  | 6        | 2.77          |
| (1,2623) | 1:156:A:ARG:HH21 | 1:198:A:PHE:HD2  | 6        | 2.77          |
| (1,1081) | 1:164:A:ARG:HD2  | 1:168:A:GLN:HG2  | 9        | 2.76          |
| (1,428)  | 1:127:A:GLY:HA2  | 1:164:A:ARG:HD3  | 9        | 2.72          |
| (1,312)  | 1:166:A:VAL:HG21 | 1:170:A:SER:HB3  | 17       | 2.68          |
| (1,312)  | 1:166:A:VAL:HG22 | 1:170:A:SER:HB3  | 17       | 2.68          |
| (1,312)  | 1:166:A:VAL:HG23 | 1:170:A:SER:HB3  | 17       | 2.68          |
| (1,428)  | 1:127:A:GLY:HA2  | 1:164:A:ARG:HD3  | 12       | 2.67          |
| (1,428)  | 1:127:A:GLY:HA2  | 1:164:A:ARG:HD3  | 10       | 2.66          |
| (1,601)  | 1:166:A:VAL:HG21 | 1:170:A:SER:HB2  | 17       | 2.64          |
| (1,601)  | 1:166:A:VAL:HG22 | 1:170:A:SER:HB2  | 17       | 2.64          |
| (1,601)  | 1:166:A:VAL:HG23 | 1:170:A:SER:HB2  | 17       | 2.64          |
| (1,470)  | 1:122:A:VAL:HG21 | 1:125:A:LEU:HB2  | 8        | 2.64          |
| (1,470)  | 1:122:A:VAL:HG22 | 1:125:A:LEU:HB2  | 8        | 2.64          |
| (1,470)  | 1:122:A:VAL:HG23 | 1:125:A:LEU:HB2  | 8        | 2.64          |
| (1,2682) | 1:141:A:PHE:HZ   | 1:209:A:VAL:HG11 | 4        | 2.63          |
| (1,2682) | 1:141:A:PHE:HZ   | 1:209:A:VAL:HG12 | 4        | 2.63          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2682) | 1:141:A:PHE:HZ   | 1:209:A:VAL:HG13 | 4        | 2.63          |
| (1,428)  | 1:127:A:GLY:HA2  | 1:164:A:ARG:HD3  | 11       | 2.61          |
| (1,2682) | 1:141:A:PHE:HZ   | 1:209:A:VAL:HG11 | 8        | 2.55          |
| (1,2682) | 1:141:A:PHE:HZ   | 1:209:A:VAL:HG12 | 8        | 2.55          |
| (1,2682) | 1:141:A:PHE:HZ   | 1:209:A:VAL:HG13 | 8        | 2.55          |
| (1,2682) | 1:141:A:PHE:HZ   | 1:209:A:VAL:HG11 | 1        | 2.54          |
| (1,2682) | 1:141:A:PHE:HZ   | 1:209:A:VAL:HG12 | 1        | 2.54          |
| (1,2682) | 1:141:A:PHE:HZ   | 1:209:A:VAL:HG13 | 1        | 2.54          |
| (1,2682) | 1:141:A:PHE:HZ   | 1:209:A:VAL:HG11 | 14       | 2.54          |
| (1,2682) | 1:141:A:PHE:HZ   | 1:209:A:VAL:HG12 | 14       | 2.54          |
| (1,2682) | 1:141:A:PHE:HZ   | 1:209:A:VAL:HG13 | 14       | 2.54          |
| (1,2682) | 1:141:A:PHE:HZ   | 1:209:A:VAL:HG11 | 13       | 2.53          |
| (1,2682) | 1:141:A:PHE:HZ   | 1:209:A:VAL:HG12 | 13       | 2.53          |
| (1,2682) | 1:141:A:PHE:HZ   | 1:209:A:VAL:HG13 | 13       | 2.53          |
| (1,428)  | 1:127:A:GLY:HA2  | 1:164:A:ARG:HD3  | 18       | 2.53          |
| (1,1459) | 1:136:A:ARG:HB3  | 1:159:A:ASN:HB3  | 10       | 2.52          |
| (1,470)  | 1:122:A:VAL:HG21 | 1:125:A:LEU:HB2  | 15       | 2.49          |
| (1,470)  | 1:122:A:VAL:HG22 | 1:125:A:LEU:HB2  | 15       | 2.49          |
| (1,470)  | 1:122:A:VAL:HG23 | 1:125:A:LEU:HB2  | 15       | 2.49          |
| (1,362)  | 1:172:A:GLN:HG3  | 1:215:A:VAL:HG21 | 17       | 2.49          |
| (1,362)  | 1:172:A:GLN:HG3  | 1:215:A:VAL:HG22 | 17       | 2.49          |
| (1,362)  | 1:172:A:GLN:HG3  | 1:215:A:VAL:HG23 | 17       | 2.49          |
| (1,23)   | 1:220:A:LYS:HG2  | 1:221:A:GLU:HG3  | 7        | 2.48          |
| (1,2682) | 1:141:A:PHE:HZ   | 1:209:A:VAL:HG11 | 11       | 2.47          |
| (1,2682) | 1:141:A:PHE:HZ   | 1:209:A:VAL:HG12 | 11       | 2.47          |
| (1,2682) | 1:141:A:PHE:HZ   | 1:209:A:VAL:HG13 | 11       | 2.47          |
| (1,2682) | 1:141:A:PHE:HZ   | 1:209:A:VAL:HG11 | 16       | 2.45          |
| (1,2682) | 1:141:A:PHE:HZ   | 1:209:A:VAL:HG12 | 16       | 2.45          |
| (1,2682) | 1:141:A:PHE:HZ   | 1:209:A:VAL:HG13 | 16       | 2.45          |
| (1,1081) | 1:164:A:ARG:HD2  | 1:168:A:GLN:HG2  | 20       | 2.45          |
| (1,312)  | 1:166:A:VAL:HG21 | 1:170:A:SER:HB3  | 1        | 2.45          |
| (1,312)  | 1:166:A:VAL:HG22 | 1:170:A:SER:HB3  | 1        | 2.45          |
| (1,312)  | 1:166:A:VAL:HG23 | 1:170:A:SER:HB3  | 1        | 2.45          |
| (1,1459) | 1:136:A:ARG:HB3  | 1:159:A:ASN:HB3  | 19       | 2.44          |
| (1,357)  | 1:122:A:VAL:HG21 | 1:125:A:LEU:HG   | 8        | 2.44          |
| (1,357)  | 1:122:A:VAL:HG22 | 1:125:A:LEU:HG   | 8        | 2.44          |
| (1,357)  | 1:122:A:VAL:HG23 | 1:125:A:LEU:HG   | 8        | 2.44          |
| (1,2682) | 1:141:A:PHE:HZ   | 1:209:A:VAL:HG11 | 10       | 2.42          |
| (1,2682) | 1:141:A:PHE:HZ   | 1:209:A:VAL:HG12 | 10       | 2.42          |
| (1,2682) | 1:141:A:PHE:HZ   | 1:209:A:VAL:HG13 | 10       | 2.42          |
| (1,2354) | 1:170:A:SER:HB2  | 1:174:A:ASN:HD21 | 3        | 2.42          |
| (1,1081) | 1:164:A:ARG:HD2  | 1:168:A:GLN:HG2  | 10       | 2.42          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,377)  | 1:209:A:VAL:HG21 | 1:213:A:MET:HG2  | 20       | 2.42          |
| (1,377)  | 1:209:A:VAL:HG22 | 1:213:A:MET:HG2  | 20       | 2.42          |
| (1,377)  | 1:209:A:VAL:HG23 | 1:213:A:MET:HG2  | 20       | 2.42          |
| (1,601)  | 1:166:A:VAL:HG21 | 1:170:A:SER:HB2  | 12       | 2.41          |
| (1,601)  | 1:166:A:VAL:HG22 | 1:170:A:SER:HB2  | 12       | 2.41          |
| (1,601)  | 1:166:A:VAL:HG23 | 1:170:A:SER:HB2  | 12       | 2.41          |
| (1,23)   | 1:220:A:LYS:HG2  | 1:221:A:GLU:HG3  | 15       | 2.4           |
| (1,1)    | 1:138:A:MET:HG3  | 1:139:A:ILE:HG12 | 19       | 2.39          |
| (1,23)   | 1:220:A:LYS:HG2  | 1:221:A:GLU:HG3  | 20       | 2.38          |
| (1,1)    | 1:138:A:MET:HG3  | 1:139:A:ILE:HG12 | 12       | 2.38          |
| (1,2682) | 1:141:A:PHE:HZ   | 1:209:A:VAL:HG11 | 19       | 2.36          |
| (1,2682) | 1:141:A:PHE:HZ   | 1:209:A:VAL:HG12 | 19       | 2.36          |
| (1,2682) | 1:141:A:PHE:HZ   | 1:209:A:VAL:HG13 | 19       | 2.36          |
| (1,428)  | 1:127:A:GLY:HA2  | 1:164:A:ARG:HD3  | 20       | 2.35          |
| (1,2682) | 1:141:A:PHE:HZ   | 1:209:A:VAL:HG11 | 7        | 2.33          |
| (1,2682) | 1:141:A:PHE:HZ   | 1:209:A:VAL:HG12 | 7        | 2.33          |
| (1,2682) | 1:141:A:PHE:HZ   | 1:209:A:VAL:HG13 | 7        | 2.33          |
| (1,2623) | 1:156:A:ARG:HH21 | 1:198:A:PHE:HD1  | 2        | 2.33          |
| (1,2623) | 1:156:A:ARG:HH21 | 1:198:A:PHE:HD2  | 2        | 2.33          |
| (1,377)  | 1:209:A:VAL:HG21 | 1:213:A:MET:HG2  | 2        | 2.33          |
| (1,377)  | 1:209:A:VAL:HG22 | 1:213:A:MET:HG2  | 2        | 2.33          |
| (1,377)  | 1:209:A:VAL:HG23 | 1:213:A:MET:HG2  | 2        | 2.33          |
| (1,428)  | 1:127:A:GLY:HA2  | 1:164:A:ARG:HD3  | 2        | 2.32          |
| (1,1081) | 1:164:A:ARG:HD2  | 1:168:A:GLN:HG2  | 6        | 2.31          |
| (1,370)  | 1:158:A:PRO:HG2  | 1:209:A:VAL:HG21 | 8        | 2.31          |
| (1,370)  | 1:158:A:PRO:HG2  | 1:209:A:VAL:HG22 | 8        | 2.31          |
| (1,370)  | 1:158:A:PRO:HG2  | 1:209:A:VAL:HG23 | 8        | 2.31          |
| (1,1)    | 1:138:A:MET:HG3  | 1:139:A:ILE:HG12 | 8        | 2.31          |
| (1,312)  | 1:166:A:VAL:HG21 | 1:170:A:SER:HB3  | 3        | 2.29          |
| (1,312)  | 1:166:A:VAL:HG22 | 1:170:A:SER:HB3  | 3        | 2.29          |
| (1,312)  | 1:166:A:VAL:HG23 | 1:170:A:SER:HB3  | 3        | 2.29          |
| (1,23)   | 1:220:A:LYS:HG2  | 1:221:A:GLU:HG3  | 9        | 2.29          |
| (1,1)    | 1:138:A:MET:HG3  | 1:139:A:ILE:HG12 | 15       | 2.29          |
| (1,2682) | 1:141:A:PHE:HZ   | 1:209:A:VAL:HG11 | 12       | 2.28          |
| (1,2682) | 1:141:A:PHE:HZ   | 1:209:A:VAL:HG12 | 12       | 2.28          |
| (1,2682) | 1:141:A:PHE:HZ   | 1:209:A:VAL:HG13 | 12       | 2.28          |
| (1,370)  | 1:158:A:PRO:HG2  | 1:209:A:VAL:HG21 | 7        | 2.28          |
| (1,370)  | 1:158:A:PRO:HG2  | 1:209:A:VAL:HG22 | 7        | 2.28          |
| (1,370)  | 1:158:A:PRO:HG2  | 1:209:A:VAL:HG23 | 7        | 2.28          |
| (1,309)  | 1:186:A:GLN:HE21 | 1:189:A:VAL:HG11 | 11       | 2.28          |
| (1,309)  | 1:186:A:GLN:HE21 | 1:189:A:VAL:HG12 | 11       | 2.28          |
| (1,309)  | 1:186:A:GLN:HE21 | 1:189:A:VAL:HG13 | 11       | 2.28          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1)    | 1:138:A:MET:HG3  | 1:139:A:ILE:HG12 | 20       | 2.27          |
| (1,970)  | 1:161:A:VAL:HG21 | 1:217:A:GLN:HA   | 10       | 2.26          |
| (1,970)  | 1:161:A:VAL:HG22 | 1:217:A:GLN:HA   | 10       | 2.26          |
| (1,970)  | 1:161:A:VAL:HG23 | 1:217:A:GLN:HA   | 10       | 2.26          |
| (1,1)    | 1:138:A:MET:HG3  | 1:139:A:ILE:HG12 | 6        | 2.26          |
| (1,355)  | 1:203:A:VAL:HG21 | 1:204:A:LYS:HD2  | 18       | 2.25          |
| (1,355)  | 1:203:A:VAL:HG21 | 1:204:A:LYS:HD3  | 18       | 2.25          |
| (1,355)  | 1:203:A:VAL:HG22 | 1:204:A:LYS:HD2  | 18       | 2.25          |
| (1,355)  | 1:203:A:VAL:HG22 | 1:204:A:LYS:HD3  | 18       | 2.25          |
| (1,355)  | 1:203:A:VAL:HG23 | 1:204:A:LYS:HD2  | 18       | 2.25          |
| (1,355)  | 1:203:A:VAL:HG23 | 1:204:A:LYS:HD3  | 18       | 2.25          |
| (1,1662) | 1:198:A:PHE:H    | 1:203:A:VAL:HG11 | 18       | 2.24          |
| (1,1662) | 1:198:A:PHE:H    | 1:203:A:VAL:HG12 | 18       | 2.24          |
| (1,1662) | 1:198:A:PHE:H    | 1:203:A:VAL:HG13 | 18       | 2.24          |
| (1,370)  | 1:158:A:PRO:HG2  | 1:209:A:VAL:HG21 | 11       | 2.24          |
| (1,370)  | 1:158:A:PRO:HG2  | 1:209:A:VAL:HG22 | 11       | 2.24          |
| (1,370)  | 1:158:A:PRO:HG2  | 1:209:A:VAL:HG23 | 11       | 2.24          |
| (1,370)  | 1:158:A:PRO:HG2  | 1:209:A:VAL:HG21 | 17       | 2.23          |
| (1,370)  | 1:158:A:PRO:HG2  | 1:209:A:VAL:HG22 | 17       | 2.23          |
| (1,370)  | 1:158:A:PRO:HG2  | 1:209:A:VAL:HG23 | 17       | 2.23          |
| (1,258)  | 1:122:A:VAL:HG11 | 1:190:A:THR:HG21 | 16       | 2.23          |
| (1,258)  | 1:122:A:VAL:HG11 | 1:190:A:THR:HG22 | 16       | 2.23          |
| (1,258)  | 1:122:A:VAL:HG11 | 1:190:A:THR:HG23 | 16       | 2.23          |
| (1,258)  | 1:122:A:VAL:HG12 | 1:190:A:THR:HG21 | 16       | 2.23          |
| (1,258)  | 1:122:A:VAL:HG12 | 1:190:A:THR:HG22 | 16       | 2.23          |
| (1,258)  | 1:122:A:VAL:HG12 | 1:190:A:THR:HG23 | 16       | 2.23          |
| (1,258)  | 1:122:A:VAL:HG13 | 1:190:A:THR:HG21 | 16       | 2.23          |
| (1,258)  | 1:122:A:VAL:HG13 | 1:190:A:THR:HG22 | 16       | 2.23          |
| (1,258)  | 1:122:A:VAL:HG13 | 1:190:A:THR:HG23 | 16       | 2.23          |
| (1,23)   | 1:220:A:LYS:HG2  | 1:221:A:GLU:HG3  | 11       | 2.23          |
| (1,428)  | 1:127:A:GLY:HA2  | 1:164:A:ARG:HD3  | 13       | 2.22          |
| (1,358)  | 1:203:A:VAL:HG21 | 1:204:A:LYS:HG3  | 8        | 2.21          |
| (1,358)  | 1:203:A:VAL:HG22 | 1:204:A:LYS:HG3  | 8        | 2.21          |
| (1,358)  | 1:203:A:VAL:HG23 | 1:204:A:LYS:HG3  | 8        | 2.21          |
| (1,2682) | 1:141:A:PHE:HZ   | 1:209:A:VAL:HG11 | 20       | 2.2           |
| (1,2682) | 1:141:A:PHE:HZ   | 1:209:A:VAL:HG12 | 20       | 2.2           |
| (1,2682) | 1:141:A:PHE:HZ   | 1:209:A:VAL:HG13 | 20       | 2.2           |
| (1,23)   | 1:220:A:LYS:HG2  | 1:221:A:GLU:HG3  | 18       | 2.2           |
| (1,1)    | 1:138:A:MET:HG3  | 1:139:A:ILE:HG12 | 2        | 2.2           |
| (1,1)    | 1:138:A:MET:HG3  | 1:139:A:ILE:HG12 | 11       | 2.2           |
| (1,370)  | 1:158:A:PRO:HG2  | 1:209:A:VAL:HG21 | 4        | 2.19          |
| (1,370)  | 1:158:A:PRO:HG2  | 1:209:A:VAL:HG22 | 4        | 2.19          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,370)  | 1:158:A:PRO:HG2  | 1:209:A:VAL:HG23 | 4        | 2.19          |
| (1,2634) | 1:198:A:PHE:HD1  | 1:203:A:VAL:HG11 | 5        | 2.18          |
| (1,2634) | 1:198:A:PHE:HD1  | 1:203:A:VAL:HG12 | 5        | 2.18          |
| (1,2634) | 1:198:A:PHE:HD1  | 1:203:A:VAL:HG13 | 5        | 2.18          |
| (1,2634) | 1:198:A:PHE:HD2  | 1:203:A:VAL:HG11 | 5        | 2.18          |
| (1,2634) | 1:198:A:PHE:HD2  | 1:203:A:VAL:HG12 | 5        | 2.18          |
| (1,2634) | 1:198:A:PHE:HD2  | 1:203:A:VAL:HG13 | 5        | 2.18          |
| (1,2634) | 1:198:A:PHE:HD1  | 1:203:A:VAL:HG11 | 7        | 2.18          |
| (1,2634) | 1:198:A:PHE:HD1  | 1:203:A:VAL:HG12 | 7        | 2.18          |
| (1,2634) | 1:198:A:PHE:HD1  | 1:203:A:VAL:HG13 | 7        | 2.18          |
| (1,2634) | 1:198:A:PHE:HD2  | 1:203:A:VAL:HG11 | 7        | 2.18          |
| (1,2634) | 1:198:A:PHE:HD2  | 1:203:A:VAL:HG12 | 7        | 2.18          |
| (1,2634) | 1:198:A:PHE:HD2  | 1:203:A:VAL:HG13 | 7        | 2.18          |
| (1,1081) | 1:164:A:ARG:HD2  | 1:168:A:GLN:HG2  | 13       | 2.18          |
| (1,377)  | 1:209:A:VAL:HG21 | 1:213:A:MET:HG2  | 1        | 2.18          |
| (1,377)  | 1:209:A:VAL:HG22 | 1:213:A:MET:HG2  | 1        | 2.18          |
| (1,377)  | 1:209:A:VAL:HG23 | 1:213:A:MET:HG2  | 1        | 2.18          |
| (1,2634) | 1:198:A:PHE:HD1  | 1:203:A:VAL:HG11 | 8        | 2.17          |
| (1,2634) | 1:198:A:PHE:HD1  | 1:203:A:VAL:HG12 | 8        | 2.17          |
| (1,2634) | 1:198:A:PHE:HD1  | 1:203:A:VAL:HG13 | 8        | 2.17          |
| (1,2634) | 1:198:A:PHE:HD2  | 1:203:A:VAL:HG11 | 8        | 2.17          |
| (1,2634) | 1:198:A:PHE:HD2  | 1:203:A:VAL:HG12 | 8        | 2.17          |
| (1,2634) | 1:198:A:PHE:HD2  | 1:203:A:VAL:HG13 | 8        | 2.17          |
| (1,1662) | 1:198:A:PHE:H    | 1:203:A:VAL:HG11 | 8        | 2.17          |
| (1,1662) | 1:198:A:PHE:H    | 1:203:A:VAL:HG12 | 8        | 2.17          |
| (1,1662) | 1:198:A:PHE:H    | 1:203:A:VAL:HG13 | 8        | 2.17          |
| (1,370)  | 1:158:A:PRO:HG2  | 1:209:A:VAL:HG21 | 2        | 2.17          |
| (1,370)  | 1:158:A:PRO:HG2  | 1:209:A:VAL:HG22 | 2        | 2.17          |
| (1,370)  | 1:158:A:PRO:HG2  | 1:209:A:VAL:HG23 | 2        | 2.17          |
| (1,23)   | 1:220:A:LYS:HG2  | 1:221:A:GLU:HG3  | 12       | 2.17          |
| (1,934)  | 1:166:A:VAL:HG11 | 1:221:A:GLU:HG2  | 12       | 2.16          |
| (1,934)  | 1:166:A:VAL:HG12 | 1:221:A:GLU:HG2  | 12       | 2.16          |
| (1,934)  | 1:166:A:VAL:HG13 | 1:221:A:GLU:HG2  | 12       | 2.16          |
| (1,355)  | 1:203:A:VAL:HG21 | 1:204:A:LYS:HD2  | 7        | 2.16          |
| (1,355)  | 1:203:A:VAL:HG21 | 1:204:A:LYS:HD3  | 7        | 2.16          |
| (1,355)  | 1:203:A:VAL:HG22 | 1:204:A:LYS:HD2  | 7        | 2.16          |
| (1,355)  | 1:203:A:VAL:HG22 | 1:204:A:LYS:HD3  | 7        | 2.16          |
| (1,355)  | 1:203:A:VAL:HG23 | 1:204:A:LYS:HD2  | 7        | 2.16          |
| (1,355)  | 1:203:A:VAL:HG23 | 1:204:A:LYS:HD3  | 7        | 2.16          |
| (1,377)  | 1:209:A:VAL:HG21 | 1:213:A:MET:HG2  | 4        | 2.15          |
| (1,377)  | 1:209:A:VAL:HG22 | 1:213:A:MET:HG2  | 4        | 2.15          |
| (1,377)  | 1:209:A:VAL:HG23 | 1:213:A:MET:HG2  | 4        | 2.15          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,258)  | 1:122:A:VAL:HG11 | 1:190:A:THR:HG21 | 18       | 2.15          |
| (1,258)  | 1:122:A:VAL:HG11 | 1:190:A:THR:HG22 | 18       | 2.15          |
| (1,258)  | 1:122:A:VAL:HG11 | 1:190:A:THR:HG23 | 18       | 2.15          |
| (1,258)  | 1:122:A:VAL:HG12 | 1:190:A:THR:HG21 | 18       | 2.15          |
| (1,258)  | 1:122:A:VAL:HG12 | 1:190:A:THR:HG22 | 18       | 2.15          |
| (1,258)  | 1:122:A:VAL:HG12 | 1:190:A:THR:HG23 | 18       | 2.15          |
| (1,258)  | 1:122:A:VAL:HG13 | 1:190:A:THR:HG21 | 18       | 2.15          |
| (1,258)  | 1:122:A:VAL:HG13 | 1:190:A:THR:HG22 | 18       | 2.15          |
| (1,258)  | 1:122:A:VAL:HG13 | 1:190:A:THR:HG23 | 18       | 2.15          |
| (1,1)    | 1:138:A:MET:HG3  | 1:139:A:ILE:HG12 | 4        | 2.15          |
| (1,1459) | 1:136:A:ARG:HB3  | 1:159:A:ASN:HB3  | 4        | 2.14          |
| (1,2682) | 1:141:A:PHE:HZ   | 1:209:A:VAL:HG11 | 2        | 2.13          |
| (1,2682) | 1:141:A:PHE:HZ   | 1:209:A:VAL:HG12 | 2        | 2.13          |
| (1,2682) | 1:141:A:PHE:HZ   | 1:209:A:VAL:HG13 | 2        | 2.13          |
| (1,1235) | 1:205:A:MET:HG3  | 1:206:A:MET:HG2  | 2        | 2.13          |
| (1,1081) | 1:164:A:ARG:HD2  | 1:168:A:GLN:HG2  | 16       | 2.13          |
| (1,377)  | 1:209:A:VAL:HG21 | 1:213:A:MET:HG2  | 12       | 2.13          |
| (1,377)  | 1:209:A:VAL:HG22 | 1:213:A:MET:HG2  | 12       | 2.13          |
| (1,377)  | 1:209:A:VAL:HG23 | 1:213:A:MET:HG2  | 12       | 2.13          |
| (1,370)  | 1:158:A:PRO:HG2  | 1:209:A:VAL:HG21 | 19       | 2.13          |
| (1,370)  | 1:158:A:PRO:HG2  | 1:209:A:VAL:HG22 | 19       | 2.13          |
| (1,370)  | 1:158:A:PRO:HG2  | 1:209:A:VAL:HG23 | 19       | 2.13          |
| (1,355)  | 1:203:A:VAL:HG21 | 1:204:A:LYS:HD2  | 8        | 2.13          |
| (1,355)  | 1:203:A:VAL:HG21 | 1:204:A:LYS:HD3  | 8        | 2.13          |
| (1,355)  | 1:203:A:VAL:HG22 | 1:204:A:LYS:HD2  | 8        | 2.13          |
| (1,355)  | 1:203:A:VAL:HG22 | 1:204:A:LYS:HD3  | 8        | 2.13          |
| (1,355)  | 1:203:A:VAL:HG23 | 1:204:A:LYS:HD2  | 8        | 2.13          |
| (1,355)  | 1:203:A:VAL:HG23 | 1:204:A:LYS:HD3  | 8        | 2.13          |
| (1,392)  | 1:122:A:VAL:HG11 | 1:190:A:THR:HB   | 16       | 2.12          |
| (1,392)  | 1:122:A:VAL:HG12 | 1:190:A:THR:HB   | 16       | 2.12          |
| (1,392)  | 1:122:A:VAL:HG13 | 1:190:A:THR:HB   | 16       | 2.12          |
| (1,377)  | 1:209:A:VAL:HG21 | 1:213:A:MET:HG2  | 19       | 2.12          |
| (1,377)  | 1:209:A:VAL:HG22 | 1:213:A:MET:HG2  | 19       | 2.12          |
| (1,377)  | 1:209:A:VAL:HG23 | 1:213:A:MET:HG2  | 19       | 2.12          |
| (1,2634) | 1:198:A:PHE:HD1  | 1:203:A:VAL:HG11 | 18       | 2.11          |
| (1,2634) | 1:198:A:PHE:HD1  | 1:203:A:VAL:HG12 | 18       | 2.11          |
| (1,2634) | 1:198:A:PHE:HD1  | 1:203:A:VAL:HG13 | 18       | 2.11          |
| (1,2634) | 1:198:A:PHE:HD2  | 1:203:A:VAL:HG11 | 18       | 2.11          |
| (1,2634) | 1:198:A:PHE:HD2  | 1:203:A:VAL:HG12 | 18       | 2.11          |
| (1,2634) | 1:198:A:PHE:HD2  | 1:203:A:VAL:HG13 | 18       | 2.11          |
| (1,377)  | 1:209:A:VAL:HG21 | 1:213:A:MET:HG2  | 17       | 2.11          |
| (1,377)  | 1:209:A:VAL:HG22 | 1:213:A:MET:HG2  | 17       | 2.11          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,377)  | 1:209:A:VAL:HG23 | 1:213:A:MET:HG2  | 17       | 2.11          |
| (1,370)  | 1:158:A:PRO:HG2  | 1:209:A:VAL:HG21 | 16       | 2.11          |
| (1,370)  | 1:158:A:PRO:HG2  | 1:209:A:VAL:HG22 | 16       | 2.11          |
| (1,370)  | 1:158:A:PRO:HG2  | 1:209:A:VAL:HG23 | 16       | 2.11          |
| (1,377)  | 1:209:A:VAL:HG21 | 1:213:A:MET:HG2  | 14       | 2.1           |
| (1,377)  | 1:209:A:VAL:HG22 | 1:213:A:MET:HG2  | 14       | 2.1           |
| (1,377)  | 1:209:A:VAL:HG23 | 1:213:A:MET:HG2  | 14       | 2.1           |
| (1,370)  | 1:158:A:PRO:HG2  | 1:209:A:VAL:HG21 | 14       | 2.1           |
| (1,370)  | 1:158:A:PRO:HG2  | 1:209:A:VAL:HG22 | 14       | 2.1           |
| (1,370)  | 1:158:A:PRO:HG2  | 1:209:A:VAL:HG23 | 14       | 2.1           |
| (1,2634) | 1:198:A:PHE:HD1  | 1:203:A:VAL:HG11 | 2        | 2.09          |
| (1,2634) | 1:198:A:PHE:HD1  | 1:203:A:VAL:HG12 | 2        | 2.09          |
| (1,2634) | 1:198:A:PHE:HD1  | 1:203:A:VAL:HG13 | 2        | 2.09          |
| (1,2634) | 1:198:A:PHE:HD2  | 1:203:A:VAL:HG11 | 2        | 2.09          |
| (1,2634) | 1:198:A:PHE:HD2  | 1:203:A:VAL:HG12 | 2        | 2.09          |
| (1,2634) | 1:198:A:PHE:HD2  | 1:203:A:VAL:HG13 | 2        | 2.09          |
| (1,377)  | 1:209:A:VAL:HG21 | 1:213:A:MET:HG2  | 18       | 2.09          |
| (1,377)  | 1:209:A:VAL:HG22 | 1:213:A:MET:HG2  | 18       | 2.09          |
| (1,377)  | 1:209:A:VAL:HG23 | 1:213:A:MET:HG2  | 18       | 2.09          |
| (1,358)  | 1:203:A:VAL:HG21 | 1:204:A:LYS:HG3  | 7        | 2.09          |
| (1,358)  | 1:203:A:VAL:HG22 | 1:204:A:LYS:HG3  | 7        | 2.09          |
| (1,358)  | 1:203:A:VAL:HG23 | 1:204:A:LYS:HG3  | 7        | 2.09          |
| (1,370)  | 1:158:A:PRO:HG2  | 1:209:A:VAL:HG21 | 1        | 2.08          |
| (1,370)  | 1:158:A:PRO:HG2  | 1:209:A:VAL:HG22 | 1        | 2.08          |
| (1,370)  | 1:158:A:PRO:HG2  | 1:209:A:VAL:HG23 | 1        | 2.08          |
| (1,23)   | 1:220:A:LYS:HG2  | 1:221:A:GLU:HG3  | 4        | 2.08          |
| (1,370)  | 1:158:A:PRO:HG2  | 1:209:A:VAL:HG21 | 12       | 2.07          |
| (1,370)  | 1:158:A:PRO:HG2  | 1:209:A:VAL:HG22 | 12       | 2.07          |
| (1,370)  | 1:158:A:PRO:HG2  | 1:209:A:VAL:HG23 | 12       | 2.07          |
| (1,355)  | 1:203:A:VAL:HG21 | 1:204:A:LYS:HD2  | 12       | 2.07          |
| (1,355)  | 1:203:A:VAL:HG21 | 1:204:A:LYS:HD3  | 12       | 2.07          |
| (1,355)  | 1:203:A:VAL:HG22 | 1:204:A:LYS:HD2  | 12       | 2.07          |
| (1,355)  | 1:203:A:VAL:HG22 | 1:204:A:LYS:HD3  | 12       | 2.07          |
| (1,355)  | 1:203:A:VAL:HG23 | 1:204:A:LYS:HD2  | 12       | 2.07          |
| (1,355)  | 1:203:A:VAL:HG23 | 1:204:A:LYS:HD3  | 12       | 2.07          |
| (1,258)  | 1:122:A:VAL:HG11 | 1:190:A:THR:HG21 | 2        | 2.07          |
| (1,258)  | 1:122:A:VAL:HG11 | 1:190:A:THR:HG22 | 2        | 2.07          |
| (1,258)  | 1:122:A:VAL:HG11 | 1:190:A:THR:HG23 | 2        | 2.07          |
| (1,258)  | 1:122:A:VAL:HG12 | 1:190:A:THR:HG21 | 2        | 2.07          |
| (1,258)  | 1:122:A:VAL:HG12 | 1:190:A:THR:HG22 | 2        | 2.07          |
| (1,258)  | 1:122:A:VAL:HG12 | 1:190:A:THR:HG23 | 2        | 2.07          |
| (1,258)  | 1:122:A:VAL:HG13 | 1:190:A:THR:HG21 | 2        | 2.07          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,258)  | 1:122:A:VAL:HG13 | 1:190:A:THR:HG22 | 2        | 2.07          |
| (1,258)  | 1:122:A:VAL:HG13 | 1:190:A:THR:HG23 | 2        | 2.07          |
| (1,1)    | 1:138:A:MET:HG3  | 1:139:A:ILE:HG12 | 9        | 2.07          |
| (1,1662) | 1:198:A:PHE:H    | 1:203:A:VAL:HG11 | 2        | 2.06          |
| (1,1662) | 1:198:A:PHE:H    | 1:203:A:VAL:HG12 | 2        | 2.06          |
| (1,1662) | 1:198:A:PHE:H    | 1:203:A:VAL:HG13 | 2        | 2.06          |
| (1,428)  | 1:127:A:GLY:HA2  | 1:164:A:ARG:HD3  | 8        | 2.06          |
| (1,23)   | 1:220:A:LYS:HG2  | 1:221:A:GLU:HG3  | 6        | 2.06          |
| (1,1)    | 1:138:A:MET:HG3  | 1:139:A:ILE:HG12 | 3        | 2.06          |
| (1,2491) | 1:150:A:TYR:HD1  | 1:209:A:VAL:HG11 | 10       | 2.05          |
| (1,2491) | 1:150:A:TYR:HD1  | 1:209:A:VAL:HG12 | 10       | 2.05          |
| (1,2491) | 1:150:A:TYR:HD1  | 1:209:A:VAL:HG13 | 10       | 2.05          |
| (1,2491) | 1:150:A:TYR:HD2  | 1:209:A:VAL:HG11 | 10       | 2.05          |
| (1,2491) | 1:150:A:TYR:HD2  | 1:209:A:VAL:HG12 | 10       | 2.05          |
| (1,2491) | 1:150:A:TYR:HD2  | 1:209:A:VAL:HG13 | 10       | 2.05          |
| (1,355)  | 1:203:A:VAL:HG21 | 1:204:A:LYS:HD2  | 2        | 2.05          |
| (1,355)  | 1:203:A:VAL:HG21 | 1:204:A:LYS:HD3  | 2        | 2.05          |
| (1,355)  | 1:203:A:VAL:HG22 | 1:204:A:LYS:HD2  | 2        | 2.05          |
| (1,355)  | 1:203:A:VAL:HG22 | 1:204:A:LYS:HD3  | 2        | 2.05          |
| (1,355)  | 1:203:A:VAL:HG23 | 1:204:A:LYS:HD2  | 2        | 2.05          |
| (1,355)  | 1:203:A:VAL:HG23 | 1:204:A:LYS:HD3  | 2        | 2.05          |
| (1,2634) | 1:198:A:PHE:HD1  | 1:203:A:VAL:HG11 | 12       | 2.04          |
| (1,2634) | 1:198:A:PHE:HD1  | 1:203:A:VAL:HG12 | 12       | 2.04          |
| (1,2634) | 1:198:A:PHE:HD1  | 1:203:A:VAL:HG13 | 12       | 2.04          |
| (1,2634) | 1:198:A:PHE:HD2  | 1:203:A:VAL:HG11 | 12       | 2.04          |
| (1,2634) | 1:198:A:PHE:HD2  | 1:203:A:VAL:HG12 | 12       | 2.04          |
| (1,2634) | 1:198:A:PHE:HD2  | 1:203:A:VAL:HG13 | 12       | 2.04          |
| (1,392)  | 1:122:A:VAL:HG11 | 1:190:A:THR:HB   | 18       | 2.04          |
| (1,392)  | 1:122:A:VAL:HG12 | 1:190:A:THR:HB   | 18       | 2.04          |
| (1,392)  | 1:122:A:VAL:HG13 | 1:190:A:THR:HB   | 18       | 2.04          |
| (1,356)  | 1:203:A:VAL:HG21 | 1:204:A:LYS:HG2  | 18       | 2.04          |
| (1,356)  | 1:203:A:VAL:HG22 | 1:204:A:LYS:HG2  | 18       | 2.04          |
| (1,356)  | 1:203:A:VAL:HG23 | 1:204:A:LYS:HG2  | 18       | 2.04          |
| (1,2682) | 1:141:A:PHE:HZ   | 1:209:A:VAL:HG11 | 17       | 2.03          |
| (1,2682) | 1:141:A:PHE:HZ   | 1:209:A:VAL:HG12 | 17       | 2.03          |
| (1,2682) | 1:141:A:PHE:HZ   | 1:209:A:VAL:HG13 | 17       | 2.03          |
| (1,1459) | 1:136:A:ARG:HB3  | 1:159:A:ASN:HB3  | 1        | 2.03          |
| (1,1459) | 1:136:A:ARG:HB3  | 1:159:A:ASN:HB3  | 12       | 2.03          |
| (1,377)  | 1:209:A:VAL:HG21 | 1:213:A:MET:HG2  | 8        | 2.03          |
| (1,377)  | 1:209:A:VAL:HG22 | 1:213:A:MET:HG2  | 8        | 2.03          |
| (1,377)  | 1:209:A:VAL:HG23 | 1:213:A:MET:HG2  | 8        | 2.03          |
| (1,58)   | 1:122:A:VAL:HG21 | 1:125:A:LEU:HD11 | 15       | 2.02          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,58)   | 1:122:A:VAL:HG21 | 1:125:A:LEU:HD12 | 15       | 2.02          |
| (1,58)   | 1:122:A:VAL:HG21 | 1:125:A:LEU:HD13 | 15       | 2.02          |
| (1,58)   | 1:122:A:VAL:HG22 | 1:125:A:LEU:HD11 | 15       | 2.02          |
| (1,58)   | 1:122:A:VAL:HG22 | 1:125:A:LEU:HD12 | 15       | 2.02          |
| (1,58)   | 1:122:A:VAL:HG22 | 1:125:A:LEU:HD13 | 15       | 2.02          |
| (1,58)   | 1:122:A:VAL:HG23 | 1:125:A:LEU:HD11 | 15       | 2.02          |
| (1,58)   | 1:122:A:VAL:HG23 | 1:125:A:LEU:HD12 | 15       | 2.02          |
| (1,58)   | 1:122:A:VAL:HG23 | 1:125:A:LEU:HD13 | 15       | 2.02          |
| (1,2825) | 1:176:A:VAL:HG21 | 1:218:A:TYR:HE1  | 12       | 2.0           |
| (1,2825) | 1:176:A:VAL:HG21 | 1:218:A:TYR:HE2  | 12       | 2.0           |
| (1,2825) | 1:176:A:VAL:HG22 | 1:218:A:TYR:HE1  | 12       | 2.0           |
| (1,2825) | 1:176:A:VAL:HG22 | 1:218:A:TYR:HE2  | 12       | 2.0           |
| (1,2825) | 1:176:A:VAL:HG23 | 1:218:A:TYR:HE1  | 12       | 2.0           |
| (1,2825) | 1:176:A:VAL:HG23 | 1:218:A:TYR:HE2  | 12       | 2.0           |
| (1,370)  | 1:158:A:PRO:HG2  | 1:209:A:VAL:HG21 | 20       | 2.0           |
| (1,370)  | 1:158:A:PRO:HG2  | 1:209:A:VAL:HG22 | 20       | 2.0           |
| (1,370)  | 1:158:A:PRO:HG2  | 1:209:A:VAL:HG23 | 20       | 2.0           |
| (1,1081) | 1:164:A:ARG:HD2  | 1:168:A:GLN:HG2  | 11       | 1.99          |
| (1,23)   | 1:220:A:LYS:HG2  | 1:221:A:GLU:HG3  | 5        | 1.99          |
| (1,428)  | 1:127:A:GLY:HA2  | 1:164:A:ARG:HD3  | 6        | 1.98          |
| (1,2682) | 1:141:A:PHE:HZ   | 1:209:A:VAL:HG11 | 18       | 1.97          |
| (1,2682) | 1:141:A:PHE:HZ   | 1:209:A:VAL:HG12 | 18       | 1.97          |
| (1,2682) | 1:141:A:PHE:HZ   | 1:209:A:VAL:HG13 | 18       | 1.97          |
| (1,355)  | 1:203:A:VAL:HG21 | 1:204:A:LYS:HD2  | 5        | 1.97          |
| (1,355)  | 1:203:A:VAL:HG21 | 1:204:A:LYS:HD3  | 5        | 1.97          |
| (1,355)  | 1:203:A:VAL:HG22 | 1:204:A:LYS:HD2  | 5        | 1.97          |
| (1,355)  | 1:203:A:VAL:HG22 | 1:204:A:LYS:HD3  | 5        | 1.97          |
| (1,355)  | 1:203:A:VAL:HG23 | 1:204:A:LYS:HD2  | 5        | 1.97          |
| (1,355)  | 1:203:A:VAL:HG23 | 1:204:A:LYS:HD3  | 5        | 1.97          |
| (1,1662) | 1:198:A:PHE:H    | 1:203:A:VAL:HG11 | 7        | 1.96          |
| (1,1662) | 1:198:A:PHE:H    | 1:203:A:VAL:HG12 | 7        | 1.96          |
| (1,1662) | 1:198:A:PHE:H    | 1:203:A:VAL:HG13 | 7        | 1.96          |
| (1,1081) | 1:164:A:ARG:HD2  | 1:168:A:GLN:HG2  | 2        | 1.96          |
| (1,377)  | 1:209:A:VAL:HG21 | 1:213:A:MET:HG2  | 11       | 1.95          |
| (1,377)  | 1:209:A:VAL:HG22 | 1:213:A:MET:HG2  | 11       | 1.95          |
| (1,377)  | 1:209:A:VAL:HG23 | 1:213:A:MET:HG2  | 11       | 1.95          |
| (1,258)  | 1:122:A:VAL:HG11 | 1:190:A:THR:HG21 | 9        | 1.95          |
| (1,258)  | 1:122:A:VAL:HG11 | 1:190:A:THR:HG22 | 9        | 1.95          |
| (1,258)  | 1:122:A:VAL:HG11 | 1:190:A:THR:HG23 | 9        | 1.95          |
| (1,258)  | 1:122:A:VAL:HG12 | 1:190:A:THR:HG21 | 9        | 1.95          |
| (1,258)  | 1:122:A:VAL:HG12 | 1:190:A:THR:HG22 | 9        | 1.95          |
| (1,258)  | 1:122:A:VAL:HG12 | 1:190:A:THR:HG23 | 9        | 1.95          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,258)  | 1:122:A:VAL:HG13 | 1:190:A:THR:HG21 | 9        | 1.95          |
| (1,258)  | 1:122:A:VAL:HG13 | 1:190:A:THR:HG22 | 9        | 1.95          |
| (1,258)  | 1:122:A:VAL:HG13 | 1:190:A:THR:HG23 | 9        | 1.95          |
| (1,2582) | 1:175:A:PHE:HE1  | 1:176:A:VAL:HG21 | 12       | 1.94          |
| (1,2582) | 1:175:A:PHE:HE1  | 1:176:A:VAL:HG22 | 12       | 1.94          |
| (1,2582) | 1:175:A:PHE:HE1  | 1:176:A:VAL:HG23 | 12       | 1.94          |
| (1,2582) | 1:175:A:PHE:HE2  | 1:176:A:VAL:HG21 | 12       | 1.94          |
| (1,2582) | 1:175:A:PHE:HE2  | 1:176:A:VAL:HG22 | 12       | 1.94          |
| (1,2582) | 1:175:A:PHE:HE2  | 1:176:A:VAL:HG23 | 12       | 1.94          |
| (1,2356) | 1:169:A:TYR:HB2  | 1:174:A:ASN:HD21 | 7        | 1.94          |
| (1,1)    | 1:138:A:MET:HG3  | 1:139:A:ILE:HG12 | 5        | 1.94          |
| (1,2623) | 1:156:A:ARG:HH21 | 1:198:A:PHE:HD1  | 18       | 1.93          |
| (1,2623) | 1:156:A:ARG:HH21 | 1:198:A:PHE:HD2  | 18       | 1.93          |
| (1,370)  | 1:158:A:PRO:HG2  | 1:209:A:VAL:HG21 | 13       | 1.93          |
| (1,370)  | 1:158:A:PRO:HG2  | 1:209:A:VAL:HG22 | 13       | 1.93          |
| (1,370)  | 1:158:A:PRO:HG2  | 1:209:A:VAL:HG23 | 13       | 1.93          |
| (1,377)  | 1:209:A:VAL:HG21 | 1:213:A:MET:HG2  | 7        | 1.92          |
| (1,377)  | 1:209:A:VAL:HG22 | 1:213:A:MET:HG2  | 7        | 1.92          |
| (1,377)  | 1:209:A:VAL:HG23 | 1:213:A:MET:HG2  | 7        | 1.92          |
| (1,356)  | 1:203:A:VAL:HG21 | 1:204:A:LYS:HG2  | 2        | 1.92          |
| (1,356)  | 1:203:A:VAL:HG22 | 1:204:A:LYS:HG2  | 2        | 1.92          |
| (1,356)  | 1:203:A:VAL:HG23 | 1:204:A:LYS:HG2  | 2        | 1.92          |
| (1,2491) | 1:150:A:TYR:HD1  | 1:209:A:VAL:HG11 | 14       | 1.91          |
| (1,2491) | 1:150:A:TYR:HD1  | 1:209:A:VAL:HG12 | 14       | 1.91          |
| (1,2491) | 1:150:A:TYR:HD1  | 1:209:A:VAL:HG13 | 14       | 1.91          |
| (1,2491) | 1:150:A:TYR:HD2  | 1:209:A:VAL:HG11 | 14       | 1.91          |
| (1,2491) | 1:150:A:TYR:HD2  | 1:209:A:VAL:HG12 | 14       | 1.91          |
| (1,2491) | 1:150:A:TYR:HD2  | 1:209:A:VAL:HG13 | 14       | 1.91          |
| (1,2491) | 1:150:A:TYR:HD1  | 1:209:A:VAL:HG11 | 16       | 1.91          |
| (1,2491) | 1:150:A:TYR:HD1  | 1:209:A:VAL:HG12 | 16       | 1.91          |
| (1,2491) | 1:150:A:TYR:HD1  | 1:209:A:VAL:HG13 | 16       | 1.91          |
| (1,2491) | 1:150:A:TYR:HD2  | 1:209:A:VAL:HG11 | 16       | 1.91          |
| (1,2491) | 1:150:A:TYR:HD2  | 1:209:A:VAL:HG12 | 16       | 1.91          |
| (1,2491) | 1:150:A:TYR:HD2  | 1:209:A:VAL:HG13 | 16       | 1.91          |
| (1,1283) | 1:206:A:MET:HG2  | 1:207:A:GLU:HG3  | 12       | 1.91          |
| (1,52)   | 1:176:A:VAL:HG21 | 1:217:A:GLN:HB3  | 12       | 1.91          |
| (1,52)   | 1:176:A:VAL:HG22 | 1:217:A:GLN:HB3  | 12       | 1.91          |
| (1,52)   | 1:176:A:VAL:HG23 | 1:217:A:GLN:HB3  | 12       | 1.91          |
| (1,1265) | 1:161:A:VAL:HG21 | 1:217:A:GLN:HG3  | 10       | 1.9           |
| (1,1265) | 1:161:A:VAL:HG22 | 1:217:A:GLN:HG3  | 10       | 1.9           |
| (1,1265) | 1:161:A:VAL:HG23 | 1:217:A:GLN:HG3  | 10       | 1.9           |
| (1,348)  | 1:122:A:VAL:HG21 | 1:124:A:GLY:HA2  | 18       | 1.9           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,348)  | 1:122:A:VAL:HG21 | 1:124:A:GLY:HA3  | 18       | 1.9           |
| (1,348)  | 1:122:A:VAL:HG22 | 1:124:A:GLY:HA2  | 18       | 1.9           |
| (1,348)  | 1:122:A:VAL:HG22 | 1:124:A:GLY:HA3  | 18       | 1.9           |
| (1,348)  | 1:122:A:VAL:HG23 | 1:124:A:GLY:HA2  | 18       | 1.9           |
| (1,348)  | 1:122:A:VAL:HG23 | 1:124:A:GLY:HA3  | 18       | 1.9           |
| (1,362)  | 1:172:A:GLN:HG3  | 1:215:A:VAL:HG21 | 13       | 1.89          |
| (1,362)  | 1:172:A:GLN:HG3  | 1:215:A:VAL:HG22 | 13       | 1.89          |
| (1,362)  | 1:172:A:GLN:HG3  | 1:215:A:VAL:HG23 | 13       | 1.89          |
| (1,429)  | 1:122:A:VAL:HG11 | 1:186:A:GLN:HA   | 9        | 1.88          |
| (1,429)  | 1:122:A:VAL:HG12 | 1:186:A:GLN:HA   | 9        | 1.88          |
| (1,429)  | 1:122:A:VAL:HG13 | 1:186:A:GLN:HA   | 9        | 1.88          |
| (1,1283) | 1:206:A:MET:HG2  | 1:207:A:GLU:HG3  | 10       | 1.87          |
| (1,1081) | 1:164:A:ARG:HD2  | 1:168:A:GLN:HG2  | 12       | 1.87          |
| (1,470)  | 1:122:A:VAL:HG21 | 1:125:A:LEU:HB2  | 1        | 1.87          |
| (1,470)  | 1:122:A:VAL:HG22 | 1:125:A:LEU:HB2  | 1        | 1.87          |
| (1,470)  | 1:122:A:VAL:HG23 | 1:125:A:LEU:HB2  | 1        | 1.87          |
| (1,370)  | 1:158:A:PRO:HG2  | 1:209:A:VAL:HG21 | 18       | 1.87          |
| (1,370)  | 1:158:A:PRO:HG2  | 1:209:A:VAL:HG22 | 18       | 1.87          |
| (1,370)  | 1:158:A:PRO:HG2  | 1:209:A:VAL:HG23 | 18       | 1.87          |
| (1,362)  | 1:172:A:GLN:HG3  | 1:215:A:VAL:HG21 | 2        | 1.87          |
| (1,362)  | 1:172:A:GLN:HG3  | 1:215:A:VAL:HG22 | 2        | 1.87          |
| (1,362)  | 1:172:A:GLN:HG3  | 1:215:A:VAL:HG23 | 2        | 1.87          |
| (1,470)  | 1:122:A:VAL:HG21 | 1:125:A:LEU:HB2  | 19       | 1.86          |
| (1,470)  | 1:122:A:VAL:HG22 | 1:125:A:LEU:HB2  | 19       | 1.86          |
| (1,470)  | 1:122:A:VAL:HG23 | 1:125:A:LEU:HB2  | 19       | 1.86          |
| (1,362)  | 1:172:A:GLN:HG3  | 1:215:A:VAL:HG21 | 19       | 1.86          |
| (1,362)  | 1:172:A:GLN:HG3  | 1:215:A:VAL:HG22 | 19       | 1.86          |
| (1,362)  | 1:172:A:GLN:HG3  | 1:215:A:VAL:HG23 | 19       | 1.86          |
| (1,23)   | 1:220:A:LYS:HG2  | 1:221:A:GLU:HG3  | 8        | 1.84          |
| (1,1)    | 1:138:A:MET:HG3  | 1:139:A:ILE:HG12 | 17       | 1.83          |
| (1,2491) | 1:150:A:TYR:HD1  | 1:209:A:VAL:HG11 | 13       | 1.82          |
| (1,2491) | 1:150:A:TYR:HD1  | 1:209:A:VAL:HG12 | 13       | 1.82          |
| (1,2491) | 1:150:A:TYR:HD1  | 1:209:A:VAL:HG13 | 13       | 1.82          |
| (1,2491) | 1:150:A:TYR:HD2  | 1:209:A:VAL:HG11 | 13       | 1.82          |
| (1,2491) | 1:150:A:TYR:HD2  | 1:209:A:VAL:HG12 | 13       | 1.82          |
| (1,2491) | 1:150:A:TYR:HD2  | 1:209:A:VAL:HG13 | 13       | 1.82          |
| (1,189)  | 1:123:A:GLY:HA2  | 1:125:A:LEU:HD21 | 14       | 1.82          |
| (1,189)  | 1:123:A:GLY:HA2  | 1:125:A:LEU:HD22 | 14       | 1.82          |
| (1,189)  | 1:123:A:GLY:HA2  | 1:125:A:LEU:HD23 | 14       | 1.82          |
| (1,189)  | 1:123:A:GLY:HA3  | 1:125:A:LEU:HD21 | 14       | 1.82          |
| (1,189)  | 1:123:A:GLY:HA3  | 1:125:A:LEU:HD22 | 14       | 1.82          |
| (1,189)  | 1:123:A:GLY:HA3  | 1:125:A:LEU:HD23 | 14       | 1.82          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,429)  | 1:122:A:VAL:HG11 | 1:186:A:GLN:HA   | 2        | 1.81          |
| (1,429)  | 1:122:A:VAL:HG12 | 1:186:A:GLN:HA   | 2        | 1.81          |
| (1,429)  | 1:122:A:VAL:HG13 | 1:186:A:GLN:HA   | 2        | 1.81          |
| (1,78)   | 1:139:A:ILE:HB   | 1:209:A:VAL:HG11 | 18       | 1.81          |
| (1,78)   | 1:139:A:ILE:HB   | 1:209:A:VAL:HG12 | 18       | 1.81          |
| (1,78)   | 1:139:A:ILE:HB   | 1:209:A:VAL:HG13 | 18       | 1.81          |
| (1,470)  | 1:122:A:VAL:HG21 | 1:125:A:LEU:HB2  | 12       | 1.8           |
| (1,470)  | 1:122:A:VAL:HG22 | 1:125:A:LEU:HB2  | 12       | 1.8           |
| (1,470)  | 1:122:A:VAL:HG23 | 1:125:A:LEU:HB2  | 12       | 1.8           |
| (1,58)   | 1:122:A:VAL:HG21 | 1:125:A:LEU:HD11 | 6        | 1.8           |
| (1,58)   | 1:122:A:VAL:HG21 | 1:125:A:LEU:HD12 | 6        | 1.8           |
| (1,58)   | 1:122:A:VAL:HG21 | 1:125:A:LEU:HD13 | 6        | 1.8           |
| (1,58)   | 1:122:A:VAL:HG22 | 1:125:A:LEU:HD11 | 6        | 1.8           |
| (1,58)   | 1:122:A:VAL:HG22 | 1:125:A:LEU:HD12 | 6        | 1.8           |
| (1,58)   | 1:122:A:VAL:HG22 | 1:125:A:LEU:HD13 | 6        | 1.8           |
| (1,58)   | 1:122:A:VAL:HG23 | 1:125:A:LEU:HD11 | 6        | 1.8           |
| (1,58)   | 1:122:A:VAL:HG23 | 1:125:A:LEU:HD12 | 6        | 1.8           |
| (1,58)   | 1:122:A:VAL:HG23 | 1:125:A:LEU:HD13 | 6        | 1.8           |
| (1,23)   | 1:220:A:LYS:HG2  | 1:221:A:GLU:HG3  | 17       | 1.8           |
| (1,2414) | 1:136:A:ARG:HB3  | 1:159:A:ASN:HD21 | 15       | 1.79          |
| (1,377)  | 1:209:A:VAL:HG21 | 1:213:A:MET:HG2  | 16       | 1.79          |
| (1,377)  | 1:209:A:VAL:HG22 | 1:213:A:MET:HG2  | 16       | 1.79          |
| (1,377)  | 1:209:A:VAL:HG23 | 1:213:A:MET:HG2  | 16       | 1.79          |
| (1,2851) | 1:184:A:ILE:HG13 | 1:187:A:HIS:HE1  | 8        | 1.78          |
| (1,2491) | 1:150:A:TYR:HD1  | 1:209:A:VAL:HG11 | 7        | 1.78          |
| (1,2491) | 1:150:A:TYR:HD1  | 1:209:A:VAL:HG12 | 7        | 1.78          |
| (1,2491) | 1:150:A:TYR:HD1  | 1:209:A:VAL:HG13 | 7        | 1.78          |
| (1,2491) | 1:150:A:TYR:HD2  | 1:209:A:VAL:HG11 | 7        | 1.78          |
| (1,2491) | 1:150:A:TYR:HD2  | 1:209:A:VAL:HG12 | 7        | 1.78          |
| (1,2491) | 1:150:A:TYR:HD2  | 1:209:A:VAL:HG13 | 7        | 1.78          |
| (1,2414) | 1:136:A:ARG:HB3  | 1:159:A:ASN:HD21 | 17       | 1.78          |
| (1,2407) | 1:136:A:ARG:HE   | 1:159:A:ASN:HB3  | 1        | 1.78          |
| (1,934)  | 1:166:A:VAL:HG11 | 1:221:A:GLU:HG2  | 3        | 1.78          |
| (1,934)  | 1:166:A:VAL:HG12 | 1:221:A:GLU:HG2  | 3        | 1.78          |
| (1,934)  | 1:166:A:VAL:HG13 | 1:221:A:GLU:HG2  | 3        | 1.78          |
| (1,362)  | 1:172:A:GLN:HG3  | 1:215:A:VAL:HG21 | 14       | 1.78          |
| (1,362)  | 1:172:A:GLN:HG3  | 1:215:A:VAL:HG22 | 14       | 1.78          |
| (1,362)  | 1:172:A:GLN:HG3  | 1:215:A:VAL:HG23 | 14       | 1.78          |
| (1,2491) | 1:150:A:TYR:HD1  | 1:209:A:VAL:HG11 | 8        | 1.77          |
| (1,2491) | 1:150:A:TYR:HD1  | 1:209:A:VAL:HG12 | 8        | 1.77          |
| (1,2491) | 1:150:A:TYR:HD1  | 1:209:A:VAL:HG13 | 8        | 1.77          |
| (1,2491) | 1:150:A:TYR:HD2  | 1:209:A:VAL:HG11 | 8        | 1.77          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2491) | 1:150:A:TYR:HD2  | 1:209:A:VAL:HG12 | 8        | 1.77          |
| (1,2491) | 1:150:A:TYR:HD2  | 1:209:A:VAL:HG13 | 8        | 1.77          |
| (1,2414) | 1:136:A:ARG:HB3  | 1:159:A:ASN:HD21 | 18       | 1.77          |
| (1,2354) | 1:170:A:SER:HB2  | 1:174:A:ASN:HD21 | 8        | 1.77          |
| (1,1344) | 1:206:A:MET:HB3  | 1:210:A:VAL:HB   | 19       | 1.77          |
| (1,599)  | 1:161:A:VAL:HG21 | 1:217:A:GLN:HG2  | 10       | 1.77          |
| (1,599)  | 1:161:A:VAL:HG22 | 1:217:A:GLN:HG2  | 10       | 1.77          |
| (1,599)  | 1:161:A:VAL:HG23 | 1:217:A:GLN:HG2  | 10       | 1.77          |
| (1,362)  | 1:172:A:GLN:HG3  | 1:215:A:VAL:HG21 | 8        | 1.77          |
| (1,362)  | 1:172:A:GLN:HG3  | 1:215:A:VAL:HG22 | 8        | 1.77          |
| (1,362)  | 1:172:A:GLN:HG3  | 1:215:A:VAL:HG23 | 8        | 1.77          |
| (1,357)  | 1:122:A:VAL:HG21 | 1:125:A:LEU:HG   | 19       | 1.77          |
| (1,357)  | 1:122:A:VAL:HG22 | 1:125:A:LEU:HG   | 19       | 1.77          |
| (1,357)  | 1:122:A:VAL:HG23 | 1:125:A:LEU:HG   | 19       | 1.77          |
| (1,2491) | 1:150:A:TYR:HD1  | 1:209:A:VAL:HG11 | 4        | 1.75          |
| (1,2491) | 1:150:A:TYR:HD1  | 1:209:A:VAL:HG12 | 4        | 1.75          |
| (1,2491) | 1:150:A:TYR:HD1  | 1:209:A:VAL:HG13 | 4        | 1.75          |
| (1,2491) | 1:150:A:TYR:HD2  | 1:209:A:VAL:HG11 | 4        | 1.75          |
| (1,2491) | 1:150:A:TYR:HD2  | 1:209:A:VAL:HG12 | 4        | 1.75          |
| (1,2491) | 1:150:A:TYR:HD2  | 1:209:A:VAL:HG13 | 4        | 1.75          |
| (1,2356) | 1:169:A:TYR:HB2  | 1:174:A:ASN:HD21 | 6        | 1.75          |
| (1,392)  | 1:122:A:VAL:HG11 | 1:190:A:THR:HB   | 9        | 1.75          |
| (1,392)  | 1:122:A:VAL:HG12 | 1:190:A:THR:HB   | 9        | 1.75          |
| (1,392)  | 1:122:A:VAL:HG13 | 1:190:A:THR:HB   | 9        | 1.75          |
| (1,356)  | 1:203:A:VAL:HG21 | 1:204:A:LYS:HG2  | 12       | 1.75          |
| (1,356)  | 1:203:A:VAL:HG22 | 1:204:A:LYS:HG2  | 12       | 1.75          |
| (1,356)  | 1:203:A:VAL:HG23 | 1:204:A:LYS:HG2  | 12       | 1.75          |
| (1,258)  | 1:122:A:VAL:HG11 | 1:190:A:THR:HG21 | 4        | 1.75          |
| (1,258)  | 1:122:A:VAL:HG11 | 1:190:A:THR:HG22 | 4        | 1.75          |
| (1,258)  | 1:122:A:VAL:HG11 | 1:190:A:THR:HG23 | 4        | 1.75          |
| (1,258)  | 1:122:A:VAL:HG12 | 1:190:A:THR:HG21 | 4        | 1.75          |
| (1,258)  | 1:122:A:VAL:HG12 | 1:190:A:THR:HG22 | 4        | 1.75          |
| (1,258)  | 1:122:A:VAL:HG12 | 1:190:A:THR:HG23 | 4        | 1.75          |
| (1,258)  | 1:122:A:VAL:HG13 | 1:190:A:THR:HG21 | 4        | 1.75          |
| (1,258)  | 1:122:A:VAL:HG13 | 1:190:A:THR:HG22 | 4        | 1.75          |
| (1,258)  | 1:122:A:VAL:HG13 | 1:190:A:THR:HG23 | 4        | 1.75          |
| (1,1283) | 1:206:A:MET:HG2  | 1:207:A:GLU:HG3  | 2        | 1.74          |
| (1,362)  | 1:172:A:GLN:HG3  | 1:215:A:VAL:HG21 | 4        | 1.74          |
| (1,362)  | 1:172:A:GLN:HG3  | 1:215:A:VAL:HG22 | 4        | 1.74          |
| (1,362)  | 1:172:A:GLN:HG3  | 1:215:A:VAL:HG23 | 4        | 1.74          |
| (1,356)  | 1:203:A:VAL:HG21 | 1:204:A:LYS:HG2  | 5        | 1.74          |
| (1,356)  | 1:203:A:VAL:HG22 | 1:204:A:LYS:HG2  | 5        | 1.74          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,356)  | 1:203:A:VAL:HG23 | 1:204:A:LYS:HG2  | 5        | 1.74          |
| (1,130)  | 1:161:A:VAL:HG11 | 1:210:A:VAL:H    | 10       | 1.74          |
| (1,130)  | 1:161:A:VAL:HG12 | 1:210:A:VAL:H    | 10       | 1.74          |
| (1,130)  | 1:161:A:VAL:HG13 | 1:210:A:VAL:H    | 10       | 1.74          |
| (1,23)   | 1:220:A:LYS:HG2  | 1:221:A:GLU:HG3  | 14       | 1.74          |
| (1,1344) | 1:206:A:MET:HB3  | 1:210:A:VAL:HB   | 15       | 1.73          |
| (1,1235) | 1:205:A:MET:HG3  | 1:206:A:MET:HG2  | 10       | 1.73          |
| (1,428)  | 1:127:A:GLY:HA2  | 1:164:A:ARG:HD3  | 17       | 1.73          |
| (1,392)  | 1:122:A:VAL:HG11 | 1:190:A:THR:HB   | 2        | 1.73          |
| (1,392)  | 1:122:A:VAL:HG12 | 1:190:A:THR:HB   | 2        | 1.73          |
| (1,392)  | 1:122:A:VAL:HG13 | 1:190:A:THR:HB   | 2        | 1.73          |
| (1,2421) | 1:127:A:GLY:H    | 1:164:A:ARG:HD3  | 12       | 1.72          |
| (1,1459) | 1:136:A:ARG:HB3  | 1:159:A:ASN:HB3  | 18       | 1.72          |
| (1,2374) | 1:168:A:GLN:HE22 | 1:169:A:TYR:HE1  | 18       | 1.71          |
| (1,2374) | 1:168:A:GLN:HE22 | 1:169:A:TYR:HE2  | 18       | 1.71          |
| (1,2374) | 1:168:A:GLN:HE22 | 1:169:A:TYR:HE1  | 20       | 1.71          |
| (1,2374) | 1:168:A:GLN:HE22 | 1:169:A:TYR:HE2  | 20       | 1.71          |
| (1,1344) | 1:206:A:MET:HB3  | 1:210:A:VAL:HB   | 4        | 1.71          |
| (1,1344) | 1:206:A:MET:HB3  | 1:210:A:VAL:HB   | 12       | 1.71          |
| (1,377)  | 1:209:A:VAL:HG21 | 1:213:A:MET:HG2  | 10       | 1.71          |
| (1,377)  | 1:209:A:VAL:HG22 | 1:213:A:MET:HG2  | 10       | 1.71          |
| (1,377)  | 1:209:A:VAL:HG23 | 1:213:A:MET:HG2  | 10       | 1.71          |
| (1,2414) | 1:136:A:ARG:HB3  | 1:159:A:ASN:HD21 | 19       | 1.7           |
| (1,1344) | 1:206:A:MET:HB3  | 1:210:A:VAL:HB   | 14       | 1.7           |
| (1,677)  | 1:135:A:SER:HB2  | 1:213:A:MET:HA   | 5        | 1.7           |
| (1,2491) | 1:150:A:TYR:HD1  | 1:209:A:VAL:HG11 | 11       | 1.69          |
| (1,2491) | 1:150:A:TYR:HD1  | 1:209:A:VAL:HG12 | 11       | 1.69          |
| (1,2491) | 1:150:A:TYR:HD1  | 1:209:A:VAL:HG13 | 11       | 1.69          |
| (1,2491) | 1:150:A:TYR:HD2  | 1:209:A:VAL:HG11 | 11       | 1.69          |
| (1,2491) | 1:150:A:TYR:HD2  | 1:209:A:VAL:HG12 | 11       | 1.69          |
| (1,2491) | 1:150:A:TYR:HD2  | 1:209:A:VAL:HG13 | 11       | 1.69          |
| (1,2374) | 1:168:A:GLN:HE22 | 1:169:A:TYR:HE1  | 13       | 1.69          |
| (1,2374) | 1:168:A:GLN:HE22 | 1:169:A:TYR:HE2  | 13       | 1.69          |
| (1,1081) | 1:164:A:ARG:HD2  | 1:168:A:GLN:HG2  | 17       | 1.69          |
| (1,220)  | 1:127:A:GLY:HA2  | 1:164:A:ARG:HE   | 3        | 1.69          |
| (1,23)   | 1:220:A:LYS:HG2  | 1:221:A:GLU:HG3  | 16       | 1.69          |
| (1,2421) | 1:127:A:GLY:H    | 1:164:A:ARG:HD3  | 18       | 1.68          |
| (1,2374) | 1:168:A:GLN:HE22 | 1:169:A:TYR:HE1  | 4        | 1.68          |
| (1,2374) | 1:168:A:GLN:HE22 | 1:169:A:TYR:HE2  | 4        | 1.68          |
| (1,2374) | 1:168:A:GLN:HE22 | 1:169:A:TYR:HE1  | 10       | 1.68          |
| (1,2374) | 1:168:A:GLN:HE22 | 1:169:A:TYR:HE2  | 10       | 1.68          |
| (1,1344) | 1:206:A:MET:HB3  | 1:210:A:VAL:HB   | 6        | 1.68          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1164) | 1:215:A:VAL:HG21 | 1:219:A:GLN:HG2  | 4        | 1.68          |
| (1,1164) | 1:215:A:VAL:HG22 | 1:219:A:GLN:HG2  | 4        | 1.68          |
| (1,1164) | 1:215:A:VAL:HG23 | 1:219:A:GLN:HG2  | 4        | 1.68          |
| (1,220)  | 1:127:A:GLY:HA2  | 1:164:A:ARG:HE   | 5        | 1.68          |
| (1,196)  | 1:161:A:VAL:HG21 | 1:216:A:THR:HG21 | 10       | 1.68          |
| (1,196)  | 1:161:A:VAL:HG21 | 1:216:A:THR:HG22 | 10       | 1.68          |
| (1,196)  | 1:161:A:VAL:HG21 | 1:216:A:THR:HG23 | 10       | 1.68          |
| (1,196)  | 1:161:A:VAL:HG22 | 1:216:A:THR:HG21 | 10       | 1.68          |
| (1,196)  | 1:161:A:VAL:HG22 | 1:216:A:THR:HG22 | 10       | 1.68          |
| (1,196)  | 1:161:A:VAL:HG22 | 1:216:A:THR:HG23 | 10       | 1.68          |
| (1,196)  | 1:161:A:VAL:HG23 | 1:216:A:THR:HG21 | 10       | 1.68          |
| (1,196)  | 1:161:A:VAL:HG23 | 1:216:A:THR:HG22 | 10       | 1.68          |
| (1,196)  | 1:161:A:VAL:HG23 | 1:216:A:THR:HG23 | 10       | 1.68          |
| (1,2491) | 1:150:A:TYR:HD1  | 1:209:A:VAL:HG11 | 1        | 1.67          |
| (1,2491) | 1:150:A:TYR:HD1  | 1:209:A:VAL:HG12 | 1        | 1.67          |
| (1,2491) | 1:150:A:TYR:HD1  | 1:209:A:VAL:HG13 | 1        | 1.67          |
| (1,2491) | 1:150:A:TYR:HD2  | 1:209:A:VAL:HG11 | 1        | 1.67          |
| (1,2491) | 1:150:A:TYR:HD2  | 1:209:A:VAL:HG12 | 1        | 1.67          |
| (1,2491) | 1:150:A:TYR:HD2  | 1:209:A:VAL:HG13 | 1        | 1.67          |
| (1,2414) | 1:136:A:ARG:HB3  | 1:159:A:ASN:HD21 | 11       | 1.67          |
| (1,1344) | 1:206:A:MET:HB3  | 1:210:A:VAL:HB   | 20       | 1.67          |
| (1,934)  | 1:166:A:VAL:HG11 | 1:221:A:GLU:HG2  | 17       | 1.67          |
| (1,934)  | 1:166:A:VAL:HG12 | 1:221:A:GLU:HG2  | 17       | 1.67          |
| (1,934)  | 1:166:A:VAL:HG13 | 1:221:A:GLU:HG2  | 17       | 1.67          |
| (1,2374) | 1:168:A:GLN:HE22 | 1:169:A:TYR:HE1  | 11       | 1.66          |
| (1,2374) | 1:168:A:GLN:HE22 | 1:169:A:TYR:HE2  | 11       | 1.66          |
| (1,220)  | 1:127:A:GLY:HA2  | 1:164:A:ARG:HE   | 7        | 1.66          |
| (1,2407) | 1:136:A:ARG:HE   | 1:159:A:ASN:HB3  | 19       | 1.65          |
| (1,2356) | 1:169:A:TYR:HB2  | 1:174:A:ASN:HD21 | 18       | 1.65          |
| (1,704)  | 1:209:A:VAL:HG21 | 1:213:A:MET:HE1  | 20       | 1.65          |
| (1,704)  | 1:209:A:VAL:HG21 | 1:213:A:MET:HE2  | 20       | 1.65          |
| (1,704)  | 1:209:A:VAL:HG21 | 1:213:A:MET:HE3  | 20       | 1.65          |
| (1,704)  | 1:209:A:VAL:HG22 | 1:213:A:MET:HE1  | 20       | 1.65          |
| (1,704)  | 1:209:A:VAL:HG22 | 1:213:A:MET:HE2  | 20       | 1.65          |
| (1,704)  | 1:209:A:VAL:HG22 | 1:213:A:MET:HE3  | 20       | 1.65          |
| (1,704)  | 1:209:A:VAL:HG23 | 1:213:A:MET:HE1  | 20       | 1.65          |
| (1,704)  | 1:209:A:VAL:HG23 | 1:213:A:MET:HE2  | 20       | 1.65          |
| (1,704)  | 1:209:A:VAL:HG23 | 1:213:A:MET:HE3  | 20       | 1.65          |
| (1,567)  | 1:230:A:ARG:HB2  | 1:231:A:SER:HB3  | 12       | 1.65          |
| (1,567)  | 1:230:A:ARG:HB2  | 1:231:A:SER:HB3  | 14       | 1.65          |
| (1,2374) | 1:168:A:GLN:HE22 | 1:169:A:TYR:HE1  | 5        | 1.64          |
| (1,2374) | 1:168:A:GLN:HE22 | 1:169:A:TYR:HE2  | 5        | 1.64          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2374) | 1:168:A:GLN:HE22 | 1:169:A:TYR:HE1  | 8        | 1.64          |
| (1,2374) | 1:168:A:GLN:HE22 | 1:169:A:TYR:HE2  | 8        | 1.64          |
| (1,2374) | 1:168:A:GLN:HE22 | 1:169:A:TYR:HE1  | 14       | 1.64          |
| (1,2374) | 1:168:A:GLN:HE22 | 1:169:A:TYR:HE2  | 14       | 1.64          |
| (1,1375) | 1:136:A:ARG:HD2  | 1:154:A:MET:HG3  | 17       | 1.64          |
| (1,1344) | 1:206:A:MET:HB3  | 1:210:A:VAL:HB   | 7        | 1.64          |
| (1,1125) | 1:198:A:PHE:HA   | 1:203:A:VAL:HG11 | 18       | 1.64          |
| (1,1125) | 1:198:A:PHE:HA   | 1:203:A:VAL:HG12 | 18       | 1.64          |
| (1,1125) | 1:198:A:PHE:HA   | 1:203:A:VAL:HG13 | 18       | 1.64          |
| (1,1344) | 1:206:A:MET:HB3  | 1:210:A:VAL:HB   | 1        | 1.63          |
| (1,1344) | 1:206:A:MET:HB3  | 1:210:A:VAL:HB   | 17       | 1.63          |
| (1,377)  | 1:209:A:VAL:HG21 | 1:213:A:MET:HG2  | 13       | 1.63          |
| (1,377)  | 1:209:A:VAL:HG22 | 1:213:A:MET:HG2  | 13       | 1.63          |
| (1,377)  | 1:209:A:VAL:HG23 | 1:213:A:MET:HG2  | 13       | 1.63          |
| (1,2587) | 1:176:A:VAL:HG21 | 1:218:A:TYR:HD1  | 12       | 1.62          |
| (1,2587) | 1:176:A:VAL:HG21 | 1:218:A:TYR:HD2  | 12       | 1.62          |
| (1,2587) | 1:176:A:VAL:HG22 | 1:218:A:TYR:HD1  | 12       | 1.62          |
| (1,2587) | 1:176:A:VAL:HG22 | 1:218:A:TYR:HD2  | 12       | 1.62          |
| (1,2587) | 1:176:A:VAL:HG23 | 1:218:A:TYR:HD1  | 12       | 1.62          |
| (1,2587) | 1:176:A:VAL:HG23 | 1:218:A:TYR:HD2  | 12       | 1.62          |
| (1,2483) | 1:161:A:VAL:HG21 | 1:163:A:TYR:HD1  | 10       | 1.62          |
| (1,2483) | 1:161:A:VAL:HG21 | 1:163:A:TYR:HD2  | 10       | 1.62          |
| (1,2483) | 1:161:A:VAL:HG22 | 1:163:A:TYR:HD1  | 10       | 1.62          |
| (1,2483) | 1:161:A:VAL:HG22 | 1:163:A:TYR:HD2  | 10       | 1.62          |
| (1,2483) | 1:161:A:VAL:HG23 | 1:163:A:TYR:HD1  | 10       | 1.62          |
| (1,2483) | 1:161:A:VAL:HG23 | 1:163:A:TYR:HD2  | 10       | 1.62          |
| (1,2374) | 1:168:A:GLN:HE22 | 1:169:A:TYR:HE1  | 17       | 1.62          |
| (1,2374) | 1:168:A:GLN:HE22 | 1:169:A:TYR:HE2  | 17       | 1.62          |
| (1,1480) | 1:203:A:VAL:HG21 | 1:207:A:GLU:HB2  | 2        | 1.62          |
| (1,1480) | 1:203:A:VAL:HG22 | 1:207:A:GLU:HB2  | 2        | 1.62          |
| (1,1480) | 1:203:A:VAL:HG23 | 1:207:A:GLU:HB2  | 2        | 1.62          |
| (1,1235) | 1:205:A:MET:HG3  | 1:206:A:MET:HG2  | 12       | 1.62          |
| (1,677)  | 1:135:A:SER:HB2  | 1:213:A:MET:HA   | 10       | 1.62          |
| (1,362)  | 1:172:A:GLN:HG3  | 1:215:A:VAL:HG21 | 12       | 1.62          |
| (1,362)  | 1:172:A:GLN:HG3  | 1:215:A:VAL:HG22 | 12       | 1.62          |
| (1,362)  | 1:172:A:GLN:HG3  | 1:215:A:VAL:HG23 | 12       | 1.62          |
| (1,189)  | 1:123:A:GLY:HA2  | 1:125:A:LEU:HD21 | 1        | 1.62          |
| (1,189)  | 1:123:A:GLY:HA2  | 1:125:A:LEU:HD22 | 1        | 1.62          |
| (1,189)  | 1:123:A:GLY:HA2  | 1:125:A:LEU:HD23 | 1        | 1.62          |
| (1,189)  | 1:123:A:GLY:HA3  | 1:125:A:LEU:HD21 | 1        | 1.62          |
| (1,189)  | 1:123:A:GLY:HA3  | 1:125:A:LEU:HD22 | 1        | 1.62          |
| (1,189)  | 1:123:A:GLY:HA3  | 1:125:A:LEU:HD23 | 1        | 1.62          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2482) | 1:163:A:TYR:HD1  | 1:221:A:GLU:HG2  | 20       | 1.61          |
| (1,2482) | 1:163:A:TYR:HD2  | 1:221:A:GLU:HG2  | 20       | 1.61          |
| (1,927)  | 1:212:A:GLN:HA   | 1:213:A:MET:HG2  | 6        | 1.61          |
| (1,23)   | 1:220:A:LYS:HG2  | 1:221:A:GLU:HG3  | 1        | 1.61          |
| (1,1344) | 1:206:A:MET:HB3  | 1:210:A:VAL:HB   | 18       | 1.6           |
| (1,704)  | 1:209:A:VAL:HG21 | 1:213:A:MET:HE1  | 14       | 1.6           |
| (1,704)  | 1:209:A:VAL:HG21 | 1:213:A:MET:HE2  | 14       | 1.6           |
| (1,704)  | 1:209:A:VAL:HG21 | 1:213:A:MET:HE3  | 14       | 1.6           |
| (1,704)  | 1:209:A:VAL:HG22 | 1:213:A:MET:HE1  | 14       | 1.6           |
| (1,704)  | 1:209:A:VAL:HG22 | 1:213:A:MET:HE2  | 14       | 1.6           |
| (1,704)  | 1:209:A:VAL:HG22 | 1:213:A:MET:HE3  | 14       | 1.6           |
| (1,704)  | 1:209:A:VAL:HG23 | 1:213:A:MET:HE1  | 14       | 1.6           |
| (1,704)  | 1:209:A:VAL:HG23 | 1:213:A:MET:HE2  | 14       | 1.6           |
| (1,704)  | 1:209:A:VAL:HG23 | 1:213:A:MET:HE3  | 14       | 1.6           |
| (1,23)   | 1:220:A:LYS:HG2  | 1:221:A:GLU:HG3  | 13       | 1.6           |
| (1,2421) | 1:127:A:GLY:H    | 1:164:A:ARG:HD3  | 10       | 1.59          |
| (1,2374) | 1:168:A:GLN:HE22 | 1:169:A:TYR:HE1  | 3        | 1.59          |
| (1,2374) | 1:168:A:GLN:HE22 | 1:169:A:TYR:HE2  | 3        | 1.59          |
| (1,2374) | 1:168:A:GLN:HE22 | 1:169:A:TYR:HE1  | 9        | 1.59          |
| (1,2374) | 1:168:A:GLN:HE22 | 1:169:A:TYR:HE2  | 9        | 1.59          |
| (1,1662) | 1:198:A:PHE:H    | 1:203:A:VAL:HG11 | 12       | 1.59          |
| (1,1662) | 1:198:A:PHE:H    | 1:203:A:VAL:HG12 | 12       | 1.59          |
| (1,1662) | 1:198:A:PHE:H    | 1:203:A:VAL:HG13 | 12       | 1.59          |
| (1,1344) | 1:206:A:MET:HB3  | 1:210:A:VAL:HB   | 8        | 1.59          |
| (1,927)  | 1:212:A:GLN:HA   | 1:213:A:MET:HG2  | 2        | 1.59          |
| (1,927)  | 1:212:A:GLN:HA   | 1:213:A:MET:HG2  | 3        | 1.59          |
| (1,927)  | 1:212:A:GLN:HA   | 1:213:A:MET:HG2  | 5        | 1.59          |
| (1,927)  | 1:212:A:GLN:HA   | 1:213:A:MET:HG2  | 11       | 1.59          |
| (1,927)  | 1:212:A:GLN:HA   | 1:213:A:MET:HG2  | 17       | 1.59          |
| (1,677)  | 1:135:A:SER:HB2  | 1:213:A:MET:HA   | 3        | 1.59          |
| (1,314)  | 1:166:A:VAL:HG21 | 1:169:A:TYR:HB3  | 1        | 1.59          |
| (1,314)  | 1:166:A:VAL:HG22 | 1:169:A:TYR:HB3  | 1        | 1.59          |
| (1,314)  | 1:166:A:VAL:HG23 | 1:169:A:TYR:HB3  | 1        | 1.59          |
| (1,78)   | 1:139:A:ILE:HB   | 1:209:A:VAL:HG11 | 10       | 1.59          |
| (1,78)   | 1:139:A:ILE:HB   | 1:209:A:VAL:HG12 | 10       | 1.59          |
| (1,78)   | 1:139:A:ILE:HB   | 1:209:A:VAL:HG13 | 10       | 1.59          |
| (1,2352) | 1:171:A:ASN:HA   | 1:174:A:ASN:HD21 | 2        | 1.58          |
| (1,2320) | 1:160:A:GLN:HE22 | 1:213:A:MET:HB2  | 16       | 1.58          |
| (1,983)  | 1:149:A:TYR:H    | 1:152:A:GLU:HG2  | 13       | 1.58          |
| (1,177)  | 1:195:A:GLY:HA3  | 1:197:A:ASN:HD21 | 6        | 1.58          |
| (1,159)  | 1:228:A:GLY:HA2  | 1:230:A:ARG:HD2  | 10       | 1.58          |
| (1,159)  | 1:228:A:GLY:HA3  | 1:230:A:ARG:HD2  | 10       | 1.58          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,927)  | 1:212:A:GLN:HA   | 1:213:A:MET:HG2  | 9        | 1.57          |
| (1,927)  | 1:212:A:GLN:HA   | 1:213:A:MET:HG2  | 18       | 1.57          |
| (1,23)   | 1:220:A:LYS:HG2  | 1:221:A:GLU:HG3  | 10       | 1.57          |
| (1,1662) | 1:198:A:PHE:H    | 1:203:A:VAL:HG11 | 5        | 1.56          |
| (1,1662) | 1:198:A:PHE:H    | 1:203:A:VAL:HG12 | 5        | 1.56          |
| (1,1662) | 1:198:A:PHE:H    | 1:203:A:VAL:HG13 | 5        | 1.56          |
| (1,927)  | 1:212:A:GLN:HA   | 1:213:A:MET:HG2  | 10       | 1.56          |
| (1,269)  | 1:165:A:PRO:HB3  | 1:166:A:VAL:HG11 | 17       | 1.56          |
| (1,269)  | 1:165:A:PRO:HB3  | 1:166:A:VAL:HG12 | 17       | 1.56          |
| (1,269)  | 1:165:A:PRO:HB3  | 1:166:A:VAL:HG13 | 17       | 1.56          |
| (1,160)  | 1:223:A:GLN:HE21 | 1:228:A:GLY:HA2  | 10       | 1.56          |
| (1,160)  | 1:223:A:GLN:HE21 | 1:228:A:GLY:HA3  | 10       | 1.56          |
| (1,2846) | 1:157:A:TYR:HE1  | 1:206:A:MET:HB2  | 3        | 1.55          |
| (1,2846) | 1:157:A:TYR:HE2  | 1:206:A:MET:HB2  | 3        | 1.55          |
| (1,2352) | 1:171:A:ASN:HA   | 1:174:A:ASN:HD21 | 3        | 1.55          |
| (1,2315) | 1:160:A:GLN:HE21 | 1:213:A:MET:HB2  | 7        | 1.55          |
| (1,983)  | 1:149:A:TYR:H    | 1:152:A:GLU:HG2  | 8        | 1.55          |
| (1,601)  | 1:166:A:VAL:HG21 | 1:170:A:SER:HB2  | 3        | 1.55          |
| (1,601)  | 1:166:A:VAL:HG22 | 1:170:A:SER:HB2  | 3        | 1.55          |
| (1,601)  | 1:166:A:VAL:HG23 | 1:170:A:SER:HB2  | 3        | 1.55          |
| (1,362)  | 1:172:A:GLN:HG3  | 1:215:A:VAL:HG21 | 6        | 1.55          |
| (1,362)  | 1:172:A:GLN:HG3  | 1:215:A:VAL:HG22 | 6        | 1.55          |
| (1,362)  | 1:172:A:GLN:HG3  | 1:215:A:VAL:HG23 | 6        | 1.55          |
| (1,173)  | 1:198:A:PHE:HB2  | 1:203:A:VAL:HG11 | 18       | 1.55          |
| (1,173)  | 1:198:A:PHE:HB2  | 1:203:A:VAL:HG12 | 18       | 1.55          |
| (1,173)  | 1:198:A:PHE:HB2  | 1:203:A:VAL:HG13 | 18       | 1.55          |
| (1,160)  | 1:223:A:GLN:HE21 | 1:228:A:GLY:HA2  | 5        | 1.55          |
| (1,160)  | 1:223:A:GLN:HE21 | 1:228:A:GLY:HA3  | 5        | 1.55          |
| (1,1459) | 1:136:A:ARG:HB3  | 1:159:A:ASN:HB3  | 17       | 1.54          |
| (1,78)   | 1:139:A:ILE:HB   | 1:209:A:VAL:HG11 | 14       | 1.54          |
| (1,78)   | 1:139:A:ILE:HB   | 1:209:A:VAL:HG12 | 14       | 1.54          |
| (1,78)   | 1:139:A:ILE:HB   | 1:209:A:VAL:HG13 | 14       | 1.54          |
| (1,23)   | 1:220:A:LYS:HG2  | 1:221:A:GLU:HG3  | 19       | 1.54          |
| (1,2414) | 1:136:A:ARG:HB3  | 1:159:A:ASN:HD21 | 1        | 1.53          |
| (1,2414) | 1:136:A:ARG:HB3  | 1:159:A:ASN:HD21 | 10       | 1.53          |
| (1,476)  | 1:203:A:VAL:HG21 | 1:204:A:LYS:HE2  | 8        | 1.53          |
| (1,476)  | 1:203:A:VAL:HG21 | 1:204:A:LYS:HE3  | 8        | 1.53          |
| (1,476)  | 1:203:A:VAL:HG22 | 1:204:A:LYS:HE2  | 8        | 1.53          |
| (1,476)  | 1:203:A:VAL:HG22 | 1:204:A:LYS:HE3  | 8        | 1.53          |
| (1,476)  | 1:203:A:VAL:HG23 | 1:204:A:LYS:HE2  | 8        | 1.53          |
| (1,476)  | 1:203:A:VAL:HG23 | 1:204:A:LYS:HE3  | 8        | 1.53          |
| (1,428)  | 1:127:A:GLY:HA2  | 1:164:A:ARG:HD3  | 16       | 1.53          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2374) | 1:168:A:GLN:HE22 | 1:169:A:TYR:HE1  | 1        | 1.52          |
| (1,2374) | 1:168:A:GLN:HE22 | 1:169:A:TYR:HE2  | 1        | 1.52          |
| (1,1125) | 1:198:A:PHE:HA   | 1:203:A:VAL:HG11 | 8        | 1.52          |
| (1,1125) | 1:198:A:PHE:HA   | 1:203:A:VAL:HG12 | 8        | 1.52          |
| (1,1125) | 1:198:A:PHE:HA   | 1:203:A:VAL:HG13 | 8        | 1.52          |
| (1,596)  | 1:131:A:GLY:HA3  | 1:161:A:VAL:HG21 | 10       | 1.52          |
| (1,596)  | 1:131:A:GLY:HA3  | 1:161:A:VAL:HG22 | 10       | 1.52          |
| (1,596)  | 1:131:A:GLY:HA3  | 1:161:A:VAL:HG23 | 10       | 1.52          |
| (1,89)   | 1:206:A:MET:HB3  | 1:210:A:VAL:HG21 | 20       | 1.52          |
| (1,89)   | 1:206:A:MET:HB3  | 1:210:A:VAL:HG22 | 20       | 1.52          |
| (1,89)   | 1:206:A:MET:HB3  | 1:210:A:VAL:HG23 | 20       | 1.52          |
| (1,2315) | 1:160:A:GLN:HE21 | 1:213:A:MET:HB2  | 12       | 1.51          |
| (1,1283) | 1:206:A:MET:HG2  | 1:207:A:GLU:HG3  | 19       | 1.51          |
| (1,220)  | 1:127:A:GLY:HA2  | 1:164:A:ARG:HE   | 19       | 1.51          |
| (1,78)   | 1:139:A:ILE:HB   | 1:209:A:VAL:HG11 | 13       | 1.51          |
| (1,78)   | 1:139:A:ILE:HB   | 1:209:A:VAL:HG12 | 13       | 1.51          |
| (1,78)   | 1:139:A:ILE:HB   | 1:209:A:VAL:HG13 | 13       | 1.51          |
| (1,2421) | 1:127:A:GLY:H    | 1:164:A:ARG:HD3  | 11       | 1.5           |
| (1,1459) | 1:136:A:ARG:HB3  | 1:159:A:ASN:HB3  | 15       | 1.5           |
| (1,1283) | 1:206:A:MET:HG2  | 1:207:A:GLU:HG3  | 17       | 1.5           |
| (1,220)  | 1:127:A:GLY:HA2  | 1:164:A:ARG:HE   | 14       | 1.5           |
| (1,2571) | 1:215:A:VAL:HG21 | 1:218:A:TYR:HD1  | 17       | 1.49          |
| (1,2571) | 1:215:A:VAL:HG21 | 1:218:A:TYR:HD2  | 17       | 1.49          |
| (1,2571) | 1:215:A:VAL:HG22 | 1:218:A:TYR:HD1  | 17       | 1.49          |
| (1,2571) | 1:215:A:VAL:HG22 | 1:218:A:TYR:HD2  | 17       | 1.49          |
| (1,2571) | 1:215:A:VAL:HG23 | 1:218:A:TYR:HD1  | 17       | 1.49          |
| (1,2571) | 1:215:A:VAL:HG23 | 1:218:A:TYR:HD2  | 17       | 1.49          |
| (1,2482) | 1:163:A:TYR:HD1  | 1:221:A:GLU:HG2  | 3        | 1.49          |
| (1,2482) | 1:163:A:TYR:HD2  | 1:221:A:GLU:HG2  | 3        | 1.49          |
| (1,2421) | 1:127:A:GLY:H    | 1:164:A:ARG:HD3  | 9        | 1.49          |
| (1,2407) | 1:136:A:ARG:HE   | 1:159:A:ASN:HB3  | 10       | 1.49          |
| (1,1235) | 1:205:A:MET:HG3  | 1:206:A:MET:HG2  | 6        | 1.49          |
| (1,1125) | 1:198:A:PHE:HA   | 1:203:A:VAL:HG11 | 2        | 1.49          |
| (1,1125) | 1:198:A:PHE:HA   | 1:203:A:VAL:HG12 | 2        | 1.49          |
| (1,1125) | 1:198:A:PHE:HA   | 1:203:A:VAL:HG13 | 2        | 1.49          |
| (1,160)  | 1:223:A:GLN:HE21 | 1:228:A:GLY:HA2  | 8        | 1.49          |
| (1,160)  | 1:223:A:GLN:HE21 | 1:228:A:GLY:HA3  | 8        | 1.49          |
| (1,2491) | 1:150:A:TYR:HD1  | 1:209:A:VAL:HG11 | 12       | 1.48          |
| (1,2491) | 1:150:A:TYR:HD1  | 1:209:A:VAL:HG12 | 12       | 1.48          |
| (1,2491) | 1:150:A:TYR:HD1  | 1:209:A:VAL:HG13 | 12       | 1.48          |
| (1,2491) | 1:150:A:TYR:HD2  | 1:209:A:VAL:HG11 | 12       | 1.48          |
| (1,2491) | 1:150:A:TYR:HD2  | 1:209:A:VAL:HG12 | 12       | 1.48          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2491) | 1:150:A:TYR:HD2  | 1:209:A:VAL:HG13 | 12       | 1.48          |
| (1,2374) | 1:168:A:GLN:HE22 | 1:169:A:TYR:HE1  | 2        | 1.48          |
| (1,2374) | 1:168:A:GLN:HE22 | 1:169:A:TYR:HE2  | 2        | 1.48          |
| (1,1256) | 1:184:A:ILE:HG13 | 1:206:A:MET:HG3  | 2        | 1.48          |
| (1,1256) | 1:184:A:ILE:HG13 | 1:206:A:MET:HG3  | 6        | 1.48          |
| (1,258)  | 1:122:A:VAL:HG11 | 1:190:A:THR:HG21 | 6        | 1.48          |
| (1,258)  | 1:122:A:VAL:HG11 | 1:190:A:THR:HG22 | 6        | 1.48          |
| (1,258)  | 1:122:A:VAL:HG11 | 1:190:A:THR:HG23 | 6        | 1.48          |
| (1,258)  | 1:122:A:VAL:HG12 | 1:190:A:THR:HG21 | 6        | 1.48          |
| (1,258)  | 1:122:A:VAL:HG12 | 1:190:A:THR:HG22 | 6        | 1.48          |
| (1,258)  | 1:122:A:VAL:HG12 | 1:190:A:THR:HG23 | 6        | 1.48          |
| (1,258)  | 1:122:A:VAL:HG13 | 1:190:A:THR:HG21 | 6        | 1.48          |
| (1,258)  | 1:122:A:VAL:HG13 | 1:190:A:THR:HG22 | 6        | 1.48          |
| (1,258)  | 1:122:A:VAL:HG13 | 1:190:A:THR:HG23 | 6        | 1.48          |
| (1,2851) | 1:184:A:ILE:HG13 | 1:187:A:HIS:HE1  | 10       | 1.47          |
| (1,2354) | 1:170:A:SER:HB2  | 1:174:A:ASN:HD21 | 18       | 1.47          |
| (1,1344) | 1:206:A:MET:HB3  | 1:210:A:VAL:HB   | 2        | 1.47          |
| (1,927)  | 1:212:A:GLN:HA   | 1:213:A:MET:HG2  | 8        | 1.47          |
| (1,396)  | 1:210:A:VAL:HA   | 1:213:A:MET:HB3  | 13       | 1.47          |
| (1,160)  | 1:223:A:GLN:HE21 | 1:228:A:GLY:HA2  | 7        | 1.47          |
| (1,160)  | 1:223:A:GLN:HE21 | 1:228:A:GLY:HA3  | 7        | 1.47          |
| (1,78)   | 1:139:A:ILE:HB   | 1:209:A:VAL:HG11 | 11       | 1.47          |
| (1,78)   | 1:139:A:ILE:HB   | 1:209:A:VAL:HG12 | 11       | 1.47          |
| (1,78)   | 1:139:A:ILE:HB   | 1:209:A:VAL:HG13 | 11       | 1.47          |
| (1,2482) | 1:163:A:TYR:HD1  | 1:221:A:GLU:HG2  | 13       | 1.46          |
| (1,2482) | 1:163:A:TYR:HD2  | 1:221:A:GLU:HG2  | 13       | 1.46          |
| (1,1344) | 1:206:A:MET:HB3  | 1:210:A:VAL:HB   | 10       | 1.46          |
| (1,927)  | 1:212:A:GLN:HA   | 1:213:A:MET:HG2  | 4        | 1.46          |
| (1,927)  | 1:212:A:GLN:HA   | 1:213:A:MET:HG2  | 13       | 1.46          |
| (1,927)  | 1:212:A:GLN:HA   | 1:213:A:MET:HG2  | 14       | 1.46          |
| (1,927)  | 1:212:A:GLN:HA   | 1:213:A:MET:HG2  | 20       | 1.46          |
| (1,159)  | 1:228:A:GLY:HA2  | 1:230:A:ARG:HD2  | 9        | 1.46          |
| (1,159)  | 1:228:A:GLY:HA3  | 1:230:A:ARG:HD2  | 9        | 1.46          |
| (1,159)  | 1:228:A:GLY:HA2  | 1:230:A:ARG:HD2  | 14       | 1.46          |
| (1,159)  | 1:228:A:GLY:HA3  | 1:230:A:ARG:HD2  | 14       | 1.46          |
| (1,158)  | 1:126:A:GLY:HA2  | 1:164:A:ARG:HD3  | 12       | 1.46          |
| (1,1912) | 1:213:A:MET:H    | 1:215:A:VAL:HG11 | 19       | 1.45          |
| (1,1912) | 1:213:A:MET:H    | 1:215:A:VAL:HG12 | 19       | 1.45          |
| (1,1912) | 1:213:A:MET:H    | 1:215:A:VAL:HG13 | 19       | 1.45          |
| (1,1125) | 1:198:A:PHE:HA   | 1:203:A:VAL:HG11 | 5        | 1.45          |
| (1,1125) | 1:198:A:PHE:HA   | 1:203:A:VAL:HG12 | 5        | 1.45          |
| (1,1125) | 1:198:A:PHE:HA   | 1:203:A:VAL:HG13 | 5        | 1.45          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,677)  | 1:135:A:SER:HB2  | 1:213:A:MET:HA   | 14       | 1.45          |
| (1,358)  | 1:203:A:VAL:HG21 | 1:204:A:LYS:HG3  | 18       | 1.45          |
| (1,358)  | 1:203:A:VAL:HG22 | 1:204:A:LYS:HG3  | 18       | 1.45          |
| (1,358)  | 1:203:A:VAL:HG23 | 1:204:A:LYS:HG3  | 18       | 1.45          |
| (1,314)  | 1:166:A:VAL:HG21 | 1:169:A:TYR:HB3  | 17       | 1.45          |
| (1,314)  | 1:166:A:VAL:HG22 | 1:169:A:TYR:HB3  | 17       | 1.45          |
| (1,314)  | 1:166:A:VAL:HG23 | 1:169:A:TYR:HB3  | 17       | 1.45          |
| (1,158)  | 1:126:A:GLY:HA2  | 1:164:A:ARG:HD3  | 18       | 1.45          |
| (1,89)   | 1:206:A:MET:HB3  | 1:210:A:VAL:HG21 | 14       | 1.45          |
| (1,89)   | 1:206:A:MET:HB3  | 1:210:A:VAL:HG22 | 14       | 1.45          |
| (1,89)   | 1:206:A:MET:HB3  | 1:210:A:VAL:HG23 | 14       | 1.45          |
| (1,78)   | 1:139:A:ILE:HB   | 1:209:A:VAL:HG11 | 8        | 1.45          |
| (1,78)   | 1:139:A:ILE:HB   | 1:209:A:VAL:HG12 | 8        | 1.45          |
| (1,78)   | 1:139:A:ILE:HB   | 1:209:A:VAL:HG13 | 8        | 1.45          |
| (1,23)   | 1:220:A:LYS:HG2  | 1:221:A:GLU:HG3  | 2        | 1.45          |
| (1,2177) | 1:212:A:GLN:H    | 1:213:A:MET:HG2  | 6        | 1.44          |
| (1,1912) | 1:213:A:MET:H    | 1:215:A:VAL:HG11 | 6        | 1.44          |
| (1,1912) | 1:213:A:MET:H    | 1:215:A:VAL:HG12 | 6        | 1.44          |
| (1,1912) | 1:213:A:MET:H    | 1:215:A:VAL:HG13 | 6        | 1.44          |
| (1,1689) | 1:134:A:MET:H    | 1:159:A:ASN:HB2  | 4        | 1.44          |
| (1,1283) | 1:206:A:MET:HG2  | 1:207:A:GLU:HG3  | 18       | 1.44          |
| (1,1164) | 1:215:A:VAL:HG21 | 1:219:A:GLN:HG2  | 14       | 1.44          |
| (1,1164) | 1:215:A:VAL:HG22 | 1:219:A:GLN:HG2  | 14       | 1.44          |
| (1,1164) | 1:215:A:VAL:HG23 | 1:219:A:GLN:HG2  | 14       | 1.44          |
| (1,1131) | 1:223:A:GLN:HG2  | 1:226:A:TYR:H    | 14       | 1.44          |
| (1,322)  | 1:158:A:PRO:HD3  | 1:209:A:VAL:HG21 | 17       | 1.44          |
| (1,322)  | 1:158:A:PRO:HD3  | 1:209:A:VAL:HG22 | 17       | 1.44          |
| (1,322)  | 1:158:A:PRO:HD3  | 1:209:A:VAL:HG23 | 17       | 1.44          |
| (1,89)   | 1:206:A:MET:HB3  | 1:210:A:VAL:HG21 | 7        | 1.44          |
| (1,89)   | 1:206:A:MET:HB3  | 1:210:A:VAL:HG22 | 7        | 1.44          |
| (1,89)   | 1:206:A:MET:HB3  | 1:210:A:VAL:HG23 | 7        | 1.44          |
| (1,2491) | 1:150:A:TYR:HD1  | 1:209:A:VAL:HG11 | 17       | 1.43          |
| (1,2491) | 1:150:A:TYR:HD1  | 1:209:A:VAL:HG12 | 17       | 1.43          |
| (1,2491) | 1:150:A:TYR:HD1  | 1:209:A:VAL:HG13 | 17       | 1.43          |
| (1,2491) | 1:150:A:TYR:HD2  | 1:209:A:VAL:HG11 | 17       | 1.43          |
| (1,2491) | 1:150:A:TYR:HD2  | 1:209:A:VAL:HG12 | 17       | 1.43          |
| (1,2491) | 1:150:A:TYR:HD2  | 1:209:A:VAL:HG13 | 17       | 1.43          |
| (1,2491) | 1:150:A:TYR:HD1  | 1:209:A:VAL:HG11 | 19       | 1.43          |
| (1,2491) | 1:150:A:TYR:HD1  | 1:209:A:VAL:HG12 | 19       | 1.43          |
| (1,2491) | 1:150:A:TYR:HD1  | 1:209:A:VAL:HG13 | 19       | 1.43          |
| (1,2491) | 1:150:A:TYR:HD2  | 1:209:A:VAL:HG11 | 19       | 1.43          |
| (1,2491) | 1:150:A:TYR:HD2  | 1:209:A:VAL:HG12 | 19       | 1.43          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2491) | 1:150:A:TYR:HD2  | 1:209:A:VAL:HG13 | 19       | 1.43          |
| (1,2374) | 1:168:A:GLN:HE22 | 1:169:A:TYR:HE1  | 16       | 1.43          |
| (1,2374) | 1:168:A:GLN:HE22 | 1:169:A:TYR:HE2  | 16       | 1.43          |
| (1,2354) | 1:170:A:SER:HB2  | 1:174:A:ASN:HD21 | 2        | 1.43          |
| (1,927)  | 1:212:A:GLN:HA   | 1:213:A:MET:HG2  | 16       | 1.43          |
| (1,704)  | 1:209:A:VAL:HG21 | 1:213:A:MET:HE1  | 11       | 1.43          |
| (1,704)  | 1:209:A:VAL:HG21 | 1:213:A:MET:HE2  | 11       | 1.43          |
| (1,704)  | 1:209:A:VAL:HG21 | 1:213:A:MET:HE3  | 11       | 1.43          |
| (1,704)  | 1:209:A:VAL:HG22 | 1:213:A:MET:HE1  | 11       | 1.43          |
| (1,704)  | 1:209:A:VAL:HG22 | 1:213:A:MET:HE2  | 11       | 1.43          |
| (1,704)  | 1:209:A:VAL:HG22 | 1:213:A:MET:HE3  | 11       | 1.43          |
| (1,704)  | 1:209:A:VAL:HG23 | 1:213:A:MET:HE1  | 11       | 1.43          |
| (1,704)  | 1:209:A:VAL:HG23 | 1:213:A:MET:HE2  | 11       | 1.43          |
| (1,704)  | 1:209:A:VAL:HG23 | 1:213:A:MET:HE3  | 11       | 1.43          |
| (1,437)  | 1:229:A:ARG:HB3  | 1:230:A:ARG:HD3  | 3        | 1.43          |
| (1,437)  | 1:229:A:ARG:HB2  | 1:230:A:ARG:HD3  | 3        | 1.43          |
| (1,315)  | 1:166:A:VAL:HG11 | 1:221:A:GLU:HB2  | 12       | 1.43          |
| (1,315)  | 1:166:A:VAL:HG12 | 1:221:A:GLU:HB2  | 12       | 1.43          |
| (1,315)  | 1:166:A:VAL:HG13 | 1:221:A:GLU:HB2  | 12       | 1.43          |
| (1,2315) | 1:160:A:GLN:HE21 | 1:213:A:MET:HB2  | 18       | 1.42          |
| (1,1283) | 1:206:A:MET:HG2  | 1:207:A:GLU:HG3  | 9        | 1.42          |
| (1,1081) | 1:164:A:ARG:HD2  | 1:168:A:GLN:HG2  | 4        | 1.42          |
| (1,1081) | 1:164:A:ARG:HD2  | 1:168:A:GLN:HG2  | 14       | 1.42          |
| (1,437)  | 1:229:A:ARG:HB3  | 1:230:A:ARG:HD3  | 4        | 1.42          |
| (1,437)  | 1:229:A:ARG:HB2  | 1:230:A:ARG:HD3  | 4        | 1.42          |
| (1,348)  | 1:122:A:VAL:HG21 | 1:124:A:GLY:HA2  | 16       | 1.42          |
| (1,348)  | 1:122:A:VAL:HG21 | 1:124:A:GLY:HA3  | 16       | 1.42          |
| (1,348)  | 1:122:A:VAL:HG22 | 1:124:A:GLY:HA2  | 16       | 1.42          |
| (1,348)  | 1:122:A:VAL:HG22 | 1:124:A:GLY:HA3  | 16       | 1.42          |
| (1,348)  | 1:122:A:VAL:HG23 | 1:124:A:GLY:HA2  | 16       | 1.42          |
| (1,348)  | 1:122:A:VAL:HG23 | 1:124:A:GLY:HA3  | 16       | 1.42          |
| (1,2421) | 1:127:A:GLY:H    | 1:164:A:ARG:HD3  | 2        | 1.41          |
| (1,2315) | 1:160:A:GLN:HE21 | 1:213:A:MET:HB2  | 1        | 1.41          |
| (1,1679) | 1:122:A:VAL:HG21 | 1:125:A:LEU:H    | 19       | 1.41          |
| (1,1679) | 1:122:A:VAL:HG22 | 1:125:A:LEU:H    | 19       | 1.41          |
| (1,1679) | 1:122:A:VAL:HG23 | 1:125:A:LEU:H    | 19       | 1.41          |
| (1,1131) | 1:223:A:GLN:HG2  | 1:226:A:TYR:H    | 16       | 1.41          |
| (1,921)  | 1:167:A:SER:HA   | 1:168:A:GLN:HG3  | 14       | 1.41          |
| (1,370)  | 1:158:A:PRO:HG2  | 1:209:A:VAL:HG21 | 10       | 1.41          |
| (1,370)  | 1:158:A:PRO:HG2  | 1:209:A:VAL:HG22 | 10       | 1.41          |
| (1,370)  | 1:158:A:PRO:HG2  | 1:209:A:VAL:HG23 | 10       | 1.41          |
| (1,2846) | 1:157:A:TYR:HE1  | 1:206:A:MET:HB2  | 1        | 1.4           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2846) | 1:157:A:TYR:HE2  | 1:206:A:MET:HB2  | 1        | 1.4           |
| (1,2559) | 1:128:A:TYR:HD1  | 1:164:A:ARG:HD3  | 18       | 1.4           |
| (1,2559) | 1:128:A:TYR:HD2  | 1:164:A:ARG:HD3  | 18       | 1.4           |
| (1,1689) | 1:134:A:MET:H    | 1:159:A:ASN:HB2  | 19       | 1.4           |
| (1,602)  | 1:230:A:ARG:H    | 1:231:A:SER:HB3  | 2        | 1.4           |
| (1,396)  | 1:210:A:VAL:HA   | 1:213:A:MET:HB3  | 14       | 1.4           |
| (1,311)  | 1:201:A:THR:HA   | 1:203:A:VAL:HG21 | 12       | 1.4           |
| (1,311)  | 1:201:A:THR:HA   | 1:203:A:VAL:HG22 | 12       | 1.4           |
| (1,311)  | 1:201:A:THR:HA   | 1:203:A:VAL:HG23 | 12       | 1.4           |
| (1,269)  | 1:165:A:PRO:HB3  | 1:166:A:VAL:HG11 | 12       | 1.4           |
| (1,269)  | 1:165:A:PRO:HB3  | 1:166:A:VAL:HG12 | 12       | 1.4           |
| (1,269)  | 1:165:A:PRO:HB3  | 1:166:A:VAL:HG13 | 12       | 1.4           |
| (1,158)  | 1:126:A:GLY:HA2  | 1:164:A:ARG:HD3  | 10       | 1.4           |
| (1,58)   | 1:122:A:VAL:HG21 | 1:125:A:LEU:HD11 | 8        | 1.4           |
| (1,58)   | 1:122:A:VAL:HG21 | 1:125:A:LEU:HD12 | 8        | 1.4           |
| (1,58)   | 1:122:A:VAL:HG21 | 1:125:A:LEU:HD13 | 8        | 1.4           |
| (1,58)   | 1:122:A:VAL:HG22 | 1:125:A:LEU:HD11 | 8        | 1.4           |
| (1,58)   | 1:122:A:VAL:HG22 | 1:125:A:LEU:HD12 | 8        | 1.4           |
| (1,58)   | 1:122:A:VAL:HG22 | 1:125:A:LEU:HD13 | 8        | 1.4           |
| (1,58)   | 1:122:A:VAL:HG23 | 1:125:A:LEU:HD11 | 8        | 1.4           |
| (1,58)   | 1:122:A:VAL:HG23 | 1:125:A:LEU:HD12 | 8        | 1.4           |
| (1,58)   | 1:122:A:VAL:HG23 | 1:125:A:LEU:HD13 | 8        | 1.4           |
| (1,2315) | 1:160:A:GLN:HE21 | 1:213:A:MET:HB2  | 3        | 1.39          |
| (1,1344) | 1:206:A:MET:HB3  | 1:210:A:VAL:HB   | 11       | 1.39          |
| (1,927)  | 1:212:A:GLN:HA   | 1:213:A:MET:HG2  | 19       | 1.39          |
| (1,704)  | 1:209:A:VAL:HG21 | 1:213:A:MET:HE1  | 13       | 1.39          |
| (1,704)  | 1:209:A:VAL:HG21 | 1:213:A:MET:HE2  | 13       | 1.39          |
| (1,704)  | 1:209:A:VAL:HG21 | 1:213:A:MET:HE3  | 13       | 1.39          |
| (1,704)  | 1:209:A:VAL:HG22 | 1:213:A:MET:HE1  | 13       | 1.39          |
| (1,704)  | 1:209:A:VAL:HG22 | 1:213:A:MET:HE2  | 13       | 1.39          |
| (1,704)  | 1:209:A:VAL:HG22 | 1:213:A:MET:HE3  | 13       | 1.39          |
| (1,704)  | 1:209:A:VAL:HG23 | 1:213:A:MET:HE1  | 13       | 1.39          |
| (1,704)  | 1:209:A:VAL:HG23 | 1:213:A:MET:HE2  | 13       | 1.39          |
| (1,704)  | 1:209:A:VAL:HG23 | 1:213:A:MET:HE3  | 13       | 1.39          |
| (1,429)  | 1:122:A:VAL:HG11 | 1:186:A:GLN:HA   | 4        | 1.39          |
| (1,429)  | 1:122:A:VAL:HG12 | 1:186:A:GLN:HA   | 4        | 1.39          |
| (1,429)  | 1:122:A:VAL:HG13 | 1:186:A:GLN:HA   | 4        | 1.39          |
| (1,269)  | 1:165:A:PRO:HB3  | 1:166:A:VAL:HG11 | 3        | 1.39          |
| (1,269)  | 1:165:A:PRO:HB3  | 1:166:A:VAL:HG12 | 3        | 1.39          |
| (1,269)  | 1:165:A:PRO:HB3  | 1:166:A:VAL:HG13 | 3        | 1.39          |
| (1,158)  | 1:126:A:GLY:HA2  | 1:164:A:ARG:HD3  | 2        | 1.39          |
| (1,78)   | 1:139:A:ILE:HB   | 1:209:A:VAL:HG11 | 4        | 1.39          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,78)   | 1:139:A:ILE:HB   | 1:209:A:VAL:HG12 | 4        | 1.39          |
| (1,78)   | 1:139:A:ILE:HB   | 1:209:A:VAL:HG13 | 4        | 1.39          |
| (1,2794) | 1:128:A:TYR:HE1  | 1:164:A:ARG:HG2  | 18       | 1.38          |
| (1,2794) | 1:128:A:TYR:HE2  | 1:164:A:ARG:HG2  | 18       | 1.38          |
| (1,2491) | 1:150:A:TYR:HD1  | 1:209:A:VAL:HG11 | 20       | 1.38          |
| (1,2491) | 1:150:A:TYR:HD1  | 1:209:A:VAL:HG12 | 20       | 1.38          |
| (1,2491) | 1:150:A:TYR:HD1  | 1:209:A:VAL:HG13 | 20       | 1.38          |
| (1,2491) | 1:150:A:TYR:HD2  | 1:209:A:VAL:HG11 | 20       | 1.38          |
| (1,2491) | 1:150:A:TYR:HD2  | 1:209:A:VAL:HG12 | 20       | 1.38          |
| (1,2491) | 1:150:A:TYR:HD2  | 1:209:A:VAL:HG13 | 20       | 1.38          |
| (1,2482) | 1:163:A:TYR:HD1  | 1:221:A:GLU:HG2  | 7        | 1.38          |
| (1,2482) | 1:163:A:TYR:HD2  | 1:221:A:GLU:HG2  | 7        | 1.38          |
| (1,2356) | 1:169:A:TYR:HB2  | 1:174:A:ASN:HD21 | 4        | 1.38          |
| (1,2347) | 1:139:A:ILE:HG13 | 1:212:A:GLN:HE22 | 15       | 1.38          |
| (1,1912) | 1:213:A:MET:H    | 1:215:A:VAL:HG11 | 17       | 1.38          |
| (1,1912) | 1:213:A:MET:H    | 1:215:A:VAL:HG12 | 17       | 1.38          |
| (1,1912) | 1:213:A:MET:H    | 1:215:A:VAL:HG13 | 17       | 1.38          |
| (1,704)  | 1:209:A:VAL:HG21 | 1:213:A:MET:HE1  | 19       | 1.38          |
| (1,704)  | 1:209:A:VAL:HG21 | 1:213:A:MET:HE2  | 19       | 1.38          |
| (1,704)  | 1:209:A:VAL:HG21 | 1:213:A:MET:HE3  | 19       | 1.38          |
| (1,704)  | 1:209:A:VAL:HG22 | 1:213:A:MET:HE1  | 19       | 1.38          |
| (1,704)  | 1:209:A:VAL:HG22 | 1:213:A:MET:HE2  | 19       | 1.38          |
| (1,704)  | 1:209:A:VAL:HG22 | 1:213:A:MET:HE3  | 19       | 1.38          |
| (1,704)  | 1:209:A:VAL:HG23 | 1:213:A:MET:HE1  | 19       | 1.38          |
| (1,704)  | 1:209:A:VAL:HG23 | 1:213:A:MET:HE2  | 19       | 1.38          |
| (1,704)  | 1:209:A:VAL:HG23 | 1:213:A:MET:HE3  | 19       | 1.38          |
| (1,602)  | 1:230:A:ARG:H    | 1:231:A:SER:HB3  | 12       | 1.38          |
| (1,470)  | 1:122:A:VAL:HG21 | 1:125:A:LEU:HB2  | 6        | 1.38          |
| (1,470)  | 1:122:A:VAL:HG22 | 1:125:A:LEU:HB2  | 6        | 1.38          |
| (1,470)  | 1:122:A:VAL:HG23 | 1:125:A:LEU:HB2  | 6        | 1.38          |
| (1,396)  | 1:210:A:VAL:HA   | 1:213:A:MET:HB3  | 8        | 1.38          |
| (1,357)  | 1:122:A:VAL:HG21 | 1:125:A:LEU:HG   | 15       | 1.38          |
| (1,357)  | 1:122:A:VAL:HG22 | 1:125:A:LEU:HG   | 15       | 1.38          |
| (1,357)  | 1:122:A:VAL:HG23 | 1:125:A:LEU:HG   | 15       | 1.38          |
| (1,158)  | 1:126:A:GLY:HA2  | 1:164:A:ARG:HD3  | 8        | 1.38          |
| (1,2851) | 1:184:A:ILE:HG13 | 1:187:A:HIS:HE1  | 19       | 1.37          |
| (1,2315) | 1:160:A:GLN:HE21 | 1:213:A:MET:HB2  | 10       | 1.37          |
| (1,2315) | 1:160:A:GLN:HE21 | 1:213:A:MET:HB2  | 17       | 1.37          |
| (1,1912) | 1:213:A:MET:H    | 1:215:A:VAL:HG11 | 12       | 1.37          |
| (1,1912) | 1:213:A:MET:H    | 1:215:A:VAL:HG12 | 12       | 1.37          |
| (1,1912) | 1:213:A:MET:H    | 1:215:A:VAL:HG13 | 12       | 1.37          |
| (1,1344) | 1:206:A:MET:HB3  | 1:210:A:VAL:HB   | 3        | 1.37          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1081) | 1:164:A:ARG:HD2  | 1:168:A:GLN:HG2  | 5        | 1.37          |
| (1,704)  | 1:209:A:VAL:HG21 | 1:213:A:MET:HE1  | 4        | 1.37          |
| (1,704)  | 1:209:A:VAL:HG21 | 1:213:A:MET:HE2  | 4        | 1.37          |
| (1,704)  | 1:209:A:VAL:HG21 | 1:213:A:MET:HE3  | 4        | 1.37          |
| (1,704)  | 1:209:A:VAL:HG22 | 1:213:A:MET:HE1  | 4        | 1.37          |
| (1,704)  | 1:209:A:VAL:HG22 | 1:213:A:MET:HE2  | 4        | 1.37          |
| (1,704)  | 1:209:A:VAL:HG22 | 1:213:A:MET:HE3  | 4        | 1.37          |
| (1,704)  | 1:209:A:VAL:HG23 | 1:213:A:MET:HE1  | 4        | 1.37          |
| (1,704)  | 1:209:A:VAL:HG23 | 1:213:A:MET:HE2  | 4        | 1.37          |
| (1,704)  | 1:209:A:VAL:HG23 | 1:213:A:MET:HE3  | 4        | 1.37          |
| (1,704)  | 1:209:A:VAL:HG21 | 1:213:A:MET:HE1  | 10       | 1.37          |
| (1,704)  | 1:209:A:VAL:HG21 | 1:213:A:MET:HE2  | 10       | 1.37          |
| (1,704)  | 1:209:A:VAL:HG21 | 1:213:A:MET:HE3  | 10       | 1.37          |
| (1,704)  | 1:209:A:VAL:HG22 | 1:213:A:MET:HE1  | 10       | 1.37          |
| (1,704)  | 1:209:A:VAL:HG22 | 1:213:A:MET:HE2  | 10       | 1.37          |
| (1,704)  | 1:209:A:VAL:HG22 | 1:213:A:MET:HE3  | 10       | 1.37          |
| (1,704)  | 1:209:A:VAL:HG23 | 1:213:A:MET:HE1  | 10       | 1.37          |
| (1,704)  | 1:209:A:VAL:HG23 | 1:213:A:MET:HE2  | 10       | 1.37          |
| (1,704)  | 1:209:A:VAL:HG23 | 1:213:A:MET:HE3  | 10       | 1.37          |
| (1,602)  | 1:230:A:ARG:H    | 1:231:A:SER:HB3  | 3        | 1.37          |
| (1,348)  | 1:122:A:VAL:HG21 | 1:124:A:GLY:HA2  | 4        | 1.37          |
| (1,348)  | 1:122:A:VAL:HG21 | 1:124:A:GLY:HA3  | 4        | 1.37          |
| (1,348)  | 1:122:A:VAL:HG22 | 1:124:A:GLY:HA2  | 4        | 1.37          |
| (1,348)  | 1:122:A:VAL:HG22 | 1:124:A:GLY:HA3  | 4        | 1.37          |
| (1,348)  | 1:122:A:VAL:HG23 | 1:124:A:GLY:HA2  | 4        | 1.37          |
| (1,348)  | 1:122:A:VAL:HG23 | 1:124:A:GLY:HA3  | 4        | 1.37          |
| (1,311)  | 1:201:A:THR:HA   | 1:203:A:VAL:HG21 | 8        | 1.37          |
| (1,311)  | 1:201:A:THR:HA   | 1:203:A:VAL:HG22 | 8        | 1.37          |
| (1,311)  | 1:201:A:THR:HA   | 1:203:A:VAL:HG23 | 8        | 1.37          |
| (1,173)  | 1:198:A:PHE:HB2  | 1:203:A:VAL:HG11 | 2        | 1.37          |
| (1,173)  | 1:198:A:PHE:HB2  | 1:203:A:VAL:HG12 | 2        | 1.37          |
| (1,173)  | 1:198:A:PHE:HB2  | 1:203:A:VAL:HG13 | 2        | 1.37          |
| (1,2414) | 1:136:A:ARG:HB3  | 1:159:A:ASN:HD21 | 2        | 1.36          |
| (1,2315) | 1:160:A:GLN:HE21 | 1:213:A:MET:HB2  | 2        | 1.36          |
| (1,1073) | 1:166:A:VAL:HG11 | 1:221:A:GLU:HA   | 12       | 1.36          |
| (1,1073) | 1:166:A:VAL:HG12 | 1:221:A:GLU:HA   | 12       | 1.36          |
| (1,1073) | 1:166:A:VAL:HG13 | 1:221:A:GLU:HA   | 12       | 1.36          |
| (1,467)  | 1:122:A:VAL:HG21 | 1:125:A:LEU:HB3  | 8        | 1.36          |
| (1,467)  | 1:122:A:VAL:HG22 | 1:125:A:LEU:HB3  | 8        | 1.36          |
| (1,467)  | 1:122:A:VAL:HG23 | 1:125:A:LEU:HB3  | 8        | 1.36          |
| (1,396)  | 1:210:A:VAL:HA   | 1:213:A:MET:HB3  | 11       | 1.36          |
| (1,322)  | 1:158:A:PRO:HD3  | 1:209:A:VAL:HG21 | 2        | 1.36          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,322)  | 1:158:A:PRO:HD3  | 1:209:A:VAL:HG22 | 2        | 1.36          |
| (1,322)  | 1:158:A:PRO:HD3  | 1:209:A:VAL:HG23 | 2        | 1.36          |
| (1,311)  | 1:201:A:THR:HA   | 1:203:A:VAL:HG21 | 18       | 1.36          |
| (1,311)  | 1:201:A:THR:HA   | 1:203:A:VAL:HG22 | 18       | 1.36          |
| (1,311)  | 1:201:A:THR:HA   | 1:203:A:VAL:HG23 | 18       | 1.36          |
| (1,158)  | 1:126:A:GLY:HA2  | 1:164:A:ARG:HD3  | 16       | 1.36          |
| (1,2794) | 1:128:A:TYR:HE1  | 1:164:A:ARG:HG2  | 16       | 1.35          |
| (1,2794) | 1:128:A:TYR:HE2  | 1:164:A:ARG:HG2  | 16       | 1.35          |
| (1,2674) | 1:175:A:PHE:HZ   | 1:221:A:GLU:HG2  | 20       | 1.35          |
| (1,2491) | 1:150:A:TYR:HD1  | 1:209:A:VAL:HG11 | 2        | 1.35          |
| (1,2491) | 1:150:A:TYR:HD1  | 1:209:A:VAL:HG12 | 2        | 1.35          |
| (1,2491) | 1:150:A:TYR:HD1  | 1:209:A:VAL:HG13 | 2        | 1.35          |
| (1,2491) | 1:150:A:TYR:HD2  | 1:209:A:VAL:HG11 | 2        | 1.35          |
| (1,2491) | 1:150:A:TYR:HD2  | 1:209:A:VAL:HG12 | 2        | 1.35          |
| (1,2491) | 1:150:A:TYR:HD2  | 1:209:A:VAL:HG13 | 2        | 1.35          |
| (1,2482) | 1:163:A:TYR:HD1  | 1:221:A:GLU:HG2  | 12       | 1.35          |
| (1,2482) | 1:163:A:TYR:HD2  | 1:221:A:GLU:HG2  | 12       | 1.35          |
| (1,1131) | 1:223:A:GLN:HG2  | 1:226:A:TYR:H    | 19       | 1.35          |
| (1,996)  | 1:176:A:VAL:HA   | 1:211:A:GLU:HG3  | 15       | 1.35          |
| (1,677)  | 1:135:A:SER:HB2  | 1:213:A:MET:HA   | 19       | 1.35          |
| (1,601)  | 1:166:A:VAL:HG21 | 1:170:A:SER:HB2  | 1        | 1.35          |
| (1,601)  | 1:166:A:VAL:HG22 | 1:170:A:SER:HB2  | 1        | 1.35          |
| (1,601)  | 1:166:A:VAL:HG23 | 1:170:A:SER:HB2  | 1        | 1.35          |
| (1,567)  | 1:230:A:ARG:HB2  | 1:231:A:SER:HB3  | 2        | 1.35          |
| (1,396)  | 1:210:A:VAL:HA   | 1:213:A:MET:HB3  | 6        | 1.35          |
| (1,104)  | 1:213:A:MET:HA   | 1:215:A:VAL:HG11 | 6        | 1.35          |
| (1,104)  | 1:213:A:MET:HA   | 1:215:A:VAL:HG12 | 6        | 1.35          |
| (1,104)  | 1:213:A:MET:HA   | 1:215:A:VAL:HG13 | 6        | 1.35          |
| (1,2847) | 1:157:A:TYR:HE1  | 1:209:A:VAL:HG11 | 10       | 1.34          |
| (1,2847) | 1:157:A:TYR:HE1  | 1:209:A:VAL:HG12 | 10       | 1.34          |
| (1,2847) | 1:157:A:TYR:HE1  | 1:209:A:VAL:HG13 | 10       | 1.34          |
| (1,2847) | 1:157:A:TYR:HE2  | 1:209:A:VAL:HG11 | 10       | 1.34          |
| (1,2847) | 1:157:A:TYR:HE2  | 1:209:A:VAL:HG12 | 10       | 1.34          |
| (1,2847) | 1:157:A:TYR:HE2  | 1:209:A:VAL:HG13 | 10       | 1.34          |
| (1,2354) | 1:170:A:SER:HB2  | 1:174:A:ASN:HD21 | 4        | 1.34          |
| (1,1752) | 1:166:A:VAL:HG11 | 1:223:A:GLN:H    | 17       | 1.34          |
| (1,1752) | 1:166:A:VAL:HG12 | 1:223:A:GLN:H    | 17       | 1.34          |
| (1,1752) | 1:166:A:VAL:HG13 | 1:223:A:GLN:H    | 17       | 1.34          |
| (1,1689) | 1:134:A:MET:H    | 1:159:A:ASN:HB2  | 12       | 1.34          |
| (1,1097) | 1:165:A:PRO:HB3  | 1:168:A:GLN:HG2  | 18       | 1.34          |
| (1,597)  | 1:161:A:VAL:HG21 | 1:217:A:GLN:HB2  | 10       | 1.34          |
| (1,597)  | 1:161:A:VAL:HG22 | 1:217:A:GLN:HB2  | 10       | 1.34          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,597)  | 1:161:A:VAL:HG23 | 1:217:A:GLN:HB2  | 10       | 1.34          |
| (1,396)  | 1:210:A:VAL:HA   | 1:213:A:MET:HB3  | 4        | 1.34          |
| (1,358)  | 1:203:A:VAL:HG21 | 1:204:A:LYS:HG3  | 2        | 1.34          |
| (1,358)  | 1:203:A:VAL:HG22 | 1:204:A:LYS:HG3  | 2        | 1.34          |
| (1,358)  | 1:203:A:VAL:HG23 | 1:204:A:LYS:HG3  | 2        | 1.34          |
| (1,177)  | 1:195:A:GLY:HA3  | 1:197:A:ASN:HD21 | 7        | 1.34          |
| (1,104)  | 1:213:A:MET:HA   | 1:215:A:VAL:HG11 | 13       | 1.34          |
| (1,104)  | 1:213:A:MET:HA   | 1:215:A:VAL:HG12 | 13       | 1.34          |
| (1,104)  | 1:213:A:MET:HA   | 1:215:A:VAL:HG13 | 13       | 1.34          |
| (1,2851) | 1:184:A:ILE:HG13 | 1:187:A:HIS:HE1  | 9        | 1.33          |
| (1,2794) | 1:128:A:TYR:HE1  | 1:164:A:ARG:HG2  | 10       | 1.33          |
| (1,2794) | 1:128:A:TYR:HE2  | 1:164:A:ARG:HG2  | 10       | 1.33          |
| (1,2559) | 1:128:A:TYR:HD1  | 1:164:A:ARG:HD3  | 13       | 1.33          |
| (1,2559) | 1:128:A:TYR:HD2  | 1:164:A:ARG:HD3  | 13       | 1.33          |
| (1,2482) | 1:163:A:TYR:HD1  | 1:221:A:GLU:HG2  | 6        | 1.33          |
| (1,2482) | 1:163:A:TYR:HD2  | 1:221:A:GLU:HG2  | 6        | 1.33          |
| (1,2374) | 1:168:A:GLN:HE22 | 1:169:A:TYR:HE1  | 7        | 1.33          |
| (1,2374) | 1:168:A:GLN:HE22 | 1:169:A:TYR:HE2  | 7        | 1.33          |
| (1,2374) | 1:168:A:GLN:HE22 | 1:169:A:TYR:HE1  | 12       | 1.33          |
| (1,2374) | 1:168:A:GLN:HE22 | 1:169:A:TYR:HE2  | 12       | 1.33          |
| (1,2315) | 1:160:A:GLN:HE21 | 1:213:A:MET:HB2  | 16       | 1.33          |
| (1,1283) | 1:206:A:MET:HG2  | 1:207:A:GLU:HG3  | 4        | 1.33          |
| (1,1283) | 1:206:A:MET:HG2  | 1:207:A:GLU:HG3  | 13       | 1.33          |
| (1,1256) | 1:184:A:ILE:HG13 | 1:206:A:MET:HG3  | 12       | 1.33          |
| (1,677)  | 1:135:A:SER:HB2  | 1:213:A:MET:HA   | 1        | 1.33          |
| (1,348)  | 1:122:A:VAL:HG21 | 1:124:A:GLY:HA2  | 19       | 1.33          |
| (1,348)  | 1:122:A:VAL:HG21 | 1:124:A:GLY:HA3  | 19       | 1.33          |
| (1,348)  | 1:122:A:VAL:HG22 | 1:124:A:GLY:HA2  | 19       | 1.33          |
| (1,348)  | 1:122:A:VAL:HG22 | 1:124:A:GLY:HA3  | 19       | 1.33          |
| (1,348)  | 1:122:A:VAL:HG23 | 1:124:A:GLY:HA2  | 19       | 1.33          |
| (1,348)  | 1:122:A:VAL:HG23 | 1:124:A:GLY:HA3  | 19       | 1.33          |
| (1,104)  | 1:213:A:MET:HA   | 1:215:A:VAL:HG11 | 12       | 1.33          |
| (1,104)  | 1:213:A:MET:HA   | 1:215:A:VAL:HG12 | 12       | 1.33          |
| (1,104)  | 1:213:A:MET:HA   | 1:215:A:VAL:HG13 | 12       | 1.33          |
| (1,104)  | 1:213:A:MET:HA   | 1:215:A:VAL:HG11 | 19       | 1.33          |
| (1,104)  | 1:213:A:MET:HA   | 1:215:A:VAL:HG12 | 19       | 1.33          |
| (1,104)  | 1:213:A:MET:HA   | 1:215:A:VAL:HG13 | 19       | 1.33          |
| (1,23)   | 1:220:A:LYS:HG2  | 1:221:A:GLU:HG3  | 3        | 1.33          |
| (1,2851) | 1:184:A:ILE:HG13 | 1:187:A:HIS:HE1  | 3        | 1.32          |
| (1,2846) | 1:157:A:TYR:HE1  | 1:206:A:MET:HB2  | 13       | 1.32          |
| (1,2846) | 1:157:A:TYR:HE2  | 1:206:A:MET:HB2  | 13       | 1.32          |
| (1,2711) | 1:145:A:TRP:HZ3  | 1:146:A:GLU:HG3  | 4        | 1.32          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2356) | 1:169:A:TYR:HB2  | 1:174:A:ASN:HD21 | 5        | 1.32          |
| (1,2177) | 1:212:A:GLN:H    | 1:213:A:MET:HG2  | 2        | 1.32          |
| (1,2177) | 1:212:A:GLN:H    | 1:213:A:MET:HG2  | 19       | 1.32          |
| (1,2123) | 1:199:A:THR:H    | 1:203:A:VAL:HG11 | 2        | 1.32          |
| (1,2123) | 1:199:A:THR:H    | 1:203:A:VAL:HG12 | 2        | 1.32          |
| (1,2123) | 1:199:A:THR:H    | 1:203:A:VAL:HG13 | 2        | 1.32          |
| (1,1912) | 1:213:A:MET:H    | 1:215:A:VAL:HG11 | 13       | 1.32          |
| (1,1912) | 1:213:A:MET:H    | 1:215:A:VAL:HG12 | 13       | 1.32          |
| (1,1912) | 1:213:A:MET:H    | 1:215:A:VAL:HG13 | 13       | 1.32          |
| (1,1679) | 1:122:A:VAL:HG21 | 1:125:A:LEU:H    | 8        | 1.32          |
| (1,1679) | 1:122:A:VAL:HG22 | 1:125:A:LEU:H    | 8        | 1.32          |
| (1,1679) | 1:122:A:VAL:HG23 | 1:125:A:LEU:H    | 8        | 1.32          |
| (1,1235) | 1:205:A:MET:HG3  | 1:206:A:MET:HG2  | 3        | 1.32          |
| (1,1235) | 1:205:A:MET:HG3  | 1:206:A:MET:HG2  | 5        | 1.32          |
| (1,1131) | 1:223:A:GLN:HG2  | 1:226:A:TYR:H    | 8        | 1.32          |
| (1,1125) | 1:198:A:PHE:HA   | 1:203:A:VAL:HG11 | 7        | 1.32          |
| (1,1125) | 1:198:A:PHE:HA   | 1:203:A:VAL:HG12 | 7        | 1.32          |
| (1,1125) | 1:198:A:PHE:HA   | 1:203:A:VAL:HG13 | 7        | 1.32          |
| (1,476)  | 1:203:A:VAL:HG21 | 1:204:A:LYS:HE2  | 7        | 1.32          |
| (1,476)  | 1:203:A:VAL:HG21 | 1:204:A:LYS:HE3  | 7        | 1.32          |
| (1,476)  | 1:203:A:VAL:HG22 | 1:204:A:LYS:HE2  | 7        | 1.32          |
| (1,476)  | 1:203:A:VAL:HG22 | 1:204:A:LYS:HE3  | 7        | 1.32          |
| (1,476)  | 1:203:A:VAL:HG23 | 1:204:A:LYS:HE2  | 7        | 1.32          |
| (1,476)  | 1:203:A:VAL:HG23 | 1:204:A:LYS:HE3  | 7        | 1.32          |
| (1,429)  | 1:122:A:VAL:HG11 | 1:186:A:GLN:HA   | 16       | 1.32          |
| (1,429)  | 1:122:A:VAL:HG12 | 1:186:A:GLN:HA   | 16       | 1.32          |
| (1,429)  | 1:122:A:VAL:HG13 | 1:186:A:GLN:HA   | 16       | 1.32          |
| (1,358)  | 1:203:A:VAL:HG21 | 1:204:A:LYS:HG3  | 12       | 1.32          |
| (1,358)  | 1:203:A:VAL:HG22 | 1:204:A:LYS:HG3  | 12       | 1.32          |
| (1,358)  | 1:203:A:VAL:HG23 | 1:204:A:LYS:HG3  | 12       | 1.32          |
| (1,322)  | 1:158:A:PRO:HD3  | 1:209:A:VAL:HG21 | 12       | 1.32          |
| (1,322)  | 1:158:A:PRO:HD3  | 1:209:A:VAL:HG22 | 12       | 1.32          |
| (1,322)  | 1:158:A:PRO:HD3  | 1:209:A:VAL:HG23 | 12       | 1.32          |
| (1,220)  | 1:127:A:GLY:HA2  | 1:164:A:ARG:HE   | 4        | 1.32          |
| (1,189)  | 1:123:A:GLY:HA2  | 1:125:A:LEU:HD21 | 11       | 1.32          |
| (1,189)  | 1:123:A:GLY:HA2  | 1:125:A:LEU:HD22 | 11       | 1.32          |
| (1,189)  | 1:123:A:GLY:HA2  | 1:125:A:LEU:HD23 | 11       | 1.32          |
| (1,189)  | 1:123:A:GLY:HA3  | 1:125:A:LEU:HD21 | 11       | 1.32          |
| (1,189)  | 1:123:A:GLY:HA3  | 1:125:A:LEU:HD22 | 11       | 1.32          |
| (1,189)  | 1:123:A:GLY:HA3  | 1:125:A:LEU:HD23 | 11       | 1.32          |
| (1,159)  | 1:228:A:GLY:HA2  | 1:230:A:ARG:HD2  | 13       | 1.32          |
| (1,159)  | 1:228:A:GLY:HA3  | 1:230:A:ARG:HD2  | 13       | 1.32          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,78)   | 1:139:A:ILE:HB   | 1:209:A:VAL:HG11 | 1        | 1.32          |
| (1,78)   | 1:139:A:ILE:HB   | 1:209:A:VAL:HG12 | 1        | 1.32          |
| (1,78)   | 1:139:A:ILE:HB   | 1:209:A:VAL:HG13 | 1        | 1.32          |
| (1,78)   | 1:139:A:ILE:HB   | 1:209:A:VAL:HG11 | 16       | 1.32          |
| (1,78)   | 1:139:A:ILE:HB   | 1:209:A:VAL:HG12 | 16       | 1.32          |
| (1,78)   | 1:139:A:ILE:HB   | 1:209:A:VAL:HG13 | 16       | 1.32          |
| (1,78)   | 1:139:A:ILE:HB   | 1:209:A:VAL:HG11 | 19       | 1.32          |
| (1,78)   | 1:139:A:ILE:HB   | 1:209:A:VAL:HG12 | 19       | 1.32          |
| (1,78)   | 1:139:A:ILE:HB   | 1:209:A:VAL:HG13 | 19       | 1.32          |
| (1,2794) | 1:128:A:TYR:HE1  | 1:164:A:ARG:HG2  | 11       | 1.31          |
| (1,2794) | 1:128:A:TYR:HE2  | 1:164:A:ARG:HG2  | 11       | 1.31          |
| (1,2491) | 1:150:A:TYR:HD1  | 1:209:A:VAL:HG11 | 18       | 1.31          |
| (1,2491) | 1:150:A:TYR:HD1  | 1:209:A:VAL:HG12 | 18       | 1.31          |
| (1,2491) | 1:150:A:TYR:HD1  | 1:209:A:VAL:HG13 | 18       | 1.31          |
| (1,2491) | 1:150:A:TYR:HD2  | 1:209:A:VAL:HG11 | 18       | 1.31          |
| (1,2491) | 1:150:A:TYR:HD2  | 1:209:A:VAL:HG12 | 18       | 1.31          |
| (1,2491) | 1:150:A:TYR:HD2  | 1:209:A:VAL:HG13 | 18       | 1.31          |
| (1,2482) | 1:163:A:TYR:HD1  | 1:221:A:GLU:HG2  | 8        | 1.31          |
| (1,2482) | 1:163:A:TYR:HD2  | 1:221:A:GLU:HG2  | 8        | 1.31          |
| (1,2352) | 1:171:A:ASN:HA   | 1:174:A:ASN:HD21 | 6        | 1.31          |
| (1,2347) | 1:139:A:ILE:HG13 | 1:212:A:GLN:HE22 | 11       | 1.31          |
| (1,2315) | 1:160:A:GLN:HE21 | 1:213:A:MET:HB2  | 6        | 1.31          |
| (1,1235) | 1:205:A:MET:HG3  | 1:206:A:MET:HG2  | 14       | 1.31          |
| (1,704)  | 1:209:A:VAL:HG21 | 1:213:A:MET:HE1  | 8        | 1.31          |
| (1,704)  | 1:209:A:VAL:HG21 | 1:213:A:MET:HE2  | 8        | 1.31          |
| (1,704)  | 1:209:A:VAL:HG21 | 1:213:A:MET:HE3  | 8        | 1.31          |
| (1,704)  | 1:209:A:VAL:HG22 | 1:213:A:MET:HE1  | 8        | 1.31          |
| (1,704)  | 1:209:A:VAL:HG22 | 1:213:A:MET:HE2  | 8        | 1.31          |
| (1,704)  | 1:209:A:VAL:HG22 | 1:213:A:MET:HE3  | 8        | 1.31          |
| (1,704)  | 1:209:A:VAL:HG23 | 1:213:A:MET:HE1  | 8        | 1.31          |
| (1,704)  | 1:209:A:VAL:HG23 | 1:213:A:MET:HE2  | 8        | 1.31          |
| (1,704)  | 1:209:A:VAL:HG23 | 1:213:A:MET:HE3  | 8        | 1.31          |
| (1,311)  | 1:201:A:THR:HA   | 1:203:A:VAL:HG21 | 5        | 1.31          |
| (1,311)  | 1:201:A:THR:HA   | 1:203:A:VAL:HG22 | 5        | 1.31          |
| (1,311)  | 1:201:A:THR:HA   | 1:203:A:VAL:HG23 | 5        | 1.31          |
| (1,173)  | 1:198:A:PHE:HB2  | 1:203:A:VAL:HG11 | 8        | 1.31          |
| (1,173)  | 1:198:A:PHE:HB2  | 1:203:A:VAL:HG12 | 8        | 1.31          |
| (1,173)  | 1:198:A:PHE:HB2  | 1:203:A:VAL:HG13 | 8        | 1.31          |
| (1,159)  | 1:228:A:GLY:HA2  | 1:230:A:ARG:HD2  | 17       | 1.31          |
| (1,159)  | 1:228:A:GLY:HA3  | 1:230:A:ARG:HD2  | 17       | 1.31          |
| (1,104)  | 1:213:A:MET:HA   | 1:215:A:VAL:HG11 | 17       | 1.31          |
| (1,104)  | 1:213:A:MET:HA   | 1:215:A:VAL:HG12 | 17       | 1.31          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,104)  | 1:213:A:MET:HA   | 1:215:A:VAL:HG13 | 17       | 1.31          |
| (1,1912) | 1:213:A:MET:H    | 1:215:A:VAL:HG11 | 14       | 1.3           |
| (1,1912) | 1:213:A:MET:H    | 1:215:A:VAL:HG12 | 14       | 1.3           |
| (1,1912) | 1:213:A:MET:H    | 1:215:A:VAL:HG13 | 14       | 1.3           |
| (1,1125) | 1:198:A:PHE:HA   | 1:203:A:VAL:HG11 | 12       | 1.3           |
| (1,1125) | 1:198:A:PHE:HA   | 1:203:A:VAL:HG12 | 12       | 1.3           |
| (1,1125) | 1:198:A:PHE:HA   | 1:203:A:VAL:HG13 | 12       | 1.3           |
| (1,429)  | 1:122:A:VAL:HG11 | 1:186:A:GLN:HA   | 18       | 1.3           |
| (1,429)  | 1:122:A:VAL:HG12 | 1:186:A:GLN:HA   | 18       | 1.3           |
| (1,429)  | 1:122:A:VAL:HG13 | 1:186:A:GLN:HA   | 18       | 1.3           |
| (1,160)  | 1:223:A:GLN:HE21 | 1:228:A:GLY:HA2  | 12       | 1.3           |
| (1,160)  | 1:223:A:GLN:HE21 | 1:228:A:GLY:HA3  | 12       | 1.3           |
| (1,2711) | 1:145:A:TRP:HZ3  | 1:146:A:GLU:HG3  | 8        | 1.29          |
| (1,2421) | 1:127:A:GLY:H    | 1:164:A:ARG:HD3  | 20       | 1.29          |
| (1,2320) | 1:160:A:GLN:HE22 | 1:213:A:MET:HB2  | 1        | 1.29          |
| (1,1878) | 1:161:A:VAL:HG21 | 1:218:A:TYR:H    | 10       | 1.29          |
| (1,1878) | 1:161:A:VAL:HG22 | 1:218:A:TYR:H    | 10       | 1.29          |
| (1,1878) | 1:161:A:VAL:HG23 | 1:218:A:TYR:H    | 10       | 1.29          |
| (1,567)  | 1:230:A:ARG:HB2  | 1:231:A:SER:HB3  | 3        | 1.29          |
| (1,428)  | 1:127:A:GLY:HA2  | 1:164:A:ARG:HD3  | 5        | 1.29          |
| (1,104)  | 1:213:A:MET:HA   | 1:215:A:VAL:HG11 | 14       | 1.29          |
| (1,104)  | 1:213:A:MET:HA   | 1:215:A:VAL:HG12 | 14       | 1.29          |
| (1,104)  | 1:213:A:MET:HA   | 1:215:A:VAL:HG13 | 14       | 1.29          |
| (1,2847) | 1:157:A:TYR:HE1  | 1:209:A:VAL:HG11 | 13       | 1.28          |
| (1,2847) | 1:157:A:TYR:HE1  | 1:209:A:VAL:HG12 | 13       | 1.28          |
| (1,2847) | 1:157:A:TYR:HE1  | 1:209:A:VAL:HG13 | 13       | 1.28          |
| (1,2847) | 1:157:A:TYR:HE2  | 1:209:A:VAL:HG11 | 13       | 1.28          |
| (1,2847) | 1:157:A:TYR:HE2  | 1:209:A:VAL:HG12 | 13       | 1.28          |
| (1,2847) | 1:157:A:TYR:HE2  | 1:209:A:VAL:HG13 | 13       | 1.28          |
| (1,2482) | 1:163:A:TYR:HD1  | 1:221:A:GLU:HG2  | 14       | 1.28          |
| (1,2482) | 1:163:A:TYR:HD2  | 1:221:A:GLU:HG2  | 14       | 1.28          |
| (1,2347) | 1:139:A:ILE:HG13 | 1:212:A:GLN:HE22 | 6        | 1.28          |
| (1,2347) | 1:139:A:ILE:HG13 | 1:212:A:GLN:HE22 | 9        | 1.28          |
| (1,1231) | 1:209:A:VAL:HG21 | 1:213:A:MET:HG3  | 20       | 1.28          |
| (1,1231) | 1:209:A:VAL:HG22 | 1:213:A:MET:HG3  | 20       | 1.28          |
| (1,1231) | 1:209:A:VAL:HG23 | 1:213:A:MET:HG3  | 20       | 1.28          |
| (1,392)  | 1:122:A:VAL:HG11 | 1:190:A:THR:HB   | 4        | 1.28          |
| (1,392)  | 1:122:A:VAL:HG12 | 1:190:A:THR:HB   | 4        | 1.28          |
| (1,392)  | 1:122:A:VAL:HG13 | 1:190:A:THR:HB   | 4        | 1.28          |
| (1,356)  | 1:203:A:VAL:HG21 | 1:204:A:LYS:HG2  | 7        | 1.28          |
| (1,356)  | 1:203:A:VAL:HG22 | 1:204:A:LYS:HG2  | 7        | 1.28          |
| (1,356)  | 1:203:A:VAL:HG23 | 1:204:A:LYS:HG2  | 7        | 1.28          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,311)  | 1:201:A:THR:HA   | 1:203:A:VAL:HG21 | 7        | 1.28          |
| (1,311)  | 1:201:A:THR:HA   | 1:203:A:VAL:HG22 | 7        | 1.28          |
| (1,311)  | 1:201:A:THR:HA   | 1:203:A:VAL:HG23 | 7        | 1.28          |
| (1,169)  | 1:198:A:PHE:HB3  | 1:203:A:VAL:HG11 | 18       | 1.28          |
| (1,169)  | 1:198:A:PHE:HB3  | 1:203:A:VAL:HG12 | 18       | 1.28          |
| (1,169)  | 1:198:A:PHE:HB3  | 1:203:A:VAL:HG13 | 18       | 1.28          |
| (1,160)  | 1:223:A:GLN:HE21 | 1:228:A:GLY:HA2  | 16       | 1.28          |
| (1,160)  | 1:223:A:GLN:HE21 | 1:228:A:GLY:HA3  | 16       | 1.28          |
| (1,2847) | 1:157:A:TYR:HE1  | 1:209:A:VAL:HG11 | 8        | 1.27          |
| (1,2847) | 1:157:A:TYR:HE1  | 1:209:A:VAL:HG12 | 8        | 1.27          |
| (1,2847) | 1:157:A:TYR:HE1  | 1:209:A:VAL:HG13 | 8        | 1.27          |
| (1,2847) | 1:157:A:TYR:HE2  | 1:209:A:VAL:HG11 | 8        | 1.27          |
| (1,2847) | 1:157:A:TYR:HE2  | 1:209:A:VAL:HG12 | 8        | 1.27          |
| (1,2847) | 1:157:A:TYR:HE2  | 1:209:A:VAL:HG13 | 8        | 1.27          |
| (1,2847) | 1:157:A:TYR:HE1  | 1:209:A:VAL:HG11 | 14       | 1.27          |
| (1,2847) | 1:157:A:TYR:HE1  | 1:209:A:VAL:HG12 | 14       | 1.27          |
| (1,2847) | 1:157:A:TYR:HE1  | 1:209:A:VAL:HG13 | 14       | 1.27          |
| (1,2847) | 1:157:A:TYR:HE2  | 1:209:A:VAL:HG11 | 14       | 1.27          |
| (1,2847) | 1:157:A:TYR:HE2  | 1:209:A:VAL:HG12 | 14       | 1.27          |
| (1,2847) | 1:157:A:TYR:HE2  | 1:209:A:VAL:HG13 | 14       | 1.27          |
| (1,2846) | 1:157:A:TYR:HE1  | 1:206:A:MET:HB2  | 12       | 1.27          |
| (1,2846) | 1:157:A:TYR:HE2  | 1:206:A:MET:HB2  | 12       | 1.27          |
| (1,2510) | 1:226:A:TYR:HD1  | 1:229:A:ARG:HB2  | 20       | 1.27          |
| (1,2510) | 1:226:A:TYR:HD2  | 1:229:A:ARG:HB2  | 20       | 1.27          |
| (1,2354) | 1:170:A:SER:HB2  | 1:174:A:ASN:HD21 | 14       | 1.27          |
| (1,1235) | 1:205:A:MET:HG3  | 1:206:A:MET:HG2  | 17       | 1.27          |
| (1,1081) | 1:164:A:ARG:HD2  | 1:168:A:GLN:HG2  | 1        | 1.27          |
| (1,751)  | 1:222:A:SER:HB2  | 1:223:A:GLN:HA   | 10       | 1.27          |
| (1,318)  | 1:153:A:ASN:HB2  | 1:156:A:ARG:HD3  | 20       | 1.27          |
| (1,158)  | 1:126:A:GLY:HA2  | 1:164:A:ARG:HD3  | 6        | 1.27          |
| (1,89)   | 1:206:A:MET:HB3  | 1:210:A:VAL:HG21 | 4        | 1.27          |
| (1,89)   | 1:206:A:MET:HB3  | 1:210:A:VAL:HG22 | 4        | 1.27          |
| (1,89)   | 1:206:A:MET:HB3  | 1:210:A:VAL:HG23 | 4        | 1.27          |
| (1,2847) | 1:157:A:TYR:HE1  | 1:209:A:VAL:HG11 | 11       | 1.26          |
| (1,2847) | 1:157:A:TYR:HE1  | 1:209:A:VAL:HG12 | 11       | 1.26          |
| (1,2847) | 1:157:A:TYR:HE1  | 1:209:A:VAL:HG13 | 11       | 1.26          |
| (1,2847) | 1:157:A:TYR:HE2  | 1:209:A:VAL:HG11 | 11       | 1.26          |
| (1,2847) | 1:157:A:TYR:HE2  | 1:209:A:VAL:HG12 | 11       | 1.26          |
| (1,2847) | 1:157:A:TYR:HE2  | 1:209:A:VAL:HG13 | 11       | 1.26          |
| (1,2711) | 1:145:A:TRP:HZ3  | 1:146:A:GLU:HG3  | 16       | 1.26          |
| (1,2482) | 1:163:A:TYR:HD1  | 1:221:A:GLU:HG2  | 4        | 1.26          |
| (1,2482) | 1:163:A:TYR:HD2  | 1:221:A:GLU:HG2  | 4        | 1.26          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2482) | 1:163:A:TYR:HD1  | 1:221:A:GLU:HG2  | 11       | 1.26          |
| (1,2482) | 1:163:A:TYR:HD2  | 1:221:A:GLU:HG2  | 11       | 1.26          |
| (1,2354) | 1:170:A:SER:HB2  | 1:174:A:ASN:HD21 | 19       | 1.26          |
| (1,2177) | 1:212:A:GLN:H    | 1:213:A:MET:HG2  | 17       | 1.26          |
| (1,467)  | 1:122:A:VAL:HG21 | 1:125:A:LEU:HB3  | 12       | 1.26          |
| (1,467)  | 1:122:A:VAL:HG22 | 1:125:A:LEU:HB3  | 12       | 1.26          |
| (1,467)  | 1:122:A:VAL:HG23 | 1:125:A:LEU:HB3  | 12       | 1.26          |
| (1,437)  | 1:229:A:ARG:HB3  | 1:230:A:ARG:HD3  | 20       | 1.26          |
| (1,437)  | 1:229:A:ARG:HB2  | 1:230:A:ARG:HD3  | 20       | 1.26          |
| (1,356)  | 1:203:A:VAL:HG21 | 1:204:A:LYS:HG2  | 8        | 1.26          |
| (1,356)  | 1:203:A:VAL:HG22 | 1:204:A:LYS:HG2  | 8        | 1.26          |
| (1,356)  | 1:203:A:VAL:HG23 | 1:204:A:LYS:HG2  | 8        | 1.26          |
| (1,220)  | 1:127:A:GLY:HA2  | 1:164:A:ARG:HE   | 1        | 1.26          |
| (1,2851) | 1:184:A:ILE:HG13 | 1:187:A:HIS:HE1  | 15       | 1.25          |
| (1,2711) | 1:145:A:TRP:HZ3  | 1:146:A:GLU:HG3  | 5        | 1.25          |
| (1,2559) | 1:128:A:TYR:HD1  | 1:164:A:ARG:HD3  | 2        | 1.25          |
| (1,2559) | 1:128:A:TYR:HD2  | 1:164:A:ARG:HD3  | 2        | 1.25          |
| (1,2559) | 1:128:A:TYR:HD1  | 1:164:A:ARG:HD3  | 12       | 1.25          |
| (1,2559) | 1:128:A:TYR:HD2  | 1:164:A:ARG:HD3  | 12       | 1.25          |
| (1,2374) | 1:168:A:GLN:HE22 | 1:169:A:TYR:HE1  | 6        | 1.25          |
| (1,2374) | 1:168:A:GLN:HE22 | 1:169:A:TYR:HE2  | 6        | 1.25          |
| (1,2320) | 1:160:A:GLN:HE22 | 1:213:A:MET:HB2  | 14       | 1.25          |
| (1,2177) | 1:212:A:GLN:H    | 1:213:A:MET:HG2  | 3        | 1.25          |
| (1,1235) | 1:205:A:MET:HG3  | 1:206:A:MET:HG2  | 20       | 1.25          |
| (1,1073) | 1:166:A:VAL:HG11 | 1:221:A:GLU:HA   | 17       | 1.25          |
| (1,1073) | 1:166:A:VAL:HG12 | 1:221:A:GLU:HA   | 17       | 1.25          |
| (1,1073) | 1:166:A:VAL:HG13 | 1:221:A:GLU:HA   | 17       | 1.25          |
| (1,751)  | 1:222:A:SER:HB2  | 1:223:A:GLN:HA   | 17       | 1.25          |
| (1,593)  | 1:161:A:VAL:HG21 | 1:163:A:TYR:HE1  | 10       | 1.25          |
| (1,593)  | 1:161:A:VAL:HG21 | 1:163:A:TYR:HE2  | 10       | 1.25          |
| (1,593)  | 1:161:A:VAL:HG22 | 1:163:A:TYR:HE1  | 10       | 1.25          |
| (1,593)  | 1:161:A:VAL:HG22 | 1:163:A:TYR:HE2  | 10       | 1.25          |
| (1,593)  | 1:161:A:VAL:HG23 | 1:163:A:TYR:HE1  | 10       | 1.25          |
| (1,593)  | 1:161:A:VAL:HG23 | 1:163:A:TYR:HE2  | 10       | 1.25          |
| (1,348)  | 1:122:A:VAL:HG21 | 1:124:A:GLY:HA2  | 1        | 1.25          |
| (1,348)  | 1:122:A:VAL:HG21 | 1:124:A:GLY:HA3  | 1        | 1.25          |
| (1,348)  | 1:122:A:VAL:HG22 | 1:124:A:GLY:HA2  | 1        | 1.25          |
| (1,348)  | 1:122:A:VAL:HG22 | 1:124:A:GLY:HA3  | 1        | 1.25          |
| (1,348)  | 1:122:A:VAL:HG23 | 1:124:A:GLY:HA2  | 1        | 1.25          |
| (1,348)  | 1:122:A:VAL:HG23 | 1:124:A:GLY:HA3  | 1        | 1.25          |
| (1,2851) | 1:184:A:ILE:HG13 | 1:187:A:HIS:HE1  | 2        | 1.24          |
| (1,2847) | 1:157:A:TYR:HE1  | 1:209:A:VAL:HG11 | 12       | 1.24          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2847) | 1:157:A:TYR:HE1  | 1:209:A:VAL:HG12 | 12       | 1.24          |
| (1,2847) | 1:157:A:TYR:HE1  | 1:209:A:VAL:HG13 | 12       | 1.24          |
| (1,2847) | 1:157:A:TYR:HE2  | 1:209:A:VAL:HG11 | 12       | 1.24          |
| (1,2847) | 1:157:A:TYR:HE2  | 1:209:A:VAL:HG12 | 12       | 1.24          |
| (1,2847) | 1:157:A:TYR:HE2  | 1:209:A:VAL:HG13 | 12       | 1.24          |
| (1,2846) | 1:157:A:TYR:HE1  | 1:206:A:MET:HB2  | 6        | 1.24          |
| (1,2846) | 1:157:A:TYR:HE2  | 1:206:A:MET:HB2  | 6        | 1.24          |
| (1,2571) | 1:215:A:VAL:HG21 | 1:218:A:TYR:HD1  | 13       | 1.24          |
| (1,2571) | 1:215:A:VAL:HG21 | 1:218:A:TYR:HD2  | 13       | 1.24          |
| (1,2571) | 1:215:A:VAL:HG22 | 1:218:A:TYR:HD1  | 13       | 1.24          |
| (1,2571) | 1:215:A:VAL:HG22 | 1:218:A:TYR:HD2  | 13       | 1.24          |
| (1,2571) | 1:215:A:VAL:HG23 | 1:218:A:TYR:HD1  | 13       | 1.24          |
| (1,2571) | 1:215:A:VAL:HG23 | 1:218:A:TYR:HD2  | 13       | 1.24          |
| (1,921)  | 1:167:A:SER:HA   | 1:168:A:GLN:HG3  | 11       | 1.24          |
| (1,470)  | 1:122:A:VAL:HG21 | 1:125:A:LEU:HB2  | 18       | 1.24          |
| (1,470)  | 1:122:A:VAL:HG22 | 1:125:A:LEU:HB2  | 18       | 1.24          |
| (1,470)  | 1:122:A:VAL:HG23 | 1:125:A:LEU:HB2  | 18       | 1.24          |
| (1,380)  | 1:122:A:VAL:HG21 | 1:123:A:GLY:HA2  | 9        | 1.24          |
| (1,380)  | 1:122:A:VAL:HG21 | 1:123:A:GLY:HA3  | 9        | 1.24          |
| (1,380)  | 1:122:A:VAL:HG22 | 1:123:A:GLY:HA2  | 9        | 1.24          |
| (1,380)  | 1:122:A:VAL:HG22 | 1:123:A:GLY:HA3  | 9        | 1.24          |
| (1,380)  | 1:122:A:VAL:HG23 | 1:123:A:GLY:HA2  | 9        | 1.24          |
| (1,380)  | 1:122:A:VAL:HG23 | 1:123:A:GLY:HA3  | 9        | 1.24          |
| (1,169)  | 1:198:A:PHE:HB3  | 1:203:A:VAL:HG11 | 8        | 1.24          |
| (1,169)  | 1:198:A:PHE:HB3  | 1:203:A:VAL:HG12 | 8        | 1.24          |
| (1,169)  | 1:198:A:PHE:HB3  | 1:203:A:VAL:HG13 | 8        | 1.24          |
| (1,1)    | 1:138:A:MET:HG3  | 1:139:A:ILE:HG12 | 18       | 1.24          |
| (1,2847) | 1:157:A:TYR:HE1  | 1:209:A:VAL:HG11 | 16       | 1.23          |
| (1,2847) | 1:157:A:TYR:HE1  | 1:209:A:VAL:HG12 | 16       | 1.23          |
| (1,2847) | 1:157:A:TYR:HE1  | 1:209:A:VAL:HG13 | 16       | 1.23          |
| (1,2847) | 1:157:A:TYR:HE2  | 1:209:A:VAL:HG11 | 16       | 1.23          |
| (1,2847) | 1:157:A:TYR:HE2  | 1:209:A:VAL:HG12 | 16       | 1.23          |
| (1,2847) | 1:157:A:TYR:HE2  | 1:209:A:VAL:HG13 | 16       | 1.23          |
| (1,1235) | 1:205:A:MET:HG3  | 1:206:A:MET:HG2  | 9        | 1.23          |
| (1,1235) | 1:205:A:MET:HG3  | 1:206:A:MET:HG2  | 16       | 1.23          |
| (1,1164) | 1:215:A:VAL:HG21 | 1:219:A:GLN:HG2  | 8        | 1.23          |
| (1,1164) | 1:215:A:VAL:HG22 | 1:219:A:GLN:HG2  | 8        | 1.23          |
| (1,1164) | 1:215:A:VAL:HG23 | 1:219:A:GLN:HG2  | 8        | 1.23          |
| (1,751)  | 1:222:A:SER:HB2  | 1:223:A:GLN:HA   | 8        | 1.23          |
| (1,751)  | 1:222:A:SER:HB2  | 1:223:A:GLN:HA   | 13       | 1.23          |
| (1,637)  | 1:147:A:ASP:HB2  | 1:148:A:ARG:HG2  | 8        | 1.23          |
| (1,396)  | 1:210:A:VAL:HA   | 1:213:A:MET:HB3  | 10       | 1.23          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,380)  | 1:122:A:VAL:HG21 | 1:123:A:GLY:HA2  | 2        | 1.23          |
| (1,380)  | 1:122:A:VAL:HG21 | 1:123:A:GLY:HA3  | 2        | 1.23          |
| (1,380)  | 1:122:A:VAL:HG22 | 1:123:A:GLY:HA2  | 2        | 1.23          |
| (1,380)  | 1:122:A:VAL:HG22 | 1:123:A:GLY:HA3  | 2        | 1.23          |
| (1,380)  | 1:122:A:VAL:HG23 | 1:123:A:GLY:HA2  | 2        | 1.23          |
| (1,380)  | 1:122:A:VAL:HG23 | 1:123:A:GLY:HA3  | 2        | 1.23          |
| (1,380)  | 1:122:A:VAL:HG21 | 1:123:A:GLY:HA2  | 19       | 1.23          |
| (1,380)  | 1:122:A:VAL:HG21 | 1:123:A:GLY:HA3  | 19       | 1.23          |
| (1,380)  | 1:122:A:VAL:HG22 | 1:123:A:GLY:HA2  | 19       | 1.23          |
| (1,380)  | 1:122:A:VAL:HG22 | 1:123:A:GLY:HA3  | 19       | 1.23          |
| (1,380)  | 1:122:A:VAL:HG23 | 1:123:A:GLY:HA2  | 19       | 1.23          |
| (1,380)  | 1:122:A:VAL:HG23 | 1:123:A:GLY:HA3  | 19       | 1.23          |
| (1,358)  | 1:203:A:VAL:HG21 | 1:204:A:LYS:HG3  | 5        | 1.23          |
| (1,358)  | 1:203:A:VAL:HG22 | 1:204:A:LYS:HG3  | 5        | 1.23          |
| (1,358)  | 1:203:A:VAL:HG23 | 1:204:A:LYS:HG3  | 5        | 1.23          |
| (1,309)  | 1:186:A:GLN:HE21 | 1:189:A:VAL:HG11 | 12       | 1.23          |
| (1,309)  | 1:186:A:GLN:HE21 | 1:189:A:VAL:HG12 | 12       | 1.23          |
| (1,309)  | 1:186:A:GLN:HE21 | 1:189:A:VAL:HG13 | 12       | 1.23          |
| (1,188)  | 1:124:A:GLY:HA2  | 1:125:A:LEU:HD21 | 1        | 1.23          |
| (1,188)  | 1:124:A:GLY:HA2  | 1:125:A:LEU:HD22 | 1        | 1.23          |
| (1,188)  | 1:124:A:GLY:HA2  | 1:125:A:LEU:HD23 | 1        | 1.23          |
| (1,188)  | 1:124:A:GLY:HA3  | 1:125:A:LEU:HD21 | 1        | 1.23          |
| (1,188)  | 1:124:A:GLY:HA3  | 1:125:A:LEU:HD22 | 1        | 1.23          |
| (1,188)  | 1:124:A:GLY:HA3  | 1:125:A:LEU:HD23 | 1        | 1.23          |
| (1,158)  | 1:126:A:GLY:HA2  | 1:164:A:ARG:HD3  | 9        | 1.23          |
| (1,2851) | 1:184:A:ILE:HG13 | 1:187:A:HIS:HE1  | 14       | 1.22          |
| (1,2846) | 1:157:A:TYR:HE1  | 1:206:A:MET:HB2  | 9        | 1.22          |
| (1,2846) | 1:157:A:TYR:HE2  | 1:206:A:MET:HB2  | 9        | 1.22          |
| (1,2736) | 1:184:A:ILE:HG13 | 1:187:A:HIS:HD2  | 8        | 1.22          |
| (1,2711) | 1:145:A:TRP:HZ3  | 1:146:A:GLU:HG3  | 13       | 1.22          |
| (1,2559) | 1:128:A:TYR:HD1  | 1:164:A:ARG:HD3  | 15       | 1.22          |
| (1,2559) | 1:128:A:TYR:HD2  | 1:164:A:ARG:HD3  | 15       | 1.22          |
| (1,2421) | 1:127:A:GLY:H    | 1:164:A:ARG:HD3  | 15       | 1.22          |
| (1,2315) | 1:160:A:GLN:HE21 | 1:213:A:MET:HB2  | 4        | 1.22          |
| (1,2177) | 1:212:A:GLN:H    | 1:213:A:MET:HG2  | 5        | 1.22          |
| (1,1283) | 1:206:A:MET:HG2  | 1:207:A:GLU:HG3  | 15       | 1.22          |
| (1,1283) | 1:206:A:MET:HG2  | 1:207:A:GLU:HG3  | 16       | 1.22          |
| (1,1235) | 1:205:A:MET:HG3  | 1:206:A:MET:HG2  | 19       | 1.22          |
| (1,1231) | 1:209:A:VAL:HG21 | 1:213:A:MET:HG3  | 2        | 1.22          |
| (1,1231) | 1:209:A:VAL:HG22 | 1:213:A:MET:HG3  | 2        | 1.22          |
| (1,1231) | 1:209:A:VAL:HG23 | 1:213:A:MET:HG3  | 2        | 1.22          |
| (1,311)  | 1:201:A:THR:HA   | 1:203:A:VAL:HG21 | 2        | 1.22          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,311)  | 1:201:A:THR:HA   | 1:203:A:VAL:HG22 | 2        | 1.22          |
| (1,311)  | 1:201:A:THR:HA   | 1:203:A:VAL:HG23 | 2        | 1.22          |
| (1,159)  | 1:228:A:GLY:HA2  | 1:230:A:ARG:HD2  | 6        | 1.22          |
| (1,159)  | 1:228:A:GLY:HA3  | 1:230:A:ARG:HD2  | 6        | 1.22          |
| (1,107)  | 1:211:A:GLU:HG3  | 1:215:A:VAL:HG11 | 15       | 1.22          |
| (1,107)  | 1:211:A:GLU:HG3  | 1:215:A:VAL:HG12 | 15       | 1.22          |
| (1,107)  | 1:211:A:GLU:HG3  | 1:215:A:VAL:HG13 | 15       | 1.22          |
| (1,2851) | 1:184:A:ILE:HG13 | 1:187:A:HIS:HE1  | 20       | 1.21          |
| (1,2492) | 1:139:A:ILE:HG12 | 1:150:A:TYR:HD1  | 17       | 1.21          |
| (1,2492) | 1:139:A:ILE:HG12 | 1:150:A:TYR:HD2  | 17       | 1.21          |
| (1,2347) | 1:139:A:ILE:HG13 | 1:212:A:GLN:HE22 | 5        | 1.21          |
| (1,2320) | 1:160:A:GLN:HE22 | 1:213:A:MET:HB2  | 3        | 1.21          |
| (1,1303) | 1:137:A:PRO:HB2  | 1:213:A:MET:HG2  | 2        | 1.21          |
| (1,1131) | 1:223:A:GLN:HG2  | 1:226:A:TYR:H    | 11       | 1.21          |
| (1,931)  | 1:166:A:VAL:HG11 | 1:221:A:GLU:HG3  | 12       | 1.21          |
| (1,931)  | 1:166:A:VAL:HG12 | 1:221:A:GLU:HG3  | 12       | 1.21          |
| (1,931)  | 1:166:A:VAL:HG13 | 1:221:A:GLU:HG3  | 12       | 1.21          |
| (1,704)  | 1:209:A:VAL:HG21 | 1:213:A:MET:HE1  | 2        | 1.21          |
| (1,704)  | 1:209:A:VAL:HG21 | 1:213:A:MET:HE2  | 2        | 1.21          |
| (1,704)  | 1:209:A:VAL:HG21 | 1:213:A:MET:HE3  | 2        | 1.21          |
| (1,704)  | 1:209:A:VAL:HG22 | 1:213:A:MET:HE1  | 2        | 1.21          |
| (1,704)  | 1:209:A:VAL:HG22 | 1:213:A:MET:HE2  | 2        | 1.21          |
| (1,704)  | 1:209:A:VAL:HG22 | 1:213:A:MET:HE3  | 2        | 1.21          |
| (1,704)  | 1:209:A:VAL:HG23 | 1:213:A:MET:HE1  | 2        | 1.21          |
| (1,704)  | 1:209:A:VAL:HG23 | 1:213:A:MET:HE2  | 2        | 1.21          |
| (1,704)  | 1:209:A:VAL:HG23 | 1:213:A:MET:HE3  | 2        | 1.21          |
| (1,704)  | 1:209:A:VAL:HG21 | 1:213:A:MET:HE1  | 17       | 1.21          |
| (1,704)  | 1:209:A:VAL:HG21 | 1:213:A:MET:HE2  | 17       | 1.21          |
| (1,704)  | 1:209:A:VAL:HG21 | 1:213:A:MET:HE3  | 17       | 1.21          |
| (1,704)  | 1:209:A:VAL:HG22 | 1:213:A:MET:HE1  | 17       | 1.21          |
| (1,704)  | 1:209:A:VAL:HG22 | 1:213:A:MET:HE2  | 17       | 1.21          |
| (1,704)  | 1:209:A:VAL:HG22 | 1:213:A:MET:HE3  | 17       | 1.21          |
| (1,704)  | 1:209:A:VAL:HG23 | 1:213:A:MET:HE1  | 17       | 1.21          |
| (1,704)  | 1:209:A:VAL:HG23 | 1:213:A:MET:HE2  | 17       | 1.21          |
| (1,704)  | 1:209:A:VAL:HG23 | 1:213:A:MET:HE3  | 17       | 1.21          |
| (1,380)  | 1:122:A:VAL:HG21 | 1:123:A:GLY:HA2  | 1        | 1.21          |
| (1,380)  | 1:122:A:VAL:HG21 | 1:123:A:GLY:HA3  | 1        | 1.21          |
| (1,380)  | 1:122:A:VAL:HG22 | 1:123:A:GLY:HA2  | 1        | 1.21          |
| (1,380)  | 1:122:A:VAL:HG22 | 1:123:A:GLY:HA3  | 1        | 1.21          |
| (1,380)  | 1:122:A:VAL:HG23 | 1:123:A:GLY:HA2  | 1        | 1.21          |
| (1,380)  | 1:122:A:VAL:HG23 | 1:123:A:GLY:HA3  | 1        | 1.21          |
| (1,322)  | 1:158:A:PRO:HD3  | 1:209:A:VAL:HG21 | 18       | 1.21          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,322)  | 1:158:A:PRO:HD3  | 1:209:A:VAL:HG22 | 18       | 1.21          |
| (1,322)  | 1:158:A:PRO:HD3  | 1:209:A:VAL:HG23 | 18       | 1.21          |
| (1,231)  | 1:176:A:VAL:HG11 | 1:180:A:VAL:H    | 12       | 1.21          |
| (1,231)  | 1:176:A:VAL:HG12 | 1:180:A:VAL:H    | 12       | 1.21          |
| (1,231)  | 1:176:A:VAL:HG13 | 1:180:A:VAL:H    | 12       | 1.21          |
| (1,78)   | 1:139:A:ILE:HB   | 1:209:A:VAL:HG11 | 7        | 1.21          |
| (1,78)   | 1:139:A:ILE:HB   | 1:209:A:VAL:HG12 | 7        | 1.21          |
| (1,78)   | 1:139:A:ILE:HB   | 1:209:A:VAL:HG13 | 7        | 1.21          |
| (1,2846) | 1:157:A:TYR:HE1  | 1:206:A:MET:HB2  | 11       | 1.2           |
| (1,2846) | 1:157:A:TYR:HE2  | 1:206:A:MET:HB2  | 11       | 1.2           |
| (1,2657) | 1:141:A:PHE:HE1  | 1:208:A:ARG:HB3  | 4        | 1.2           |
| (1,2657) | 1:141:A:PHE:HE2  | 1:208:A:ARG:HB3  | 4        | 1.2           |
| (1,2615) | 1:141:A:PHE:HD1  | 1:147:A:ASP:HB3  | 12       | 1.2           |
| (1,2615) | 1:141:A:PHE:HD2  | 1:147:A:ASP:HB3  | 12       | 1.2           |
| (1,2559) | 1:128:A:TYR:HD1  | 1:164:A:ARG:HD3  | 10       | 1.2           |
| (1,2559) | 1:128:A:TYR:HD2  | 1:164:A:ARG:HD3  | 10       | 1.2           |
| (1,2414) | 1:136:A:ARG:HB3  | 1:159:A:ASN:HD21 | 6        | 1.2           |
| (1,2407) | 1:136:A:ARG:HE   | 1:159:A:ASN:HB3  | 4        | 1.2           |
| (1,1914) | 1:209:A:VAL:HG21 | 1:213:A:MET:H    | 4        | 1.2           |
| (1,1914) | 1:209:A:VAL:HG22 | 1:213:A:MET:H    | 4        | 1.2           |
| (1,1914) | 1:209:A:VAL:HG23 | 1:213:A:MET:H    | 4        | 1.2           |
| (1,1303) | 1:137:A:PRO:HB2  | 1:213:A:MET:HG2  | 18       | 1.2           |
| (1,656)  | 1:138:A:MET:HG3  | 1:154:A:MET:HE1  | 5        | 1.2           |
| (1,656)  | 1:138:A:MET:HG3  | 1:154:A:MET:HE2  | 5        | 1.2           |
| (1,656)  | 1:138:A:MET:HG3  | 1:154:A:MET:HE3  | 5        | 1.2           |
| (1,357)  | 1:122:A:VAL:HG21 | 1:125:A:LEU:HG   | 12       | 1.2           |
| (1,357)  | 1:122:A:VAL:HG22 | 1:125:A:LEU:HG   | 12       | 1.2           |
| (1,357)  | 1:122:A:VAL:HG23 | 1:125:A:LEU:HG   | 12       | 1.2           |
| (1,348)  | 1:122:A:VAL:HG21 | 1:124:A:GLY:HA2  | 12       | 1.2           |
| (1,348)  | 1:122:A:VAL:HG21 | 1:124:A:GLY:HA3  | 12       | 1.2           |
| (1,348)  | 1:122:A:VAL:HG22 | 1:124:A:GLY:HA2  | 12       | 1.2           |
| (1,348)  | 1:122:A:VAL:HG22 | 1:124:A:GLY:HA3  | 12       | 1.2           |
| (1,348)  | 1:122:A:VAL:HG23 | 1:124:A:GLY:HA2  | 12       | 1.2           |
| (1,348)  | 1:122:A:VAL:HG23 | 1:124:A:GLY:HA3  | 12       | 1.2           |
| (1,322)  | 1:158:A:PRO:HD3  | 1:209:A:VAL:HG21 | 20       | 1.2           |
| (1,322)  | 1:158:A:PRO:HD3  | 1:209:A:VAL:HG22 | 20       | 1.2           |
| (1,322)  | 1:158:A:PRO:HD3  | 1:209:A:VAL:HG23 | 20       | 1.2           |
| (1,169)  | 1:198:A:PHE:HB3  | 1:203:A:VAL:HG11 | 5        | 1.2           |
| (1,169)  | 1:198:A:PHE:HB3  | 1:203:A:VAL:HG12 | 5        | 1.2           |
| (1,169)  | 1:198:A:PHE:HB3  | 1:203:A:VAL:HG13 | 5        | 1.2           |
| (1,2711) | 1:145:A:TRP:HZ3  | 1:146:A:GLU:HG3  | 12       | 1.19          |
| (1,2657) | 1:141:A:PHE:HE1  | 1:208:A:ARG:HB3  | 5        | 1.19          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2657) | 1:141:A:PHE:HE2  | 1:208:A:ARG:HB3  | 5        | 1.19          |
| (1,2559) | 1:128:A:TYR:HD1  | 1:164:A:ARG:HD3  | 20       | 1.19          |
| (1,2559) | 1:128:A:TYR:HD2  | 1:164:A:ARG:HD3  | 20       | 1.19          |
| (1,991)  | 1:176:A:VAL:HG11 | 1:211:A:GLU:HG2  | 12       | 1.19          |
| (1,991)  | 1:176:A:VAL:HG12 | 1:211:A:GLU:HG2  | 12       | 1.19          |
| (1,991)  | 1:176:A:VAL:HG13 | 1:211:A:GLU:HG2  | 12       | 1.19          |
| (1,751)  | 1:222:A:SER:HB2  | 1:223:A:GLN:HA   | 5        | 1.19          |
| (1,622)  | 1:134:A:MET:HE1  | 1:161:A:VAL:HG21 | 10       | 1.19          |
| (1,622)  | 1:134:A:MET:HE1  | 1:161:A:VAL:HG22 | 10       | 1.19          |
| (1,622)  | 1:134:A:MET:HE1  | 1:161:A:VAL:HG23 | 10       | 1.19          |
| (1,622)  | 1:134:A:MET:HE2  | 1:161:A:VAL:HG21 | 10       | 1.19          |
| (1,622)  | 1:134:A:MET:HE2  | 1:161:A:VAL:HG22 | 10       | 1.19          |
| (1,622)  | 1:134:A:MET:HE2  | 1:161:A:VAL:HG23 | 10       | 1.19          |
| (1,622)  | 1:134:A:MET:HE3  | 1:161:A:VAL:HG21 | 10       | 1.19          |
| (1,622)  | 1:134:A:MET:HE3  | 1:161:A:VAL:HG22 | 10       | 1.19          |
| (1,622)  | 1:134:A:MET:HE3  | 1:161:A:VAL:HG23 | 10       | 1.19          |
| (1,2421) | 1:127:A:GLY:H    | 1:164:A:ARG:HD3  | 13       | 1.18          |
| (1,2356) | 1:169:A:TYR:HB2  | 1:174:A:ASN:HD21 | 8        | 1.18          |
| (1,2347) | 1:139:A:ILE:HG13 | 1:212:A:GLN:HE22 | 1        | 1.18          |
| (1,2315) | 1:160:A:GLN:HE21 | 1:213:A:MET:HB2  | 19       | 1.18          |
| (1,2315) | 1:160:A:GLN:HE21 | 1:213:A:MET:HB2  | 20       | 1.18          |
| (1,1877) | 1:176:A:VAL:HG21 | 1:218:A:TYR:H    | 12       | 1.18          |
| (1,1877) | 1:176:A:VAL:HG22 | 1:218:A:TYR:H    | 12       | 1.18          |
| (1,1877) | 1:176:A:VAL:HG23 | 1:218:A:TYR:H    | 12       | 1.18          |
| (1,1689) | 1:134:A:MET:H    | 1:159:A:ASN:HB2  | 1        | 1.18          |
| (1,704)  | 1:209:A:VAL:HG21 | 1:213:A:MET:HE1  | 18       | 1.18          |
| (1,704)  | 1:209:A:VAL:HG21 | 1:213:A:MET:HE2  | 18       | 1.18          |
| (1,704)  | 1:209:A:VAL:HG21 | 1:213:A:MET:HE3  | 18       | 1.18          |
| (1,704)  | 1:209:A:VAL:HG22 | 1:213:A:MET:HE1  | 18       | 1.18          |
| (1,704)  | 1:209:A:VAL:HG22 | 1:213:A:MET:HE2  | 18       | 1.18          |
| (1,704)  | 1:209:A:VAL:HG22 | 1:213:A:MET:HE3  | 18       | 1.18          |
| (1,704)  | 1:209:A:VAL:HG23 | 1:213:A:MET:HE1  | 18       | 1.18          |
| (1,704)  | 1:209:A:VAL:HG23 | 1:213:A:MET:HE2  | 18       | 1.18          |
| (1,704)  | 1:209:A:VAL:HG23 | 1:213:A:MET:HE3  | 18       | 1.18          |
| (1,506)  | 1:179:A:CYS:HB2  | 1:214:A:CYS:HB2  | 9        | 1.18          |
| (1,380)  | 1:122:A:VAL:HG21 | 1:123:A:GLY:HA2  | 8        | 1.18          |
| (1,380)  | 1:122:A:VAL:HG21 | 1:123:A:GLY:HA3  | 8        | 1.18          |
| (1,380)  | 1:122:A:VAL:HG22 | 1:123:A:GLY:HA2  | 8        | 1.18          |
| (1,380)  | 1:122:A:VAL:HG22 | 1:123:A:GLY:HA3  | 8        | 1.18          |
| (1,380)  | 1:122:A:VAL:HG23 | 1:123:A:GLY:HA2  | 8        | 1.18          |
| (1,380)  | 1:122:A:VAL:HG23 | 1:123:A:GLY:HA3  | 8        | 1.18          |
| (1,380)  | 1:122:A:VAL:HG21 | 1:123:A:GLY:HA2  | 12       | 1.18          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,380)  | 1:122:A:VAL:HG21 | 1:123:A:GLY:HA3  | 12       | 1.18          |
| (1,380)  | 1:122:A:VAL:HG22 | 1:123:A:GLY:HA2  | 12       | 1.18          |
| (1,380)  | 1:122:A:VAL:HG22 | 1:123:A:GLY:HA3  | 12       | 1.18          |
| (1,380)  | 1:122:A:VAL:HG23 | 1:123:A:GLY:HA2  | 12       | 1.18          |
| (1,380)  | 1:122:A:VAL:HG23 | 1:123:A:GLY:HA3  | 12       | 1.18          |
| (1,309)  | 1:186:A:GLN:HE21 | 1:189:A:VAL:HG11 | 5        | 1.18          |
| (1,309)  | 1:186:A:GLN:HE21 | 1:189:A:VAL:HG12 | 5        | 1.18          |
| (1,309)  | 1:186:A:GLN:HE21 | 1:189:A:VAL:HG13 | 5        | 1.18          |
| (1,177)  | 1:195:A:GLY:HA3  | 1:197:A:ASN:HD21 | 1        | 1.18          |
| (1,158)  | 1:126:A:GLY:HA2  | 1:164:A:ARG:HD3  | 13       | 1.18          |
| (1,2794) | 1:128:A:TYR:HE1  | 1:164:A:ARG:HG2  | 9        | 1.17          |
| (1,2794) | 1:128:A:TYR:HE2  | 1:164:A:ARG:HG2  | 9        | 1.17          |
| (1,2758) | 1:150:A:TYR:HE1  | 1:209:A:VAL:HG11 | 10       | 1.17          |
| (1,2758) | 1:150:A:TYR:HE1  | 1:209:A:VAL:HG12 | 10       | 1.17          |
| (1,2758) | 1:150:A:TYR:HE1  | 1:209:A:VAL:HG13 | 10       | 1.17          |
| (1,2758) | 1:150:A:TYR:HE2  | 1:209:A:VAL:HG11 | 10       | 1.17          |
| (1,2758) | 1:150:A:TYR:HE2  | 1:209:A:VAL:HG12 | 10       | 1.17          |
| (1,2758) | 1:150:A:TYR:HE2  | 1:209:A:VAL:HG13 | 10       | 1.17          |
| (1,2571) | 1:215:A:VAL:HG21 | 1:218:A:TYR:HD1  | 19       | 1.17          |
| (1,2571) | 1:215:A:VAL:HG21 | 1:218:A:TYR:HD2  | 19       | 1.17          |
| (1,2571) | 1:215:A:VAL:HG22 | 1:218:A:TYR:HD1  | 19       | 1.17          |
| (1,2571) | 1:215:A:VAL:HG22 | 1:218:A:TYR:HD2  | 19       | 1.17          |
| (1,2571) | 1:215:A:VAL:HG23 | 1:218:A:TYR:HD1  | 19       | 1.17          |
| (1,2571) | 1:215:A:VAL:HG23 | 1:218:A:TYR:HD2  | 19       | 1.17          |
| (1,2559) | 1:128:A:TYR:HD1  | 1:164:A:ARG:HD3  | 8        | 1.17          |
| (1,2559) | 1:128:A:TYR:HD2  | 1:164:A:ARG:HD3  | 8        | 1.17          |
| (1,2482) | 1:163:A:TYR:HD1  | 1:221:A:GLU:HG2  | 1        | 1.17          |
| (1,2482) | 1:163:A:TYR:HD2  | 1:221:A:GLU:HG2  | 1        | 1.17          |
| (1,2315) | 1:160:A:GLN:HE21 | 1:213:A:MET:HB2  | 15       | 1.17          |
| (1,2250) | 1:217:A:GLN:HE21 | 1:218:A:TYR:HA   | 11       | 1.17          |
| (1,2177) | 1:212:A:GLN:H    | 1:213:A:MET:HG2  | 18       | 1.17          |
| (1,1375) | 1:136:A:ARG:HD2  | 1:154:A:MET:HG3  | 15       | 1.17          |
| (1,1131) | 1:223:A:GLN:HG2  | 1:226:A:TYR:H    | 7        | 1.17          |
| (1,1085) | 1:129:A:MET:HB2  | 1:164:A:ARG:HA   | 15       | 1.17          |
| (1,751)  | 1:222:A:SER:HB2  | 1:223:A:GLN:HA   | 1        | 1.17          |
| (1,380)  | 1:122:A:VAL:HG21 | 1:123:A:GLY:HA2  | 16       | 1.17          |
| (1,380)  | 1:122:A:VAL:HG21 | 1:123:A:GLY:HA3  | 16       | 1.17          |
| (1,380)  | 1:122:A:VAL:HG22 | 1:123:A:GLY:HA2  | 16       | 1.17          |
| (1,380)  | 1:122:A:VAL:HG22 | 1:123:A:GLY:HA3  | 16       | 1.17          |
| (1,380)  | 1:122:A:VAL:HG23 | 1:123:A:GLY:HA2  | 16       | 1.17          |
| (1,380)  | 1:122:A:VAL:HG23 | 1:123:A:GLY:HA3  | 16       | 1.17          |
| (1,2711) | 1:145:A:TRP:HZ3  | 1:146:A:GLU:HG3  | 18       | 1.16          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2615) | 1:141:A:PHE:HD1  | 1:147:A:ASP:HB3  | 2        | 1.16          |
| (1,2615) | 1:141:A:PHE:HD2  | 1:147:A:ASP:HB3  | 2        | 1.16          |
| (1,2571) | 1:215:A:VAL:HG21 | 1:218:A:TYR:HD1  | 2        | 1.16          |
| (1,2571) | 1:215:A:VAL:HG21 | 1:218:A:TYR:HD2  | 2        | 1.16          |
| (1,2571) | 1:215:A:VAL:HG22 | 1:218:A:TYR:HD1  | 2        | 1.16          |
| (1,2571) | 1:215:A:VAL:HG22 | 1:218:A:TYR:HD2  | 2        | 1.16          |
| (1,2571) | 1:215:A:VAL:HG23 | 1:218:A:TYR:HD1  | 2        | 1.16          |
| (1,2571) | 1:215:A:VAL:HG23 | 1:218:A:TYR:HD2  | 2        | 1.16          |
| (1,2559) | 1:128:A:TYR:HD1  | 1:164:A:ARG:HD3  | 11       | 1.16          |
| (1,2559) | 1:128:A:TYR:HD2  | 1:164:A:ARG:HD3  | 11       | 1.16          |
| (1,2541) | 1:175:A:PHE:HD1  | 1:176:A:VAL:HG21 | 12       | 1.16          |
| (1,2541) | 1:175:A:PHE:HD1  | 1:176:A:VAL:HG22 | 12       | 1.16          |
| (1,2541) | 1:175:A:PHE:HD1  | 1:176:A:VAL:HG23 | 12       | 1.16          |
| (1,2541) | 1:175:A:PHE:HD2  | 1:176:A:VAL:HG21 | 12       | 1.16          |
| (1,2541) | 1:175:A:PHE:HD2  | 1:176:A:VAL:HG22 | 12       | 1.16          |
| (1,2541) | 1:175:A:PHE:HD2  | 1:176:A:VAL:HG23 | 12       | 1.16          |
| (1,2414) | 1:136:A:ARG:HB3  | 1:159:A:ASN:HD21 | 9        | 1.16          |
| (1,2347) | 1:139:A:ILE:HG13 | 1:212:A:GLN:HE22 | 2        | 1.16          |
| (1,2338) | 1:212:A:GLN:HE21 | 1:215:A:VAL:HG11 | 19       | 1.16          |
| (1,2338) | 1:212:A:GLN:HE21 | 1:215:A:VAL:HG12 | 19       | 1.16          |
| (1,2338) | 1:212:A:GLN:HE21 | 1:215:A:VAL:HG13 | 19       | 1.16          |
| (1,2315) | 1:160:A:GLN:HE21 | 1:213:A:MET:HB2  | 8        | 1.16          |
| (1,1231) | 1:209:A:VAL:HG21 | 1:213:A:MET:HG3  | 4        | 1.16          |
| (1,1231) | 1:209:A:VAL:HG22 | 1:213:A:MET:HG3  | 4        | 1.16          |
| (1,1231) | 1:209:A:VAL:HG23 | 1:213:A:MET:HG3  | 4        | 1.16          |
| (1,921)  | 1:167:A:SER:HA   | 1:168:A:GLN:HG3  | 2        | 1.16          |
| (1,445)  | 1:180:A:VAL:HA   | 1:184:A:ILE:HG12 | 11       | 1.16          |
| (1,396)  | 1:210:A:VAL:HA   | 1:213:A:MET:HB3  | 20       | 1.16          |
| (1,380)  | 1:122:A:VAL:HG21 | 1:123:A:GLY:HA2  | 15       | 1.16          |
| (1,380)  | 1:122:A:VAL:HG21 | 1:123:A:GLY:HA3  | 15       | 1.16          |
| (1,380)  | 1:122:A:VAL:HG22 | 1:123:A:GLY:HA2  | 15       | 1.16          |
| (1,380)  | 1:122:A:VAL:HG22 | 1:123:A:GLY:HA3  | 15       | 1.16          |
| (1,380)  | 1:122:A:VAL:HG23 | 1:123:A:GLY:HA2  | 15       | 1.16          |
| (1,380)  | 1:122:A:VAL:HG23 | 1:123:A:GLY:HA3  | 15       | 1.16          |
| (1,342)  | 1:189:A:VAL:HG11 | 1:190:A:THR:HA   | 11       | 1.16          |
| (1,342)  | 1:189:A:VAL:HG12 | 1:190:A:THR:HA   | 11       | 1.16          |
| (1,342)  | 1:189:A:VAL:HG13 | 1:190:A:THR:HA   | 11       | 1.16          |
| (1,309)  | 1:186:A:GLN:HE21 | 1:189:A:VAL:HG11 | 3        | 1.16          |
| (1,309)  | 1:186:A:GLN:HE21 | 1:189:A:VAL:HG12 | 3        | 1.16          |
| (1,309)  | 1:186:A:GLN:HE21 | 1:189:A:VAL:HG13 | 3        | 1.16          |
| (1,177)  | 1:195:A:GLY:HA3  | 1:197:A:ASN:HD21 | 10       | 1.16          |
| (1,169)  | 1:198:A:PHE:HB3  | 1:203:A:VAL:HG11 | 7        | 1.16          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,169)  | 1:198:A:PHE:HB3  | 1:203:A:VAL:HG12 | 7        | 1.16          |
| (1,169)  | 1:198:A:PHE:HB3  | 1:203:A:VAL:HG13 | 7        | 1.16          |
| (1,160)  | 1:223:A:GLN:HE21 | 1:228:A:GLY:HA2  | 19       | 1.16          |
| (1,160)  | 1:223:A:GLN:HE21 | 1:228:A:GLY:HA3  | 19       | 1.16          |
| (1,2846) | 1:157:A:TYR:HE1  | 1:206:A:MET:HB2  | 2        | 1.15          |
| (1,2846) | 1:157:A:TYR:HE2  | 1:206:A:MET:HB2  | 2        | 1.15          |
| (1,2571) | 1:215:A:VAL:HG21 | 1:218:A:TYR:HD1  | 12       | 1.15          |
| (1,2571) | 1:215:A:VAL:HG21 | 1:218:A:TYR:HD2  | 12       | 1.15          |
| (1,2571) | 1:215:A:VAL:HG22 | 1:218:A:TYR:HD1  | 12       | 1.15          |
| (1,2571) | 1:215:A:VAL:HG22 | 1:218:A:TYR:HD2  | 12       | 1.15          |
| (1,2571) | 1:215:A:VAL:HG23 | 1:218:A:TYR:HD1  | 12       | 1.15          |
| (1,2571) | 1:215:A:VAL:HG23 | 1:218:A:TYR:HD2  | 12       | 1.15          |
| (1,2559) | 1:128:A:TYR:HD1  | 1:164:A:ARG:HD3  | 6        | 1.15          |
| (1,2559) | 1:128:A:TYR:HD2  | 1:164:A:ARG:HD3  | 6        | 1.15          |
| (1,2254) | 1:217:A:GLN:HE22 | 1:220:A:LYS:HE2  | 7        | 1.15          |
| (1,2254) | 1:217:A:GLN:HE22 | 1:220:A:LYS:HE3  | 7        | 1.15          |
| (1,2177) | 1:212:A:GLN:H    | 1:213:A:MET:HG2  | 8        | 1.15          |
| (1,1937) | 1:220:A:LYS:H    | 1:221:A:GLU:HG3  | 7        | 1.15          |
| (1,1459) | 1:136:A:ARG:HB3  | 1:159:A:ASN:HB3  | 6        | 1.15          |
| (1,1131) | 1:223:A:GLN:HG2  | 1:226:A:TYR:H    | 9        | 1.15          |
| (1,1089) | 1:182:A:ILE:HD11 | 1:186:A:GLN:HE21 | 13       | 1.15          |
| (1,1089) | 1:182:A:ILE:HD12 | 1:186:A:GLN:HE21 | 13       | 1.15          |
| (1,1089) | 1:182:A:ILE:HD13 | 1:186:A:GLN:HE21 | 13       | 1.15          |
| (1,637)  | 1:147:A:ASP:HB2  | 1:148:A:ARG:HG2  | 13       | 1.15          |
| (1,506)  | 1:179:A:CYS:HB2  | 1:214:A:CYS:HB2  | 19       | 1.15          |
| (1,396)  | 1:210:A:VAL:HA   | 1:213:A:MET:HB3  | 16       | 1.15          |
| (1,173)  | 1:198:A:PHE:HB2  | 1:203:A:VAL:HG11 | 7        | 1.15          |
| (1,173)  | 1:198:A:PHE:HB2  | 1:203:A:VAL:HG12 | 7        | 1.15          |
| (1,173)  | 1:198:A:PHE:HB2  | 1:203:A:VAL:HG13 | 7        | 1.15          |
| (1,101)  | 1:138:A:MET:HA   | 1:209:A:VAL:HG11 | 18       | 1.15          |
| (1,101)  | 1:138:A:MET:HA   | 1:209:A:VAL:HG12 | 18       | 1.15          |
| (1,101)  | 1:138:A:MET:HA   | 1:209:A:VAL:HG13 | 18       | 1.15          |
| (1,2851) | 1:184:A:ILE:HG13 | 1:187:A:HIS:HE1  | 6        | 1.14          |
| (1,2851) | 1:184:A:ILE:HG13 | 1:187:A:HIS:HE1  | 17       | 1.14          |
| (1,2571) | 1:215:A:VAL:HG21 | 1:218:A:TYR:HD1  | 6        | 1.14          |
| (1,2571) | 1:215:A:VAL:HG21 | 1:218:A:TYR:HD2  | 6        | 1.14          |
| (1,2571) | 1:215:A:VAL:HG22 | 1:218:A:TYR:HD1  | 6        | 1.14          |
| (1,2571) | 1:215:A:VAL:HG22 | 1:218:A:TYR:HD2  | 6        | 1.14          |
| (1,2571) | 1:215:A:VAL:HG23 | 1:218:A:TYR:HD1  | 6        | 1.14          |
| (1,2571) | 1:215:A:VAL:HG23 | 1:218:A:TYR:HD2  | 6        | 1.14          |
| (1,2510) | 1:226:A:TYR:HD1  | 1:229:A:ARG:HB2  | 5        | 1.14          |
| (1,2510) | 1:226:A:TYR:HD2  | 1:229:A:ARG:HB2  | 5        | 1.14          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2421) | 1:127:A:GLY:H    | 1:164:A:ARG:HD3  | 8        | 1.14          |
| (1,2320) | 1:160:A:GLN:HE22 | 1:213:A:MET:HB2  | 5        | 1.14          |
| (1,2320) | 1:160:A:GLN:HE22 | 1:213:A:MET:HB2  | 7        | 1.14          |
| (1,2320) | 1:160:A:GLN:HE22 | 1:213:A:MET:HB2  | 8        | 1.14          |
| (1,2123) | 1:199:A:THR:H    | 1:203:A:VAL:HG11 | 7        | 1.14          |
| (1,2123) | 1:199:A:THR:H    | 1:203:A:VAL:HG12 | 7        | 1.14          |
| (1,2123) | 1:199:A:THR:H    | 1:203:A:VAL:HG13 | 7        | 1.14          |
| (1,1283) | 1:206:A:MET:HG2  | 1:207:A:GLU:HG3  | 14       | 1.14          |
| (1,1096) | 1:165:A:PRO:HD3  | 1:168:A:GLN:HG2  | 18       | 1.14          |
| (1,423)  | 1:151:A:ARG:HD3  | 1:152:A:GLU:H    | 4        | 1.14          |
| (1,396)  | 1:210:A:VAL:HA   | 1:213:A:MET:HB3  | 17       | 1.14          |
| (1,396)  | 1:210:A:VAL:HA   | 1:213:A:MET:HB3  | 19       | 1.14          |
| (1,348)  | 1:122:A:VAL:HG21 | 1:124:A:GLY:HA2  | 2        | 1.14          |
| (1,348)  | 1:122:A:VAL:HG21 | 1:124:A:GLY:HA3  | 2        | 1.14          |
| (1,348)  | 1:122:A:VAL:HG22 | 1:124:A:GLY:HA2  | 2        | 1.14          |
| (1,348)  | 1:122:A:VAL:HG22 | 1:124:A:GLY:HA3  | 2        | 1.14          |
| (1,348)  | 1:122:A:VAL:HG23 | 1:124:A:GLY:HA2  | 2        | 1.14          |
| (1,348)  | 1:122:A:VAL:HG23 | 1:124:A:GLY:HA3  | 2        | 1.14          |
| (1,2315) | 1:160:A:GLN:HE21 | 1:213:A:MET:HB2  | 5        | 1.13          |
| (1,1679) | 1:122:A:VAL:HG21 | 1:125:A:LEU:H    | 4        | 1.13          |
| (1,1679) | 1:122:A:VAL:HG22 | 1:125:A:LEU:H    | 4        | 1.13          |
| (1,1679) | 1:122:A:VAL:HG23 | 1:125:A:LEU:H    | 4        | 1.13          |
| (1,1344) | 1:206:A:MET:HB3  | 1:210:A:VAL:HB   | 13       | 1.13          |
| (1,1235) | 1:205:A:MET:HG3  | 1:206:A:MET:HG2  | 15       | 1.13          |
| (1,1131) | 1:223:A:GLN:HG2  | 1:226:A:TYR:H    | 17       | 1.13          |
| (1,169)  | 1:198:A:PHE:HB3  | 1:203:A:VAL:HG11 | 2        | 1.13          |
| (1,169)  | 1:198:A:PHE:HB3  | 1:203:A:VAL:HG12 | 2        | 1.13          |
| (1,169)  | 1:198:A:PHE:HB3  | 1:203:A:VAL:HG13 | 2        | 1.13          |
| (1,159)  | 1:228:A:GLY:HA2  | 1:230:A:ARG:HD2  | 11       | 1.13          |
| (1,159)  | 1:228:A:GLY:HA3  | 1:230:A:ARG:HD2  | 11       | 1.13          |
| (1,158)  | 1:126:A:GLY:HA2  | 1:164:A:ARG:HD3  | 20       | 1.13          |
| (1,78)   | 1:139:A:ILE:HB   | 1:209:A:VAL:HG11 | 17       | 1.13          |
| (1,78)   | 1:139:A:ILE:HB   | 1:209:A:VAL:HG12 | 17       | 1.13          |
| (1,78)   | 1:139:A:ILE:HB   | 1:209:A:VAL:HG13 | 17       | 1.13          |
| (1,2846) | 1:157:A:TYR:HE1  | 1:206:A:MET:HB2  | 18       | 1.12          |
| (1,2846) | 1:157:A:TYR:HE2  | 1:206:A:MET:HB2  | 18       | 1.12          |
| (1,2711) | 1:145:A:TRP:HZ3  | 1:146:A:GLU:HG3  | 1        | 1.12          |
| (1,2571) | 1:215:A:VAL:HG21 | 1:218:A:TYR:HD1  | 14       | 1.12          |
| (1,2571) | 1:215:A:VAL:HG21 | 1:218:A:TYR:HD2  | 14       | 1.12          |
| (1,2571) | 1:215:A:VAL:HG22 | 1:218:A:TYR:HD1  | 14       | 1.12          |
| (1,2571) | 1:215:A:VAL:HG22 | 1:218:A:TYR:HD2  | 14       | 1.12          |
| (1,2571) | 1:215:A:VAL:HG23 | 1:218:A:TYR:HD1  | 14       | 1.12          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2571) | 1:215:A:VAL:HG23 | 1:218:A:TYR:HD2  | 14       | 1.12          |
| (1,2177) | 1:212:A:GLN:H    | 1:213:A:MET:HG2  | 10       | 1.12          |
| (1,1937) | 1:220:A:LYS:H    | 1:221:A:GLU:HG3  | 6        | 1.12          |
| (1,1095) | 1:165:A:PRO:HA   | 1:168:A:GLN:HG2  | 18       | 1.12          |
| (1,751)  | 1:222:A:SER:HB2  | 1:223:A:GLN:HA   | 12       | 1.12          |
| (1,502)  | 1:162:A:TYR:HB3  | 1:183:A:THR:HA   | 10       | 1.12          |
| (1,78)   | 1:139:A:ILE:HB   | 1:209:A:VAL:HG11 | 2        | 1.12          |
| (1,78)   | 1:139:A:ILE:HB   | 1:209:A:VAL:HG12 | 2        | 1.12          |
| (1,78)   | 1:139:A:ILE:HB   | 1:209:A:VAL:HG13 | 2        | 1.12          |
| (1,78)   | 1:139:A:ILE:HB   | 1:209:A:VAL:HG11 | 12       | 1.12          |
| (1,78)   | 1:139:A:ILE:HB   | 1:209:A:VAL:HG12 | 12       | 1.12          |
| (1,78)   | 1:139:A:ILE:HB   | 1:209:A:VAL:HG13 | 12       | 1.12          |
| (1,2847) | 1:157:A:TYR:HE1  | 1:209:A:VAL:HG11 | 4        | 1.11          |
| (1,2847) | 1:157:A:TYR:HE1  | 1:209:A:VAL:HG12 | 4        | 1.11          |
| (1,2847) | 1:157:A:TYR:HE1  | 1:209:A:VAL:HG13 | 4        | 1.11          |
| (1,2847) | 1:157:A:TYR:HE2  | 1:209:A:VAL:HG11 | 4        | 1.11          |
| (1,2847) | 1:157:A:TYR:HE2  | 1:209:A:VAL:HG12 | 4        | 1.11          |
| (1,2847) | 1:157:A:TYR:HE2  | 1:209:A:VAL:HG13 | 4        | 1.11          |
| (1,2657) | 1:141:A:PHE:HE1  | 1:208:A:ARG:HB3  | 12       | 1.11          |
| (1,2657) | 1:141:A:PHE:HE2  | 1:208:A:ARG:HB3  | 12       | 1.11          |
| (1,2593) | 1:175:A:PHE:HE1  | 1:221:A:GLU:HG2  | 20       | 1.11          |
| (1,2593) | 1:175:A:PHE:HE2  | 1:221:A:GLU:HG2  | 20       | 1.11          |
| (1,2374) | 1:168:A:GLN:HE22 | 1:169:A:TYR:HE1  | 15       | 1.11          |
| (1,2374) | 1:168:A:GLN:HE22 | 1:169:A:TYR:HE2  | 15       | 1.11          |
| (1,2338) | 1:212:A:GLN:HE21 | 1:215:A:VAL:HG11 | 6        | 1.11          |
| (1,2338) | 1:212:A:GLN:HE21 | 1:215:A:VAL:HG12 | 6        | 1.11          |
| (1,2338) | 1:212:A:GLN:HE21 | 1:215:A:VAL:HG13 | 6        | 1.11          |
| (1,2338) | 1:212:A:GLN:HE21 | 1:215:A:VAL:HG11 | 14       | 1.11          |
| (1,2338) | 1:212:A:GLN:HE21 | 1:215:A:VAL:HG12 | 14       | 1.11          |
| (1,2338) | 1:212:A:GLN:HE21 | 1:215:A:VAL:HG13 | 14       | 1.11          |
| (1,1344) | 1:206:A:MET:HB3  | 1:210:A:VAL:HB   | 16       | 1.11          |
| (1,1097) | 1:165:A:PRO:HB3  | 1:168:A:GLN:HG2  | 5        | 1.11          |
| (1,751)  | 1:222:A:SER:HB2  | 1:223:A:GLN:HA   | 7        | 1.11          |
| (1,470)  | 1:122:A:VAL:HG21 | 1:125:A:LEU:HB2  | 2        | 1.11          |
| (1,470)  | 1:122:A:VAL:HG22 | 1:125:A:LEU:HB2  | 2        | 1.11          |
| (1,470)  | 1:122:A:VAL:HG23 | 1:125:A:LEU:HB2  | 2        | 1.11          |
| (1,467)  | 1:122:A:VAL:HG21 | 1:125:A:LEU:HB3  | 15       | 1.11          |
| (1,467)  | 1:122:A:VAL:HG22 | 1:125:A:LEU:HB3  | 15       | 1.11          |
| (1,467)  | 1:122:A:VAL:HG23 | 1:125:A:LEU:HB3  | 15       | 1.11          |
| (1,396)  | 1:210:A:VAL:HA   | 1:213:A:MET:HB3  | 3        | 1.11          |
| (1,309)  | 1:186:A:GLN:HE21 | 1:189:A:VAL:HG11 | 16       | 1.11          |
| (1,309)  | 1:186:A:GLN:HE21 | 1:189:A:VAL:HG12 | 16       | 1.11          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,309)  | 1:186:A:GLN:HE21 | 1:189:A:VAL:HG13 | 16       | 1.11          |
| (1,273)  | 1:166:A:VAL:HG11 | 1:225:A:TYR:HB2  | 1        | 1.11          |
| (1,273)  | 1:166:A:VAL:HG12 | 1:225:A:TYR:HB2  | 1        | 1.11          |
| (1,273)  | 1:166:A:VAL:HG13 | 1:225:A:TYR:HB2  | 1        | 1.11          |
| (1,2681) | 1:141:A:PHE:HZ   | 1:208:A:ARG:HB3  | 6        | 1.1           |
| (1,2615) | 1:141:A:PHE:HD1  | 1:147:A:ASP:HB3  | 13       | 1.1           |
| (1,2615) | 1:141:A:PHE:HD2  | 1:147:A:ASP:HB3  | 13       | 1.1           |
| (1,2571) | 1:215:A:VAL:HG21 | 1:218:A:TYR:HD1  | 8        | 1.1           |
| (1,2571) | 1:215:A:VAL:HG21 | 1:218:A:TYR:HD2  | 8        | 1.1           |
| (1,2571) | 1:215:A:VAL:HG22 | 1:218:A:TYR:HD1  | 8        | 1.1           |
| (1,2571) | 1:215:A:VAL:HG22 | 1:218:A:TYR:HD2  | 8        | 1.1           |
| (1,2571) | 1:215:A:VAL:HG23 | 1:218:A:TYR:HD1  | 8        | 1.1           |
| (1,2571) | 1:215:A:VAL:HG23 | 1:218:A:TYR:HD2  | 8        | 1.1           |
| (1,2482) | 1:163:A:TYR:HD1  | 1:221:A:GLU:HG2  | 10       | 1.1           |
| (1,2482) | 1:163:A:TYR:HD2  | 1:221:A:GLU:HG2  | 10       | 1.1           |
| (1,2414) | 1:136:A:ARG:HB3  | 1:159:A:ASN:HD21 | 13       | 1.1           |
| (1,2177) | 1:212:A:GLN:H    | 1:213:A:MET:HG2  | 12       | 1.1           |
| (1,1344) | 1:206:A:MET:HB3  | 1:210:A:VAL:HB   | 9        | 1.1           |
| (1,506)  | 1:179:A:CYS:HB2  | 1:214:A:CYS:HB2  | 20       | 1.1           |
| (1,423)  | 1:151:A:ARG:HD3  | 1:152:A:GLU:H    | 12       | 1.1           |
| (1,273)  | 1:166:A:VAL:HG11 | 1:225:A:TYR:HB2  | 12       | 1.1           |
| (1,273)  | 1:166:A:VAL:HG12 | 1:225:A:TYR:HB2  | 12       | 1.1           |
| (1,273)  | 1:166:A:VAL:HG13 | 1:225:A:TYR:HB2  | 12       | 1.1           |
| (1,2851) | 1:184:A:ILE:HG13 | 1:187:A:HIS:HE1  | 7        | 1.09          |
| (1,2356) | 1:169:A:TYR:HB2  | 1:174:A:ASN:HD21 | 20       | 1.09          |
| (1,1459) | 1:136:A:ARG:HB3  | 1:159:A:ASN:HB3  | 3        | 1.09          |
| (1,380)  | 1:122:A:VAL:HG21 | 1:123:A:GLY:HA2  | 4        | 1.09          |
| (1,380)  | 1:122:A:VAL:HG21 | 1:123:A:GLY:HA3  | 4        | 1.09          |
| (1,380)  | 1:122:A:VAL:HG22 | 1:123:A:GLY:HA2  | 4        | 1.09          |
| (1,380)  | 1:122:A:VAL:HG22 | 1:123:A:GLY:HA3  | 4        | 1.09          |
| (1,380)  | 1:122:A:VAL:HG23 | 1:123:A:GLY:HA2  | 4        | 1.09          |
| (1,380)  | 1:122:A:VAL:HG23 | 1:123:A:GLY:HA3  | 4        | 1.09          |
| (1,269)  | 1:165:A:PRO:HB3  | 1:166:A:VAL:HG11 | 1        | 1.09          |
| (1,269)  | 1:165:A:PRO:HB3  | 1:166:A:VAL:HG12 | 1        | 1.09          |
| (1,269)  | 1:165:A:PRO:HB3  | 1:166:A:VAL:HG13 | 1        | 1.09          |
| (1,258)  | 1:122:A:VAL:HG11 | 1:190:A:THR:HG21 | 19       | 1.09          |
| (1,258)  | 1:122:A:VAL:HG11 | 1:190:A:THR:HG22 | 19       | 1.09          |
| (1,258)  | 1:122:A:VAL:HG11 | 1:190:A:THR:HG23 | 19       | 1.09          |
| (1,258)  | 1:122:A:VAL:HG12 | 1:190:A:THR:HG21 | 19       | 1.09          |
| (1,258)  | 1:122:A:VAL:HG12 | 1:190:A:THR:HG22 | 19       | 1.09          |
| (1,258)  | 1:122:A:VAL:HG12 | 1:190:A:THR:HG23 | 19       | 1.09          |
| (1,258)  | 1:122:A:VAL:HG13 | 1:190:A:THR:HG21 | 19       | 1.09          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,258)  | 1:122:A:VAL:HG13 | 1:190:A:THR:HG22 | 19       | 1.09          |
| (1,258)  | 1:122:A:VAL:HG13 | 1:190:A:THR:HG23 | 19       | 1.09          |
| (1,89)   | 1:206:A:MET:HB3  | 1:210:A:VAL:HG21 | 10       | 1.09          |
| (1,89)   | 1:206:A:MET:HB3  | 1:210:A:VAL:HG22 | 10       | 1.09          |
| (1,89)   | 1:206:A:MET:HB3  | 1:210:A:VAL:HG23 | 10       | 1.09          |
| (1,2847) | 1:157:A:TYR:HE1  | 1:209:A:VAL:HG11 | 7        | 1.08          |
| (1,2847) | 1:157:A:TYR:HE1  | 1:209:A:VAL:HG12 | 7        | 1.08          |
| (1,2847) | 1:157:A:TYR:HE1  | 1:209:A:VAL:HG13 | 7        | 1.08          |
| (1,2847) | 1:157:A:TYR:HE2  | 1:209:A:VAL:HG11 | 7        | 1.08          |
| (1,2847) | 1:157:A:TYR:HE2  | 1:209:A:VAL:HG12 | 7        | 1.08          |
| (1,2847) | 1:157:A:TYR:HE2  | 1:209:A:VAL:HG13 | 7        | 1.08          |
| (1,2782) | 1:150:A:TYR:HE1  | 1:154:A:MET:HG3  | 12       | 1.08          |
| (1,2782) | 1:150:A:TYR:HE2  | 1:154:A:MET:HG3  | 12       | 1.08          |
| (1,2681) | 1:141:A:PHE:HZ   | 1:208:A:ARG:HB3  | 5        | 1.08          |
| (1,2347) | 1:139:A:ILE:HG13 | 1:212:A:GLN:HE22 | 8        | 1.08          |
| (1,2347) | 1:139:A:ILE:HG13 | 1:212:A:GLN:HE22 | 13       | 1.08          |
| (1,2338) | 1:212:A:GLN:HE21 | 1:215:A:VAL:HG11 | 13       | 1.08          |
| (1,2338) | 1:212:A:GLN:HE21 | 1:215:A:VAL:HG12 | 13       | 1.08          |
| (1,2338) | 1:212:A:GLN:HE21 | 1:215:A:VAL:HG13 | 13       | 1.08          |
| (1,2320) | 1:160:A:GLN:HE22 | 1:213:A:MET:HB2  | 20       | 1.08          |
| (1,2177) | 1:212:A:GLN:H    | 1:213:A:MET:HG2  | 14       | 1.08          |
| (1,1914) | 1:209:A:VAL:HG21 | 1:213:A:MET:H    | 20       | 1.08          |
| (1,1914) | 1:209:A:VAL:HG22 | 1:213:A:MET:H    | 20       | 1.08          |
| (1,1914) | 1:209:A:VAL:HG23 | 1:213:A:MET:H    | 20       | 1.08          |
| (1,1375) | 1:136:A:ARG:HD2  | 1:154:A:MET:HG3  | 9        | 1.08          |
| (1,1256) | 1:184:A:ILE:HG13 | 1:206:A:MET:HG3  | 10       | 1.08          |
| (1,1231) | 1:209:A:VAL:HG21 | 1:213:A:MET:HG3  | 14       | 1.08          |
| (1,1231) | 1:209:A:VAL:HG22 | 1:213:A:MET:HG3  | 14       | 1.08          |
| (1,1231) | 1:209:A:VAL:HG23 | 1:213:A:MET:HG3  | 14       | 1.08          |
| (1,567)  | 1:230:A:ARG:HB2  | 1:231:A:SER:HB3  | 4        | 1.08          |
| (1,423)  | 1:151:A:ARG:HD3  | 1:152:A:GLU:H    | 16       | 1.08          |
| (1,396)  | 1:210:A:VAL:HA   | 1:213:A:MET:HB3  | 1        | 1.08          |
| (1,396)  | 1:210:A:VAL:HA   | 1:213:A:MET:HB3  | 9        | 1.08          |
| (1,273)  | 1:166:A:VAL:HG11 | 1:225:A:TYR:HB2  | 17       | 1.08          |
| (1,273)  | 1:166:A:VAL:HG12 | 1:225:A:TYR:HB2  | 17       | 1.08          |
| (1,273)  | 1:166:A:VAL:HG13 | 1:225:A:TYR:HB2  | 17       | 1.08          |
| (1,2847) | 1:157:A:TYR:HE1  | 1:209:A:VAL:HG11 | 1        | 1.07          |
| (1,2847) | 1:157:A:TYR:HE1  | 1:209:A:VAL:HG12 | 1        | 1.07          |
| (1,2847) | 1:157:A:TYR:HE1  | 1:209:A:VAL:HG13 | 1        | 1.07          |
| (1,2847) | 1:157:A:TYR:HE2  | 1:209:A:VAL:HG11 | 1        | 1.07          |
| (1,2847) | 1:157:A:TYR:HE2  | 1:209:A:VAL:HG12 | 1        | 1.07          |
| (1,2847) | 1:157:A:TYR:HE2  | 1:209:A:VAL:HG13 | 1        | 1.07          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2347) | 1:139:A:ILE:HG13 | 1:212:A:GLN:HE22 | 14       | 1.07          |
| (1,2347) | 1:139:A:ILE:HG13 | 1:212:A:GLN:HE22 | 19       | 1.07          |
| (1,2320) | 1:160:A:GLN:HE22 | 1:213:A:MET:HB2  | 9        | 1.07          |
| (1,2054) | 1:166:A:VAL:HG11 | 1:221:A:GLU:H    | 17       | 1.07          |
| (1,2054) | 1:166:A:VAL:HG12 | 1:221:A:GLU:H    | 17       | 1.07          |
| (1,2054) | 1:166:A:VAL:HG13 | 1:221:A:GLU:H    | 17       | 1.07          |
| (1,423)  | 1:151:A:ARG:HD3  | 1:152:A:GLU:H    | 9        | 1.07          |
| (1,158)  | 1:126:A:GLY:HA2  | 1:164:A:ARG:HD3  | 17       | 1.07          |
| (1,2711) | 1:145:A:TRP:HZ3  | 1:146:A:GLU:HG3  | 9        | 1.06          |
| (1,2352) | 1:171:A:ASN:HA   | 1:174:A:ASN:HD21 | 4        | 1.06          |
| (1,2320) | 1:160:A:GLN:HE22 | 1:213:A:MET:HB2  | 11       | 1.06          |
| (1,1256) | 1:184:A:ILE:HG13 | 1:206:A:MET:HG3  | 3        | 1.06          |
| (1,1235) | 1:205:A:MET:HG3  | 1:206:A:MET:HG2  | 13       | 1.06          |
| (1,1073) | 1:166:A:VAL:HG11 | 1:221:A:GLU:HA   | 3        | 1.06          |
| (1,1073) | 1:166:A:VAL:HG12 | 1:221:A:GLU:HA   | 3        | 1.06          |
| (1,1073) | 1:166:A:VAL:HG13 | 1:221:A:GLU:HA   | 3        | 1.06          |
| (1,467)  | 1:122:A:VAL:HG21 | 1:125:A:LEU:HB3  | 1        | 1.06          |
| (1,467)  | 1:122:A:VAL:HG22 | 1:125:A:LEU:HB3  | 1        | 1.06          |
| (1,467)  | 1:122:A:VAL:HG23 | 1:125:A:LEU:HB3  | 1        | 1.06          |
| (1,380)  | 1:122:A:VAL:HG21 | 1:123:A:GLY:HA2  | 6        | 1.06          |
| (1,380)  | 1:122:A:VAL:HG21 | 1:123:A:GLY:HA3  | 6        | 1.06          |
| (1,380)  | 1:122:A:VAL:HG22 | 1:123:A:GLY:HA2  | 6        | 1.06          |
| (1,380)  | 1:122:A:VAL:HG22 | 1:123:A:GLY:HA3  | 6        | 1.06          |
| (1,380)  | 1:122:A:VAL:HG23 | 1:123:A:GLY:HA2  | 6        | 1.06          |
| (1,380)  | 1:122:A:VAL:HG23 | 1:123:A:GLY:HA3  | 6        | 1.06          |
| (1,348)  | 1:122:A:VAL:HG21 | 1:124:A:GLY:HA2  | 9        | 1.06          |
| (1,348)  | 1:122:A:VAL:HG21 | 1:124:A:GLY:HA3  | 9        | 1.06          |
| (1,348)  | 1:122:A:VAL:HG22 | 1:124:A:GLY:HA2  | 9        | 1.06          |
| (1,348)  | 1:122:A:VAL:HG22 | 1:124:A:GLY:HA3  | 9        | 1.06          |
| (1,348)  | 1:122:A:VAL:HG23 | 1:124:A:GLY:HA2  | 9        | 1.06          |
| (1,348)  | 1:122:A:VAL:HG23 | 1:124:A:GLY:HA3  | 9        | 1.06          |
| (1,2518) | 1:155:A:TYR:HD1  | 1:156:A:ARG:HD2  | 4        | 1.05          |
| (1,2518) | 1:155:A:TYR:HD2  | 1:156:A:ARG:HD2  | 4        | 1.05          |
| (1,2352) | 1:171:A:ASN:HA   | 1:174:A:ASN:HD21 | 7        | 1.05          |
| (1,2320) | 1:160:A:GLN:HE22 | 1:213:A:MET:HB2  | 12       | 1.05          |
| (1,2315) | 1:160:A:GLN:HE21 | 1:213:A:MET:HB2  | 9        | 1.05          |
| (1,1914) | 1:209:A:VAL:HG21 | 1:213:A:MET:H    | 14       | 1.05          |
| (1,1914) | 1:209:A:VAL:HG22 | 1:213:A:MET:H    | 14       | 1.05          |
| (1,1914) | 1:209:A:VAL:HG23 | 1:213:A:MET:H    | 14       | 1.05          |
| (1,1231) | 1:209:A:VAL:HG21 | 1:213:A:MET:HG3  | 8        | 1.05          |
| (1,1231) | 1:209:A:VAL:HG22 | 1:213:A:MET:HG3  | 8        | 1.05          |
| (1,1231) | 1:209:A:VAL:HG23 | 1:213:A:MET:HG3  | 8        | 1.05          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,912)  | 1:176:A:VAL:HG11 | 1:177:A:HIS:HA   | 12       | 1.05          |
| (1,912)  | 1:176:A:VAL:HG12 | 1:177:A:HIS:HA   | 12       | 1.05          |
| (1,912)  | 1:176:A:VAL:HG13 | 1:177:A:HIS:HA   | 12       | 1.05          |
| (1,396)  | 1:210:A:VAL:HA   | 1:213:A:MET:HB3  | 2        | 1.05          |
| (1,2824) | 1:218:A:TYR:HE1  | 1:222:A:SER:HB3  | 1        | 1.04          |
| (1,2824) | 1:218:A:TYR:HE2  | 1:222:A:SER:HB3  | 1        | 1.04          |
| (1,2721) | 1:177:A:HIS:HD2  | 1:178:A:ASP:HB3  | 16       | 1.04          |
| (1,2650) | 1:139:A:ILE:HG12 | 1:141:A:PHE:HE1  | 1        | 1.04          |
| (1,2650) | 1:139:A:ILE:HG12 | 1:141:A:PHE:HE2  | 1        | 1.04          |
| (1,2482) | 1:163:A:TYR:HD1  | 1:221:A:GLU:HG2  | 5        | 1.04          |
| (1,2482) | 1:163:A:TYR:HD2  | 1:221:A:GLU:HG2  | 5        | 1.04          |
| (1,2414) | 1:136:A:ARG:HB3  | 1:159:A:ASN:HD21 | 8        | 1.04          |
| (1,2315) | 1:160:A:GLN:HE21 | 1:213:A:MET:HB2  | 11       | 1.04          |
| (1,2177) | 1:212:A:GLN:H    | 1:213:A:MET:HG2  | 13       | 1.04          |
| (1,1207) | 1:168:A:GLN:HA   | 1:168:A:GLN:HE22 | 19       | 1.04          |
| (1,98)   | 1:139:A:ILE:HG21 | 1:209:A:VAL:HG11 | 18       | 1.04          |
| (1,98)   | 1:139:A:ILE:HG21 | 1:209:A:VAL:HG12 | 18       | 1.04          |
| (1,98)   | 1:139:A:ILE:HG21 | 1:209:A:VAL:HG13 | 18       | 1.04          |
| (1,98)   | 1:139:A:ILE:HG22 | 1:209:A:VAL:HG11 | 18       | 1.04          |
| (1,98)   | 1:139:A:ILE:HG22 | 1:209:A:VAL:HG12 | 18       | 1.04          |
| (1,98)   | 1:139:A:ILE:HG22 | 1:209:A:VAL:HG13 | 18       | 1.04          |
| (1,98)   | 1:139:A:ILE:HG23 | 1:209:A:VAL:HG11 | 18       | 1.04          |
| (1,98)   | 1:139:A:ILE:HG23 | 1:209:A:VAL:HG12 | 18       | 1.04          |
| (1,98)   | 1:139:A:ILE:HG23 | 1:209:A:VAL:HG13 | 18       | 1.04          |
| (1,2559) | 1:128:A:TYR:HD1  | 1:164:A:ARG:HD3  | 9        | 1.03          |
| (1,2559) | 1:128:A:TYR:HD2  | 1:164:A:ARG:HD3  | 9        | 1.03          |
| (1,2338) | 1:212:A:GLN:HE21 | 1:215:A:VAL:HG11 | 2        | 1.03          |
| (1,2338) | 1:212:A:GLN:HE21 | 1:215:A:VAL:HG12 | 2        | 1.03          |
| (1,2338) | 1:212:A:GLN:HE21 | 1:215:A:VAL:HG13 | 2        | 1.03          |
| (1,1912) | 1:213:A:MET:H    | 1:215:A:VAL:HG11 | 8        | 1.03          |
| (1,1912) | 1:213:A:MET:H    | 1:215:A:VAL:HG12 | 8        | 1.03          |
| (1,1912) | 1:213:A:MET:H    | 1:215:A:VAL:HG13 | 8        | 1.03          |
| (1,1166) | 1:215:A:VAL:HG21 | 1:219:A:GLN:HG3  | 2        | 1.03          |
| (1,1166) | 1:215:A:VAL:HG22 | 1:219:A:GLN:HG3  | 2        | 1.03          |
| (1,1166) | 1:215:A:VAL:HG23 | 1:219:A:GLN:HG3  | 2        | 1.03          |
| (1,565)  | 1:129:A:MET:HE1  | 1:132:A:SER:HB2  | 3        | 1.03          |
| (1,565)  | 1:129:A:MET:HE2  | 1:132:A:SER:HB2  | 3        | 1.03          |
| (1,565)  | 1:129:A:MET:HE3  | 1:132:A:SER:HB2  | 3        | 1.03          |
| (1,565)  | 1:129:A:MET:HE1  | 1:132:A:SER:HB2  | 6        | 1.03          |
| (1,565)  | 1:129:A:MET:HE2  | 1:132:A:SER:HB2  | 6        | 1.03          |
| (1,565)  | 1:129:A:MET:HE3  | 1:132:A:SER:HB2  | 6        | 1.03          |
| (1,565)  | 1:129:A:MET:HE1  | 1:132:A:SER:HB2  | 10       | 1.03          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,565)  | 1:129:A:MET:HE2  | 1:132:A:SER:HB2  | 10       | 1.03          |
| (1,565)  | 1:129:A:MET:HE3  | 1:132:A:SER:HB2  | 10       | 1.03          |
| (1,565)  | 1:129:A:MET:HE1  | 1:132:A:SER:HB2  | 11       | 1.03          |
| (1,565)  | 1:129:A:MET:HE2  | 1:132:A:SER:HB2  | 11       | 1.03          |
| (1,565)  | 1:129:A:MET:HE3  | 1:132:A:SER:HB2  | 11       | 1.03          |
| (1,565)  | 1:129:A:MET:HE1  | 1:132:A:SER:HB2  | 13       | 1.03          |
| (1,565)  | 1:129:A:MET:HE2  | 1:132:A:SER:HB2  | 13       | 1.03          |
| (1,565)  | 1:129:A:MET:HE3  | 1:132:A:SER:HB2  | 13       | 1.03          |
| (1,565)  | 1:129:A:MET:HE1  | 1:132:A:SER:HB2  | 14       | 1.03          |
| (1,565)  | 1:129:A:MET:HE2  | 1:132:A:SER:HB2  | 14       | 1.03          |
| (1,565)  | 1:129:A:MET:HE3  | 1:132:A:SER:HB2  | 14       | 1.03          |
| (1,322)  | 1:158:A:PRO:HD3  | 1:209:A:VAL:HG21 | 8        | 1.03          |
| (1,322)  | 1:158:A:PRO:HD3  | 1:209:A:VAL:HG22 | 8        | 1.03          |
| (1,322)  | 1:158:A:PRO:HD3  | 1:209:A:VAL:HG23 | 8        | 1.03          |
| (1,309)  | 1:186:A:GLN:HE21 | 1:189:A:VAL:HG11 | 1        | 1.03          |
| (1,309)  | 1:186:A:GLN:HE21 | 1:189:A:VAL:HG12 | 1        | 1.03          |
| (1,309)  | 1:186:A:GLN:HE21 | 1:189:A:VAL:HG13 | 1        | 1.03          |
| (1,188)  | 1:124:A:GLY:HA2  | 1:125:A:LEU:HD21 | 14       | 1.03          |
| (1,188)  | 1:124:A:GLY:HA2  | 1:125:A:LEU:HD22 | 14       | 1.03          |
| (1,188)  | 1:124:A:GLY:HA2  | 1:125:A:LEU:HD23 | 14       | 1.03          |
| (1,188)  | 1:124:A:GLY:HA3  | 1:125:A:LEU:HD21 | 14       | 1.03          |
| (1,188)  | 1:124:A:GLY:HA3  | 1:125:A:LEU:HD22 | 14       | 1.03          |
| (1,188)  | 1:124:A:GLY:HA3  | 1:125:A:LEU:HD23 | 14       | 1.03          |
| (1,155)  | 1:125:A:LEU:HB3  | 1:126:A:GLY:HA3  | 3        | 1.03          |
| (1,2759) | 1:139:A:ILE:HG12 | 1:150:A:TYR:HE1  | 20       | 1.02          |
| (1,2759) | 1:139:A:ILE:HG12 | 1:150:A:TYR:HE2  | 20       | 1.02          |
| (1,2758) | 1:150:A:TYR:HE1  | 1:209:A:VAL:HG11 | 16       | 1.02          |
| (1,2758) | 1:150:A:TYR:HE1  | 1:209:A:VAL:HG12 | 16       | 1.02          |
| (1,2758) | 1:150:A:TYR:HE1  | 1:209:A:VAL:HG13 | 16       | 1.02          |
| (1,2758) | 1:150:A:TYR:HE2  | 1:209:A:VAL:HG11 | 16       | 1.02          |
| (1,2758) | 1:150:A:TYR:HE2  | 1:209:A:VAL:HG12 | 16       | 1.02          |
| (1,2758) | 1:150:A:TYR:HE2  | 1:209:A:VAL:HG13 | 16       | 1.02          |
| (1,2650) | 1:139:A:ILE:HG12 | 1:141:A:PHE:HE1  | 17       | 1.02          |
| (1,2650) | 1:139:A:ILE:HG12 | 1:141:A:PHE:HE2  | 17       | 1.02          |
| (1,2177) | 1:212:A:GLN:H    | 1:213:A:MET:HG2  | 11       | 1.02          |
| (1,2123) | 1:199:A:THR:H    | 1:203:A:VAL:HG11 | 12       | 1.02          |
| (1,2123) | 1:199:A:THR:H    | 1:203:A:VAL:HG12 | 12       | 1.02          |
| (1,2123) | 1:199:A:THR:H    | 1:203:A:VAL:HG13 | 12       | 1.02          |
| (1,2123) | 1:199:A:THR:H    | 1:203:A:VAL:HG11 | 18       | 1.02          |
| (1,2123) | 1:199:A:THR:H    | 1:203:A:VAL:HG12 | 18       | 1.02          |
| (1,2123) | 1:199:A:THR:H    | 1:203:A:VAL:HG13 | 18       | 1.02          |
| (1,1231) | 1:209:A:VAL:HG21 | 1:213:A:MET:HG3  | 17       | 1.02          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1231) | 1:209:A:VAL:HG22 | 1:213:A:MET:HG3  | 17       | 1.02          |
| (1,1231) | 1:209:A:VAL:HG23 | 1:213:A:MET:HG3  | 17       | 1.02          |
| (1,921)  | 1:167:A:SER:HA   | 1:168:A:GLN:HG3  | 17       | 1.02          |
| (1,862)  | 1:143:A:ASN:HD22 | 1:146:A:GLU:HG2  | 1        | 1.02          |
| (1,656)  | 1:138:A:MET:HG3  | 1:154:A:MET:HE1  | 15       | 1.02          |
| (1,656)  | 1:138:A:MET:HG3  | 1:154:A:MET:HE2  | 15       | 1.02          |
| (1,656)  | 1:138:A:MET:HG3  | 1:154:A:MET:HE3  | 15       | 1.02          |
| (1,565)  | 1:129:A:MET:HE1  | 1:132:A:SER:HB2  | 2        | 1.02          |
| (1,565)  | 1:129:A:MET:HE2  | 1:132:A:SER:HB2  | 2        | 1.02          |
| (1,565)  | 1:129:A:MET:HE3  | 1:132:A:SER:HB2  | 2        | 1.02          |
| (1,565)  | 1:129:A:MET:HE1  | 1:132:A:SER:HB2  | 7        | 1.02          |
| (1,565)  | 1:129:A:MET:HE2  | 1:132:A:SER:HB2  | 7        | 1.02          |
| (1,565)  | 1:129:A:MET:HE3  | 1:132:A:SER:HB2  | 7        | 1.02          |
| (1,506)  | 1:179:A:CYS:HB2  | 1:214:A:CYS:HB2  | 12       | 1.02          |
| (1,315)  | 1:166:A:VAL:HG11 | 1:221:A:GLU:HB2  | 3        | 1.02          |
| (1,315)  | 1:166:A:VAL:HG12 | 1:221:A:GLU:HB2  | 3        | 1.02          |
| (1,315)  | 1:166:A:VAL:HG13 | 1:221:A:GLU:HB2  | 3        | 1.02          |
| (1,258)  | 1:122:A:VAL:HG11 | 1:190:A:THR:HG21 | 1        | 1.02          |
| (1,258)  | 1:122:A:VAL:HG11 | 1:190:A:THR:HG22 | 1        | 1.02          |
| (1,258)  | 1:122:A:VAL:HG11 | 1:190:A:THR:HG23 | 1        | 1.02          |
| (1,258)  | 1:122:A:VAL:HG12 | 1:190:A:THR:HG21 | 1        | 1.02          |
| (1,258)  | 1:122:A:VAL:HG12 | 1:190:A:THR:HG22 | 1        | 1.02          |
| (1,258)  | 1:122:A:VAL:HG12 | 1:190:A:THR:HG23 | 1        | 1.02          |
| (1,258)  | 1:122:A:VAL:HG13 | 1:190:A:THR:HG21 | 1        | 1.02          |
| (1,258)  | 1:122:A:VAL:HG13 | 1:190:A:THR:HG22 | 1        | 1.02          |
| (1,258)  | 1:122:A:VAL:HG13 | 1:190:A:THR:HG23 | 1        | 1.02          |
| (1,173)  | 1:198:A:PHE:HB2  | 1:203:A:VAL:HG11 | 5        | 1.02          |
| (1,173)  | 1:198:A:PHE:HB2  | 1:203:A:VAL:HG12 | 5        | 1.02          |
| (1,173)  | 1:198:A:PHE:HB2  | 1:203:A:VAL:HG13 | 5        | 1.02          |
| (1,159)  | 1:228:A:GLY:HA2  | 1:230:A:ARG:HD2  | 19       | 1.02          |
| (1,159)  | 1:228:A:GLY:HA3  | 1:230:A:ARG:HD2  | 19       | 1.02          |
| (1,2792) | 1:128:A:TYR:HE1  | 1:164:A:ARG:HD3  | 13       | 1.01          |
| (1,2792) | 1:128:A:TYR:HE2  | 1:164:A:ARG:HD3  | 13       | 1.01          |
| (1,2758) | 1:150:A:TYR:HE1  | 1:209:A:VAL:HG11 | 14       | 1.01          |
| (1,2758) | 1:150:A:TYR:HE1  | 1:209:A:VAL:HG12 | 14       | 1.01          |
| (1,2758) | 1:150:A:TYR:HE1  | 1:209:A:VAL:HG13 | 14       | 1.01          |
| (1,2758) | 1:150:A:TYR:HE2  | 1:209:A:VAL:HG11 | 14       | 1.01          |
| (1,2758) | 1:150:A:TYR:HE2  | 1:209:A:VAL:HG12 | 14       | 1.01          |
| (1,2758) | 1:150:A:TYR:HE2  | 1:209:A:VAL:HG13 | 14       | 1.01          |
| (1,2501) | 1:149:A:TYR:HD1  | 1:205:A:MET:HG2  | 9        | 1.01          |
| (1,2501) | 1:149:A:TYR:HD2  | 1:205:A:MET:HG2  | 9        | 1.01          |
| (1,2482) | 1:163:A:TYR:HD1  | 1:221:A:GLU:HG2  | 19       | 1.01          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2482) | 1:163:A:TYR:HD2  | 1:221:A:GLU:HG2  | 19       | 1.01          |
| (1,2177) | 1:212:A:GLN:H    | 1:213:A:MET:HG2  | 9        | 1.01          |
| (1,2054) | 1:166:A:VAL:HG11 | 1:221:A:GLU:H    | 3        | 1.01          |
| (1,2054) | 1:166:A:VAL:HG12 | 1:221:A:GLU:H    | 3        | 1.01          |
| (1,2054) | 1:166:A:VAL:HG13 | 1:221:A:GLU:H    | 3        | 1.01          |
| (1,1914) | 1:209:A:VAL:HG21 | 1:213:A:MET:H    | 8        | 1.01          |
| (1,1914) | 1:209:A:VAL:HG22 | 1:213:A:MET:H    | 8        | 1.01          |
| (1,1914) | 1:209:A:VAL:HG23 | 1:213:A:MET:H    | 8        | 1.01          |
| (1,1912) | 1:213:A:MET:H    | 1:215:A:VAL:HG11 | 2        | 1.01          |
| (1,1912) | 1:213:A:MET:H    | 1:215:A:VAL:HG12 | 2        | 1.01          |
| (1,1912) | 1:213:A:MET:H    | 1:215:A:VAL:HG13 | 2        | 1.01          |
| (1,1459) | 1:136:A:ARG:HB3  | 1:159:A:ASN:HB3  | 2        | 1.01          |
| (1,1164) | 1:215:A:VAL:HG21 | 1:219:A:GLN:HG2  | 12       | 1.01          |
| (1,1164) | 1:215:A:VAL:HG22 | 1:219:A:GLN:HG2  | 12       | 1.01          |
| (1,1164) | 1:215:A:VAL:HG23 | 1:219:A:GLN:HG2  | 12       | 1.01          |
| (1,1089) | 1:182:A:ILE:HD11 | 1:186:A:GLN:HE21 | 17       | 1.01          |
| (1,1089) | 1:182:A:ILE:HD12 | 1:186:A:GLN:HE21 | 17       | 1.01          |
| (1,1089) | 1:182:A:ILE:HD13 | 1:186:A:GLN:HE21 | 17       | 1.01          |
| (1,1015) | 1:152:A:GLU:HG2  | 1:153:A:ASN:HD22 | 10       | 1.01          |
| (1,567)  | 1:230:A:ARG:HB2  | 1:231:A:SER:HB3  | 13       | 1.01          |
| (1,565)  | 1:129:A:MET:HE1  | 1:132:A:SER:HB2  | 4        | 1.01          |
| (1,565)  | 1:129:A:MET:HE2  | 1:132:A:SER:HB2  | 4        | 1.01          |
| (1,565)  | 1:129:A:MET:HE3  | 1:132:A:SER:HB2  | 4        | 1.01          |
| (1,565)  | 1:129:A:MET:HE1  | 1:132:A:SER:HB2  | 5        | 1.01          |
| (1,565)  | 1:129:A:MET:HE2  | 1:132:A:SER:HB2  | 5        | 1.01          |
| (1,565)  | 1:129:A:MET:HE3  | 1:132:A:SER:HB2  | 5        | 1.01          |
| (1,565)  | 1:129:A:MET:HE1  | 1:132:A:SER:HB2  | 17       | 1.01          |
| (1,565)  | 1:129:A:MET:HE2  | 1:132:A:SER:HB2  | 17       | 1.01          |
| (1,565)  | 1:129:A:MET:HE3  | 1:132:A:SER:HB2  | 17       | 1.01          |
| (1,423)  | 1:151:A:ARG:HD3  | 1:152:A:GLU:H    | 19       | 1.01          |
| (1,362)  | 1:172:A:GLN:HG3  | 1:215:A:VAL:HG21 | 7        | 1.01          |
| (1,362)  | 1:172:A:GLN:HG3  | 1:215:A:VAL:HG22 | 7        | 1.01          |
| (1,362)  | 1:172:A:GLN:HG3  | 1:215:A:VAL:HG23 | 7        | 1.01          |
| (1,322)  | 1:158:A:PRO:HD3  | 1:209:A:VAL:HG21 | 19       | 1.01          |
| (1,322)  | 1:158:A:PRO:HD3  | 1:209:A:VAL:HG22 | 19       | 1.01          |
| (1,322)  | 1:158:A:PRO:HD3  | 1:209:A:VAL:HG23 | 19       | 1.01          |
| (1,2615) | 1:141:A:PHE:HD1  | 1:147:A:ASP:HB3  | 11       | 1.0           |
| (1,2615) | 1:141:A:PHE:HD2  | 1:147:A:ASP:HB3  | 11       | 1.0           |
| (1,2347) | 1:139:A:ILE:HG13 | 1:212:A:GLN:HE22 | 4        | 1.0           |
| (1,2123) | 1:199:A:THR:H    | 1:203:A:VAL:HG11 | 5        | 1.0           |
| (1,2123) | 1:199:A:THR:H    | 1:203:A:VAL:HG12 | 5        | 1.0           |
| (1,2123) | 1:199:A:THR:H    | 1:203:A:VAL:HG13 | 5        | 1.0           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2054) | 1:166:A:VAL:HG11 | 1:221:A:GLU:H    | 12       | 1.0           |
| (1,2054) | 1:166:A:VAL:HG12 | 1:221:A:GLU:H    | 12       | 1.0           |
| (1,2054) | 1:166:A:VAL:HG13 | 1:221:A:GLU:H    | 12       | 1.0           |
| (1,1914) | 1:209:A:VAL:HG21 | 1:213:A:MET:H    | 1        | 1.0           |
| (1,1914) | 1:209:A:VAL:HG22 | 1:213:A:MET:H    | 1        | 1.0           |
| (1,1914) | 1:209:A:VAL:HG23 | 1:213:A:MET:H    | 1        | 1.0           |
| (1,1914) | 1:209:A:VAL:HG21 | 1:213:A:MET:H    | 2        | 1.0           |
| (1,1914) | 1:209:A:VAL:HG22 | 1:213:A:MET:H    | 2        | 1.0           |
| (1,1914) | 1:209:A:VAL:HG23 | 1:213:A:MET:H    | 2        | 1.0           |
| (1,1912) | 1:213:A:MET:H    | 1:215:A:VAL:HG11 | 4        | 1.0           |
| (1,1912) | 1:213:A:MET:H    | 1:215:A:VAL:HG12 | 4        | 1.0           |
| (1,1912) | 1:213:A:MET:H    | 1:215:A:VAL:HG13 | 4        | 1.0           |
| (1,1689) | 1:134:A:MET:H    | 1:159:A:ASN:HB2  | 10       | 1.0           |
| (1,1303) | 1:137:A:PRO:HB2  | 1:213:A:MET:HG2  | 6        | 1.0           |
| (1,1166) | 1:215:A:VAL:HG21 | 1:219:A:GLN:HG3  | 19       | 1.0           |
| (1,1166) | 1:215:A:VAL:HG22 | 1:219:A:GLN:HG3  | 19       | 1.0           |
| (1,1166) | 1:215:A:VAL:HG23 | 1:219:A:GLN:HG3  | 19       | 1.0           |
| (1,1131) | 1:223:A:GLN:HG2  | 1:226:A:TYR:H    | 10       | 1.0           |
| (1,921)  | 1:167:A:SER:HA   | 1:168:A:GLN:HG3  | 3        | 1.0           |
| (1,921)  | 1:167:A:SER:HA   | 1:168:A:GLN:HG3  | 13       | 1.0           |
| (1,733)  | 1:222:A:SER:HB2  | 1:226:A:TYR:HD1  | 1        | 1.0           |
| (1,733)  | 1:222:A:SER:HB2  | 1:226:A:TYR:HD2  | 1        | 1.0           |
| (1,565)  | 1:129:A:MET:HE1  | 1:132:A:SER:HB2  | 19       | 1.0           |
| (1,565)  | 1:129:A:MET:HE2  | 1:132:A:SER:HB2  | 19       | 1.0           |
| (1,565)  | 1:129:A:MET:HE3  | 1:132:A:SER:HB2  | 19       | 1.0           |
| (1,323)  | 1:209:A:VAL:HG21 | 1:212:A:GLN:HB3  | 20       | 1.0           |
| (1,323)  | 1:209:A:VAL:HG22 | 1:212:A:GLN:HB3  | 20       | 1.0           |
| (1,323)  | 1:209:A:VAL:HG23 | 1:212:A:GLN:HB3  | 20       | 1.0           |
| (1,169)  | 1:198:A:PHE:HB3  | 1:203:A:VAL:HG11 | 12       | 1.0           |
| (1,169)  | 1:198:A:PHE:HB3  | 1:203:A:VAL:HG12 | 12       | 1.0           |
| (1,169)  | 1:198:A:PHE:HB3  | 1:203:A:VAL:HG13 | 12       | 1.0           |
| (1,2735) | 1:186:A:GLN:HB3  | 1:187:A:HIS:HD2  | 1        | 0.99          |
| (1,2735) | 1:186:A:GLN:HB3  | 1:187:A:HIS:HD2  | 7        | 0.99          |
| (1,2735) | 1:186:A:GLN:HB3  | 1:187:A:HIS:HD2  | 14       | 0.99          |
| (1,2735) | 1:186:A:GLN:HB3  | 1:187:A:HIS:HD2  | 18       | 0.99          |
| (1,2711) | 1:145:A:TRP:HZ3  | 1:146:A:GLU:HG3  | 10       | 0.99          |
| (1,2492) | 1:139:A:ILE:HG12 | 1:150:A:TYR:HD1  | 20       | 0.99          |
| (1,2492) | 1:139:A:ILE:HG12 | 1:150:A:TYR:HD2  | 20       | 0.99          |
| (1,2488) | 1:149:A:TYR:HD1  | 1:153:A:ASN:HB3  | 2        | 0.99          |
| (1,2488) | 1:149:A:TYR:HD2  | 1:153:A:ASN:HB3  | 2        | 0.99          |
| (1,2347) | 1:139:A:ILE:HG13 | 1:212:A:GLN:HE22 | 3        | 0.99          |
| (1,2338) | 1:212:A:GLN:HE21 | 1:215:A:VAL:HG11 | 12       | 0.99          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2338) | 1:212:A:GLN:HE21 | 1:215:A:VAL:HG12 | 12       | 0.99          |
| (1,2338) | 1:212:A:GLN:HE21 | 1:215:A:VAL:HG13 | 12       | 0.99          |
| (1,1231) | 1:209:A:VAL:HG21 | 1:213:A:MET:HG3  | 18       | 0.99          |
| (1,1231) | 1:209:A:VAL:HG22 | 1:213:A:MET:HG3  | 18       | 0.99          |
| (1,1231) | 1:209:A:VAL:HG23 | 1:213:A:MET:HG3  | 18       | 0.99          |
| (1,1197) | 1:160:A:GLN:HB2  | 1:183:A:THR:HG21 | 4        | 0.99          |
| (1,1197) | 1:160:A:GLN:HB2  | 1:183:A:THR:HG22 | 4        | 0.99          |
| (1,1197) | 1:160:A:GLN:HB2  | 1:183:A:THR:HG23 | 4        | 0.99          |
| (1,1131) | 1:223:A:GLN:HG2  | 1:226:A:TYR:H    | 4        | 0.99          |
| (1,751)  | 1:222:A:SER:HB2  | 1:223:A:GLN:HA   | 15       | 0.99          |
| (1,637)  | 1:147:A:ASP:HB2  | 1:148:A:ARG:HG2  | 6        | 0.99          |
| (1,602)  | 1:230:A:ARG:H    | 1:231:A:SER:HB3  | 5        | 0.99          |
| (1,78)   | 1:139:A:ILE:HB   | 1:209:A:VAL:HG11 | 20       | 0.99          |
| (1,78)   | 1:139:A:ILE:HB   | 1:209:A:VAL:HG12 | 20       | 0.99          |
| (1,78)   | 1:139:A:ILE:HB   | 1:209:A:VAL:HG13 | 20       | 0.99          |
| (1,2782) | 1:150:A:TYR:HE1  | 1:154:A:MET:HG3  | 8        | 0.98          |
| (1,2782) | 1:150:A:TYR:HE2  | 1:154:A:MET:HG3  | 8        | 0.98          |
| (1,2735) | 1:186:A:GLN:HB3  | 1:187:A:HIS:HD2  | 3        | 0.98          |
| (1,2735) | 1:186:A:GLN:HB3  | 1:187:A:HIS:HD2  | 4        | 0.98          |
| (1,2735) | 1:186:A:GLN:HB3  | 1:187:A:HIS:HD2  | 5        | 0.98          |
| (1,2735) | 1:186:A:GLN:HB3  | 1:187:A:HIS:HD2  | 12       | 0.98          |
| (1,2735) | 1:186:A:GLN:HB3  | 1:187:A:HIS:HD2  | 13       | 0.98          |
| (1,2735) | 1:186:A:GLN:HB3  | 1:187:A:HIS:HD2  | 16       | 0.98          |
| (1,2735) | 1:186:A:GLN:HB3  | 1:187:A:HIS:HD2  | 17       | 0.98          |
| (1,2735) | 1:186:A:GLN:HB3  | 1:187:A:HIS:HD2  | 19       | 0.98          |
| (1,2735) | 1:186:A:GLN:HB3  | 1:187:A:HIS:HD2  | 20       | 0.98          |
| (1,2721) | 1:177:A:HIS:HD2  | 1:178:A:ASP:HB3  | 14       | 0.98          |
| (1,2518) | 1:155:A:TYR:HD1  | 1:156:A:ARG:HD2  | 20       | 0.98          |
| (1,2518) | 1:155:A:TYR:HD2  | 1:156:A:ARG:HD2  | 20       | 0.98          |
| (1,2354) | 1:170:A:SER:HB2  | 1:174:A:ASN:HD21 | 12       | 0.98          |
| (1,2320) | 1:160:A:GLN:HE22 | 1:213:A:MET:HB2  | 13       | 0.98          |
| (1,2250) | 1:217:A:GLN:HE21 | 1:218:A:TYR:HA   | 18       | 0.98          |
| (1,1303) | 1:137:A:PRO:HB2  | 1:213:A:MET:HG2  | 3        | 0.98          |
| (1,1097) | 1:165:A:PRO:HB3  | 1:168:A:GLN:HG2  | 4        | 0.98          |
| (1,751)  | 1:222:A:SER:HB2  | 1:223:A:GLN:HA   | 20       | 0.98          |
| (1,445)  | 1:180:A:VAL:HA   | 1:184:A:ILE:HG12 | 10       | 0.98          |
| (1,380)  | 1:122:A:VAL:HG21 | 1:123:A:GLY:HA2  | 18       | 0.98          |
| (1,380)  | 1:122:A:VAL:HG21 | 1:123:A:GLY:HA3  | 18       | 0.98          |
| (1,380)  | 1:122:A:VAL:HG22 | 1:123:A:GLY:HA2  | 18       | 0.98          |
| (1,380)  | 1:122:A:VAL:HG22 | 1:123:A:GLY:HA3  | 18       | 0.98          |
| (1,380)  | 1:122:A:VAL:HG23 | 1:123:A:GLY:HA2  | 18       | 0.98          |
| (1,380)  | 1:122:A:VAL:HG23 | 1:123:A:GLY:HA3  | 18       | 0.98          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,323)  | 1:209:A:VAL:HG21 | 1:212:A:GLN:HB3  | 15       | 0.98          |
| (1,323)  | 1:209:A:VAL:HG22 | 1:212:A:GLN:HB3  | 15       | 0.98          |
| (1,323)  | 1:209:A:VAL:HG23 | 1:212:A:GLN:HB3  | 15       | 0.98          |
| (1,188)  | 1:124:A:GLY:HA2  | 1:125:A:LEU:HD21 | 15       | 0.98          |
| (1,188)  | 1:124:A:GLY:HA2  | 1:125:A:LEU:HD22 | 15       | 0.98          |
| (1,188)  | 1:124:A:GLY:HA2  | 1:125:A:LEU:HD23 | 15       | 0.98          |
| (1,188)  | 1:124:A:GLY:HA3  | 1:125:A:LEU:HD21 | 15       | 0.98          |
| (1,188)  | 1:124:A:GLY:HA3  | 1:125:A:LEU:HD22 | 15       | 0.98          |
| (1,188)  | 1:124:A:GLY:HA3  | 1:125:A:LEU:HD23 | 15       | 0.98          |
| (1,155)  | 1:125:A:LEU:HB3  | 1:126:A:GLY:HA3  | 7        | 0.98          |
| (1,155)  | 1:125:A:LEU:HB3  | 1:126:A:GLY:HA3  | 17       | 0.98          |
| (1,98)   | 1:139:A:ILE:HG21 | 1:209:A:VAL:HG11 | 1        | 0.98          |
| (1,98)   | 1:139:A:ILE:HG21 | 1:209:A:VAL:HG12 | 1        | 0.98          |
| (1,98)   | 1:139:A:ILE:HG21 | 1:209:A:VAL:HG13 | 1        | 0.98          |
| (1,98)   | 1:139:A:ILE:HG22 | 1:209:A:VAL:HG11 | 1        | 0.98          |
| (1,98)   | 1:139:A:ILE:HG22 | 1:209:A:VAL:HG12 | 1        | 0.98          |
| (1,98)   | 1:139:A:ILE:HG22 | 1:209:A:VAL:HG13 | 1        | 0.98          |
| (1,98)   | 1:139:A:ILE:HG23 | 1:209:A:VAL:HG11 | 1        | 0.98          |
| (1,98)   | 1:139:A:ILE:HG23 | 1:209:A:VAL:HG12 | 1        | 0.98          |
| (1,98)   | 1:139:A:ILE:HG23 | 1:209:A:VAL:HG13 | 1        | 0.98          |
| (1,2735) | 1:186:A:GLN:HB3  | 1:187:A:HIS:HD2  | 2        | 0.97          |
| (1,2615) | 1:141:A:PHE:HD1  | 1:147:A:ASP:HB3  | 1        | 0.97          |
| (1,2615) | 1:141:A:PHE:HD2  | 1:147:A:ASP:HB3  | 1        | 0.97          |
| (1,2347) | 1:139:A:ILE:HG13 | 1:212:A:GLN:HE22 | 7        | 0.97          |
| (1,2347) | 1:139:A:ILE:HG13 | 1:212:A:GLN:HE22 | 10       | 0.97          |
| (1,2254) | 1:217:A:GLN:HE22 | 1:220:A:LYS:HE2  | 15       | 0.97          |
| (1,2254) | 1:217:A:GLN:HE22 | 1:220:A:LYS:HE3  | 15       | 0.97          |
| (1,2177) | 1:212:A:GLN:H    | 1:213:A:MET:HG2  | 4        | 0.97          |
| (1,1375) | 1:136:A:ARG:HD2  | 1:154:A:MET:HG3  | 6        | 0.97          |
| (1,1085) | 1:129:A:MET:HB2  | 1:164:A:ARG:HA   | 7        | 0.97          |
| (1,921)  | 1:167:A:SER:HA   | 1:168:A:GLN:HG3  | 1        | 0.97          |
| (1,862)  | 1:143:A:ASN:HD22 | 1:146:A:GLU:HG2  | 14       | 0.97          |
| (1,502)  | 1:162:A:TYR:HB3  | 1:183:A:THR:HA   | 6        | 0.97          |
| (1,423)  | 1:151:A:ARG:HD3  | 1:152:A:GLU:H    | 1        | 0.97          |
| (1,423)  | 1:151:A:ARG:HD3  | 1:152:A:GLU:H    | 3        | 0.97          |
| (1,396)  | 1:210:A:VAL:HA   | 1:213:A:MET:HB3  | 5        | 0.97          |
| (1,322)  | 1:158:A:PRO:HD3  | 1:209:A:VAL:HG21 | 1        | 0.97          |
| (1,322)  | 1:158:A:PRO:HD3  | 1:209:A:VAL:HG22 | 1        | 0.97          |
| (1,322)  | 1:158:A:PRO:HD3  | 1:209:A:VAL:HG23 | 1        | 0.97          |
| (1,173)  | 1:198:A:PHE:HB2  | 1:203:A:VAL:HG11 | 12       | 0.97          |
| (1,173)  | 1:198:A:PHE:HB2  | 1:203:A:VAL:HG12 | 12       | 0.97          |
| (1,173)  | 1:198:A:PHE:HB2  | 1:203:A:VAL:HG13 | 12       | 0.97          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2457) | 1:140:A:HIS:HE1  | 1:142:A:GLY:HA3  | 16       | 0.96          |
| (1,2354) | 1:170:A:SER:HB2  | 1:174:A:ASN:HD21 | 1        | 0.96          |
| (1,921)  | 1:167:A:SER:HA   | 1:168:A:GLN:HG3  | 16       | 0.96          |
| (1,751)  | 1:222:A:SER:HB2  | 1:223:A:GLN:HA   | 6        | 0.96          |
| (1,470)  | 1:122:A:VAL:HG21 | 1:125:A:LEU:HB2  | 4        | 0.96          |
| (1,470)  | 1:122:A:VAL:HG22 | 1:125:A:LEU:HB2  | 4        | 0.96          |
| (1,470)  | 1:122:A:VAL:HG23 | 1:125:A:LEU:HB2  | 4        | 0.96          |
| (1,396)  | 1:210:A:VAL:HA   | 1:213:A:MET:HB3  | 18       | 0.96          |
| (1,357)  | 1:122:A:VAL:HG21 | 1:125:A:LEU:HG   | 6        | 0.96          |
| (1,357)  | 1:122:A:VAL:HG22 | 1:125:A:LEU:HG   | 6        | 0.96          |
| (1,357)  | 1:122:A:VAL:HG23 | 1:125:A:LEU:HG   | 6        | 0.96          |
| (1,155)  | 1:125:A:LEU:HB3  | 1:126:A:GLY:HA3  | 19       | 0.96          |
| (1,107)  | 1:211:A:GLU:HG3  | 1:215:A:VAL:HG11 | 7        | 0.96          |
| (1,107)  | 1:211:A:GLU:HG3  | 1:215:A:VAL:HG12 | 7        | 0.96          |
| (1,107)  | 1:211:A:GLU:HG3  | 1:215:A:VAL:HG13 | 7        | 0.96          |
| (1,2711) | 1:145:A:TRP:HZ3  | 1:146:A:GLU:HG3  | 20       | 0.95          |
| (1,2674) | 1:175:A:PHE:HZ   | 1:221:A:GLU:HG2  | 7        | 0.95          |
| (1,2488) | 1:149:A:TYR:HD1  | 1:153:A:ASN:HB3  | 13       | 0.95          |
| (1,2488) | 1:149:A:TYR:HD2  | 1:153:A:ASN:HB3  | 13       | 0.95          |
| (1,2315) | 1:160:A:GLN:HE21 | 1:213:A:MET:HB2  | 14       | 0.95          |
| (1,1752) | 1:166:A:VAL:HG11 | 1:223:A:GLN:H    | 12       | 0.95          |
| (1,1752) | 1:166:A:VAL:HG12 | 1:223:A:GLN:H    | 12       | 0.95          |
| (1,1752) | 1:166:A:VAL:HG13 | 1:223:A:GLN:H    | 12       | 0.95          |
| (1,1250) | 1:205:A:MET:HB2  | 1:206:A:MET:HG2  | 2        | 0.95          |
| (1,1131) | 1:223:A:GLN:HG2  | 1:226:A:TYR:H    | 18       | 0.95          |
| (1,507)  | 1:211:A:GLU:HG3  | 1:214:A:CYS:HB2  | 15       | 0.95          |
| (1,506)  | 1:179:A:CYS:HB2  | 1:214:A:CYS:HB2  | 18       | 0.95          |
| (1,155)  | 1:125:A:LEU:HB3  | 1:126:A:GLY:HA3  | 8        | 0.95          |
| (1,104)  | 1:213:A:MET:HA   | 1:215:A:VAL:HG11 | 8        | 0.95          |
| (1,104)  | 1:213:A:MET:HA   | 1:215:A:VAL:HG12 | 8        | 0.95          |
| (1,104)  | 1:213:A:MET:HA   | 1:215:A:VAL:HG13 | 8        | 0.95          |
| (1,2846) | 1:157:A:TYR:HE1  | 1:206:A:MET:HB2  | 16       | 0.94          |
| (1,2846) | 1:157:A:TYR:HE2  | 1:206:A:MET:HB2  | 16       | 0.94          |
| (1,2758) | 1:150:A:TYR:HE1  | 1:209:A:VAL:HG11 | 13       | 0.94          |
| (1,2758) | 1:150:A:TYR:HE1  | 1:209:A:VAL:HG12 | 13       | 0.94          |
| (1,2758) | 1:150:A:TYR:HE1  | 1:209:A:VAL:HG13 | 13       | 0.94          |
| (1,2758) | 1:150:A:TYR:HE2  | 1:209:A:VAL:HG11 | 13       | 0.94          |
| (1,2758) | 1:150:A:TYR:HE2  | 1:209:A:VAL:HG12 | 13       | 0.94          |
| (1,2758) | 1:150:A:TYR:HE2  | 1:209:A:VAL:HG13 | 13       | 0.94          |
| (1,2756) | 1:150:A:TYR:HE1  | 1:205:A:MET:HG2  | 6        | 0.94          |
| (1,2756) | 1:150:A:TYR:HE2  | 1:205:A:MET:HG2  | 6        | 0.94          |
| (1,2421) | 1:127:A:GLY:H    | 1:164:A:ARG:HD3  | 6        | 0.94          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2421) | 1:127:A:GLY:H    | 1:164:A:ARG:HD3  | 16       | 0.94          |
| (1,2177) | 1:212:A:GLN:H    | 1:213:A:MET:HG2  | 16       | 0.94          |
| (1,2177) | 1:212:A:GLN:H    | 1:213:A:MET:HG2  | 20       | 0.94          |
| (1,1283) | 1:206:A:MET:HG2  | 1:207:A:GLU:HG3  | 11       | 0.94          |
| (1,1256) | 1:184:A:ILE:HG13 | 1:206:A:MET:HG3  | 17       | 0.94          |
| (1,921)  | 1:167:A:SER:HA   | 1:168:A:GLN:HG3  | 10       | 0.94          |
| (1,704)  | 1:209:A:VAL:HG21 | 1:213:A:MET:HE1  | 16       | 0.94          |
| (1,704)  | 1:209:A:VAL:HG21 | 1:213:A:MET:HE2  | 16       | 0.94          |
| (1,704)  | 1:209:A:VAL:HG21 | 1:213:A:MET:HE3  | 16       | 0.94          |
| (1,704)  | 1:209:A:VAL:HG22 | 1:213:A:MET:HE1  | 16       | 0.94          |
| (1,704)  | 1:209:A:VAL:HG22 | 1:213:A:MET:HE2  | 16       | 0.94          |
| (1,704)  | 1:209:A:VAL:HG22 | 1:213:A:MET:HE3  | 16       | 0.94          |
| (1,704)  | 1:209:A:VAL:HG23 | 1:213:A:MET:HE1  | 16       | 0.94          |
| (1,704)  | 1:209:A:VAL:HG23 | 1:213:A:MET:HE2  | 16       | 0.94          |
| (1,704)  | 1:209:A:VAL:HG23 | 1:213:A:MET:HE3  | 16       | 0.94          |
| (1,525)  | 1:132:A:SER:HB2  | 1:160:A:GLN:HE21 | 1        | 0.94          |
| (1,502)  | 1:162:A:TYR:HB3  | 1:183:A:THR:HA   | 8        | 0.94          |
| (1,502)  | 1:162:A:TYR:HB3  | 1:183:A:THR:HA   | 9        | 0.94          |
| (1,318)  | 1:153:A:ASN:HB2  | 1:156:A:ARG:HD3  | 8        | 0.94          |
| (1,2821) | 1:129:A:MET:HB3  | 1:163:A:TYR:HE1  | 18       | 0.93          |
| (1,2821) | 1:129:A:MET:HB3  | 1:163:A:TYR:HE2  | 18       | 0.93          |
| (1,2593) | 1:175:A:PHE:HE1  | 1:221:A:GLU:HG2  | 12       | 0.93          |
| (1,2593) | 1:175:A:PHE:HE2  | 1:221:A:GLU:HG2  | 12       | 0.93          |
| (1,2354) | 1:170:A:SER:HB2  | 1:174:A:ASN:HD21 | 5        | 0.93          |
| (1,2338) | 1:212:A:GLN:HE21 | 1:215:A:VAL:HG11 | 4        | 0.93          |
| (1,2338) | 1:212:A:GLN:HE21 | 1:215:A:VAL:HG12 | 4        | 0.93          |
| (1,2338) | 1:212:A:GLN:HE21 | 1:215:A:VAL:HG13 | 4        | 0.93          |
| (1,2254) | 1:217:A:GLN:HE22 | 1:220:A:LYS:HE2  | 18       | 0.93          |
| (1,2254) | 1:217:A:GLN:HE22 | 1:220:A:LYS:HE3  | 18       | 0.93          |
| (1,1231) | 1:209:A:VAL:HG21 | 1:213:A:MET:HG3  | 16       | 0.93          |
| (1,1231) | 1:209:A:VAL:HG22 | 1:213:A:MET:HG3  | 16       | 0.93          |
| (1,1231) | 1:209:A:VAL:HG23 | 1:213:A:MET:HG3  | 16       | 0.93          |
| (1,322)  | 1:158:A:PRO:HD3  | 1:209:A:VAL:HG21 | 14       | 0.93          |
| (1,322)  | 1:158:A:PRO:HD3  | 1:209:A:VAL:HG22 | 14       | 0.93          |
| (1,322)  | 1:158:A:PRO:HD3  | 1:209:A:VAL:HG23 | 14       | 0.93          |
| (1,315)  | 1:166:A:VAL:HG11 | 1:221:A:GLU:HB2  | 17       | 0.93          |
| (1,315)  | 1:166:A:VAL:HG12 | 1:221:A:GLU:HB2  | 17       | 0.93          |
| (1,315)  | 1:166:A:VAL:HG13 | 1:221:A:GLU:HB2  | 17       | 0.93          |
| (1,159)  | 1:228:A:GLY:HA2  | 1:230:A:ARG:HD2  | 15       | 0.93          |
| (1,159)  | 1:228:A:GLY:HA3  | 1:230:A:ARG:HD2  | 15       | 0.93          |
| (1,155)  | 1:125:A:LEU:HB3  | 1:126:A:GLY:HA3  | 6        | 0.93          |
| (1,98)   | 1:139:A:ILE:HG21 | 1:209:A:VAL:HG11 | 11       | 0.93          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,98)   | 1:139:A:ILE:HG21 | 1:209:A:VAL:HG12 | 11       | 0.93          |
| (1,98)   | 1:139:A:ILE:HG21 | 1:209:A:VAL:HG13 | 11       | 0.93          |
| (1,98)   | 1:139:A:ILE:HG22 | 1:209:A:VAL:HG11 | 11       | 0.93          |
| (1,98)   | 1:139:A:ILE:HG22 | 1:209:A:VAL:HG12 | 11       | 0.93          |
| (1,98)   | 1:139:A:ILE:HG22 | 1:209:A:VAL:HG13 | 11       | 0.93          |
| (1,98)   | 1:139:A:ILE:HG23 | 1:209:A:VAL:HG11 | 11       | 0.93          |
| (1,98)   | 1:139:A:ILE:HG23 | 1:209:A:VAL:HG12 | 11       | 0.93          |
| (1,98)   | 1:139:A:ILE:HG23 | 1:209:A:VAL:HG13 | 11       | 0.93          |
| (1,89)   | 1:206:A:MET:HB3  | 1:210:A:VAL:HG21 | 8        | 0.93          |
| (1,89)   | 1:206:A:MET:HB3  | 1:210:A:VAL:HG22 | 8        | 0.93          |
| (1,89)   | 1:206:A:MET:HB3  | 1:210:A:VAL:HG23 | 8        | 0.93          |
| (1,2846) | 1:157:A:TYR:HE1  | 1:206:A:MET:HB2  | 19       | 0.92          |
| (1,2846) | 1:157:A:TYR:HE2  | 1:206:A:MET:HB2  | 19       | 0.92          |
| (1,2615) | 1:141:A:PHE:HD1  | 1:147:A:ASP:HB3  | 14       | 0.92          |
| (1,2615) | 1:141:A:PHE:HD2  | 1:147:A:ASP:HB3  | 14       | 0.92          |
| (1,2559) | 1:128:A:TYR:HD1  | 1:164:A:ARG:HD3  | 17       | 0.92          |
| (1,2559) | 1:128:A:TYR:HD2  | 1:164:A:ARG:HD3  | 17       | 0.92          |
| (1,2510) | 1:226:A:TYR:HD1  | 1:229:A:ARG:HB2  | 3        | 0.92          |
| (1,2510) | 1:226:A:TYR:HD2  | 1:229:A:ARG:HB2  | 3        | 0.92          |
| (1,2510) | 1:226:A:TYR:HD1  | 1:229:A:ARG:HB2  | 4        | 0.92          |
| (1,2510) | 1:226:A:TYR:HD2  | 1:229:A:ARG:HB2  | 4        | 0.92          |
| (1,2482) | 1:163:A:TYR:HD1  | 1:221:A:GLU:HG2  | 2        | 0.92          |
| (1,2482) | 1:163:A:TYR:HD2  | 1:221:A:GLU:HG2  | 2        | 0.92          |
| (1,2482) | 1:163:A:TYR:HD1  | 1:221:A:GLU:HG2  | 9        | 0.92          |
| (1,2482) | 1:163:A:TYR:HD2  | 1:221:A:GLU:HG2  | 9        | 0.92          |
| (1,2338) | 1:212:A:GLN:HE21 | 1:215:A:VAL:HG11 | 8        | 0.92          |
| (1,2338) | 1:212:A:GLN:HE21 | 1:215:A:VAL:HG12 | 8        | 0.92          |
| (1,2338) | 1:212:A:GLN:HE21 | 1:215:A:VAL:HG13 | 8        | 0.92          |
| (1,1407) | 1:134:A:MET:HB3  | 1:220:A:LYS:HD2  | 13       | 0.92          |
| (1,1407) | 1:134:A:MET:HB3  | 1:220:A:LYS:HD3  | 13       | 0.92          |
| (1,1283) | 1:206:A:MET:HG2  | 1:207:A:GLU:HG3  | 8        | 0.92          |
| (1,921)  | 1:167:A:SER:HA   | 1:168:A:GLN:HG3  | 12       | 0.92          |
| (1,309)  | 1:186:A:GLN:HE21 | 1:189:A:VAL:HG11 | 14       | 0.92          |
| (1,309)  | 1:186:A:GLN:HE21 | 1:189:A:VAL:HG12 | 14       | 0.92          |
| (1,309)  | 1:186:A:GLN:HE21 | 1:189:A:VAL:HG13 | 14       | 0.92          |
| (1,2846) | 1:157:A:TYR:HE1  | 1:206:A:MET:HB2  | 10       | 0.91          |
| (1,2846) | 1:157:A:TYR:HE2  | 1:206:A:MET:HB2  | 10       | 0.91          |
| (1,2846) | 1:157:A:TYR:HE1  | 1:206:A:MET:HB2  | 15       | 0.91          |
| (1,2846) | 1:157:A:TYR:HE2  | 1:206:A:MET:HB2  | 15       | 0.91          |
| (1,2681) | 1:141:A:PHE:HZ   | 1:208:A:ARG:HB3  | 12       | 0.91          |
| (1,2657) | 1:141:A:PHE:HE1  | 1:208:A:ARG:HB3  | 1        | 0.91          |
| (1,2657) | 1:141:A:PHE:HE2  | 1:208:A:ARG:HB3  | 1        | 0.91          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2615) | 1:141:A:PHE:HD1  | 1:147:A:ASP:HB3  | 9        | 0.91          |
| (1,2615) | 1:141:A:PHE:HD2  | 1:147:A:ASP:HB3  | 9        | 0.91          |
| (1,2571) | 1:215:A:VAL:HG21 | 1:218:A:TYR:HD1  | 4        | 0.91          |
| (1,2571) | 1:215:A:VAL:HG21 | 1:218:A:TYR:HD2  | 4        | 0.91          |
| (1,2571) | 1:215:A:VAL:HG22 | 1:218:A:TYR:HD1  | 4        | 0.91          |
| (1,2571) | 1:215:A:VAL:HG22 | 1:218:A:TYR:HD2  | 4        | 0.91          |
| (1,2571) | 1:215:A:VAL:HG23 | 1:218:A:TYR:HD1  | 4        | 0.91          |
| (1,2571) | 1:215:A:VAL:HG23 | 1:218:A:TYR:HD2  | 4        | 0.91          |
| (1,2347) | 1:139:A:ILE:HG13 | 1:212:A:GLN:HE22 | 12       | 0.91          |
| (1,2320) | 1:160:A:GLN:HE22 | 1:213:A:MET:HB2  | 19       | 0.91          |
| (1,2254) | 1:217:A:GLN:HE22 | 1:220:A:LYS:HE2  | 12       | 0.91          |
| (1,2254) | 1:217:A:GLN:HE22 | 1:220:A:LYS:HE3  | 12       | 0.91          |
| (1,1303) | 1:137:A:PRO:HB2  | 1:213:A:MET:HG2  | 5        | 0.91          |
| (1,1235) | 1:205:A:MET:HG3  | 1:206:A:MET:HG2  | 1        | 0.91          |
| (1,1015) | 1:152:A:GLU:HG2  | 1:153:A:ASN:HD22 | 4        | 0.91          |
| (1,934)  | 1:166:A:VAL:HG11 | 1:221:A:GLU:HG2  | 1        | 0.91          |
| (1,934)  | 1:166:A:VAL:HG12 | 1:221:A:GLU:HG2  | 1        | 0.91          |
| (1,934)  | 1:166:A:VAL:HG13 | 1:221:A:GLU:HG2  | 1        | 0.91          |
| (1,927)  | 1:212:A:GLN:HA   | 1:213:A:MET:HG2  | 12       | 0.91          |
| (1,677)  | 1:135:A:SER:HB2  | 1:213:A:MET:HA   | 13       | 0.91          |
| (1,602)  | 1:230:A:ARG:H    | 1:231:A:SER:HB3  | 4        | 0.91          |
| (1,104)  | 1:213:A:MET:HA   | 1:215:A:VAL:HG11 | 2        | 0.91          |
| (1,104)  | 1:213:A:MET:HA   | 1:215:A:VAL:HG12 | 2        | 0.91          |
| (1,104)  | 1:213:A:MET:HA   | 1:215:A:VAL:HG13 | 2        | 0.91          |
| (1,98)   | 1:139:A:ILE:HG21 | 1:209:A:VAL:HG11 | 10       | 0.91          |
| (1,98)   | 1:139:A:ILE:HG21 | 1:209:A:VAL:HG12 | 10       | 0.91          |
| (1,98)   | 1:139:A:ILE:HG21 | 1:209:A:VAL:HG13 | 10       | 0.91          |
| (1,98)   | 1:139:A:ILE:HG22 | 1:209:A:VAL:HG11 | 10       | 0.91          |
| (1,98)   | 1:139:A:ILE:HG22 | 1:209:A:VAL:HG12 | 10       | 0.91          |
| (1,98)   | 1:139:A:ILE:HG22 | 1:209:A:VAL:HG13 | 10       | 0.91          |
| (1,98)   | 1:139:A:ILE:HG23 | 1:209:A:VAL:HG11 | 10       | 0.91          |
| (1,98)   | 1:139:A:ILE:HG23 | 1:209:A:VAL:HG12 | 10       | 0.91          |
| (1,98)   | 1:139:A:ILE:HG23 | 1:209:A:VAL:HG13 | 10       | 0.91          |
| (1,2851) | 1:184:A:ILE:HG13 | 1:187:A:HIS:HE1  | 1        | 0.9           |
| (1,2846) | 1:157:A:TYR:HE1  | 1:206:A:MET:HB2  | 7        | 0.9           |
| (1,2846) | 1:157:A:TYR:HE2  | 1:206:A:MET:HB2  | 7        | 0.9           |
| (1,2846) | 1:157:A:TYR:HE1  | 1:206:A:MET:HB2  | 17       | 0.9           |
| (1,2846) | 1:157:A:TYR:HE2  | 1:206:A:MET:HB2  | 17       | 0.9           |
| (1,2650) | 1:139:A:ILE:HG12 | 1:141:A:PHE:HE1  | 7        | 0.9           |
| (1,2650) | 1:139:A:ILE:HG12 | 1:141:A:PHE:HE2  | 7        | 0.9           |
| (1,2492) | 1:139:A:ILE:HG12 | 1:150:A:TYR:HD1  | 12       | 0.9           |
| (1,2492) | 1:139:A:ILE:HG12 | 1:150:A:TYR:HD2  | 12       | 0.9           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2488) | 1:149:A:TYR:HD1  | 1:153:A:ASN:HB3  | 5        | 0.9           |
| (1,2488) | 1:149:A:TYR:HD2  | 1:153:A:ASN:HB3  | 5        | 0.9           |
| (1,2352) | 1:171:A:ASN:HA   | 1:174:A:ASN:HD21 | 8        | 0.9           |
| (1,2347) | 1:139:A:ILE:HG13 | 1:212:A:GLN:HE22 | 17       | 0.9           |
| (1,2338) | 1:212:A:GLN:HE21 | 1:215:A:VAL:HG11 | 17       | 0.9           |
| (1,2338) | 1:212:A:GLN:HE21 | 1:215:A:VAL:HG12 | 17       | 0.9           |
| (1,2338) | 1:212:A:GLN:HE21 | 1:215:A:VAL:HG13 | 17       | 0.9           |
| (1,2315) | 1:160:A:GLN:HE21 | 1:213:A:MET:HB2  | 13       | 0.9           |
| (1,1575) | 1:136:A:ARG:H    | 1:136:A:ARG:HD3  | 1        | 0.9           |
| (1,1523) | 1:162:A:TYR:HB3  | 1:182:A:ILE:HG12 | 12       | 0.9           |
| (1,1523) | 1:162:A:TYR:HB3  | 1:182:A:ILE:HG13 | 12       | 0.9           |
| (1,1303) | 1:137:A:PRO:HB2  | 1:213:A:MET:HG2  | 17       | 0.9           |
| (1,1231) | 1:209:A:VAL:HG21 | 1:213:A:MET:HG3  | 19       | 0.9           |
| (1,1231) | 1:209:A:VAL:HG22 | 1:213:A:MET:HG3  | 19       | 0.9           |
| (1,1231) | 1:209:A:VAL:HG23 | 1:213:A:MET:HG3  | 19       | 0.9           |
| (1,1166) | 1:215:A:VAL:HG21 | 1:219:A:GLN:HG3  | 17       | 0.9           |
| (1,1166) | 1:215:A:VAL:HG22 | 1:219:A:GLN:HG3  | 17       | 0.9           |
| (1,1166) | 1:215:A:VAL:HG23 | 1:219:A:GLN:HG3  | 17       | 0.9           |
| (1,1097) | 1:165:A:PRO:HB3  | 1:168:A:GLN:HG2  | 16       | 0.9           |
| (1,921)  | 1:167:A:SER:HA   | 1:168:A:GLN:HG3  | 8        | 0.9           |
| (1,752)  | 1:138:A:MET:HE1  | 1:139:A:ILE:HG12 | 10       | 0.9           |
| (1,752)  | 1:138:A:MET:HE2  | 1:139:A:ILE:HG12 | 10       | 0.9           |
| (1,752)  | 1:138:A:MET:HE3  | 1:139:A:ILE:HG12 | 10       | 0.9           |
| (1,704)  | 1:209:A:VAL:HG21 | 1:213:A:MET:HE1  | 7        | 0.9           |
| (1,704)  | 1:209:A:VAL:HG21 | 1:213:A:MET:HE2  | 7        | 0.9           |
| (1,704)  | 1:209:A:VAL:HG21 | 1:213:A:MET:HE3  | 7        | 0.9           |
| (1,704)  | 1:209:A:VAL:HG22 | 1:213:A:MET:HE1  | 7        | 0.9           |
| (1,704)  | 1:209:A:VAL:HG22 | 1:213:A:MET:HE2  | 7        | 0.9           |
| (1,704)  | 1:209:A:VAL:HG22 | 1:213:A:MET:HE3  | 7        | 0.9           |
| (1,704)  | 1:209:A:VAL:HG23 | 1:213:A:MET:HE1  | 7        | 0.9           |
| (1,704)  | 1:209:A:VAL:HG23 | 1:213:A:MET:HE2  | 7        | 0.9           |
| (1,704)  | 1:209:A:VAL:HG23 | 1:213:A:MET:HE3  | 7        | 0.9           |
| (1,506)  | 1:179:A:CYS:HB2  | 1:214:A:CYS:HB2  | 6        | 0.9           |
| (1,423)  | 1:151:A:ARG:HD3  | 1:152:A:GLU:H    | 5        | 0.9           |
| (1,396)  | 1:210:A:VAL:HA   | 1:213:A:MET:HB3  | 15       | 0.9           |
| (1,357)  | 1:122:A:VAL:HG21 | 1:125:A:LEU:HG   | 1        | 0.9           |
| (1,357)  | 1:122:A:VAL:HG22 | 1:125:A:LEU:HG   | 1        | 0.9           |
| (1,357)  | 1:122:A:VAL:HG23 | 1:125:A:LEU:HG   | 1        | 0.9           |
| (1,158)  | 1:126:A:GLY:HA2  | 1:164:A:ARG:HD3  | 11       | 0.9           |
| (1,98)   | 1:139:A:ILE:HG21 | 1:209:A:VAL:HG11 | 8        | 0.9           |
| (1,98)   | 1:139:A:ILE:HG21 | 1:209:A:VAL:HG12 | 8        | 0.9           |
| (1,98)   | 1:139:A:ILE:HG21 | 1:209:A:VAL:HG13 | 8        | 0.9           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,98)   | 1:139:A:ILE:HG22 | 1:209:A:VAL:HG11 | 8        | 0.9           |
| (1,98)   | 1:139:A:ILE:HG22 | 1:209:A:VAL:HG12 | 8        | 0.9           |
| (1,98)   | 1:139:A:ILE:HG22 | 1:209:A:VAL:HG13 | 8        | 0.9           |
| (1,98)   | 1:139:A:ILE:HG23 | 1:209:A:VAL:HG11 | 8        | 0.9           |
| (1,98)   | 1:139:A:ILE:HG23 | 1:209:A:VAL:HG12 | 8        | 0.9           |
| (1,98)   | 1:139:A:ILE:HG23 | 1:209:A:VAL:HG13 | 8        | 0.9           |
| (1,98)   | 1:139:A:ILE:HG21 | 1:209:A:VAL:HG11 | 13       | 0.9           |
| (1,98)   | 1:139:A:ILE:HG21 | 1:209:A:VAL:HG12 | 13       | 0.9           |
| (1,98)   | 1:139:A:ILE:HG21 | 1:209:A:VAL:HG13 | 13       | 0.9           |
| (1,98)   | 1:139:A:ILE:HG22 | 1:209:A:VAL:HG11 | 13       | 0.9           |
| (1,98)   | 1:139:A:ILE:HG22 | 1:209:A:VAL:HG12 | 13       | 0.9           |
| (1,98)   | 1:139:A:ILE:HG22 | 1:209:A:VAL:HG13 | 13       | 0.9           |
| (1,98)   | 1:139:A:ILE:HG23 | 1:209:A:VAL:HG11 | 13       | 0.9           |
| (1,98)   | 1:139:A:ILE:HG23 | 1:209:A:VAL:HG12 | 13       | 0.9           |
| (1,98)   | 1:139:A:ILE:HG23 | 1:209:A:VAL:HG13 | 13       | 0.9           |
| (1,98)   | 1:139:A:ILE:HG21 | 1:209:A:VAL:HG11 | 14       | 0.9           |
| (1,98)   | 1:139:A:ILE:HG21 | 1:209:A:VAL:HG12 | 14       | 0.9           |
| (1,98)   | 1:139:A:ILE:HG21 | 1:209:A:VAL:HG13 | 14       | 0.9           |
| (1,98)   | 1:139:A:ILE:HG22 | 1:209:A:VAL:HG11 | 14       | 0.9           |
| (1,98)   | 1:139:A:ILE:HG22 | 1:209:A:VAL:HG12 | 14       | 0.9           |
| (1,98)   | 1:139:A:ILE:HG22 | 1:209:A:VAL:HG13 | 14       | 0.9           |
| (1,98)   | 1:139:A:ILE:HG23 | 1:209:A:VAL:HG11 | 14       | 0.9           |
| (1,98)   | 1:139:A:ILE:HG23 | 1:209:A:VAL:HG12 | 14       | 0.9           |
| (1,98)   | 1:139:A:ILE:HG23 | 1:209:A:VAL:HG13 | 14       | 0.9           |
| (1,2821) | 1:129:A:MET:HB3  | 1:163:A:TYR:HE1  | 3        | 0.89          |
| (1,2821) | 1:129:A:MET:HB3  | 1:163:A:TYR:HE2  | 3        | 0.89          |
| (1,2758) | 1:150:A:TYR:HE1  | 1:209:A:VAL:HG11 | 7        | 0.89          |
| (1,2758) | 1:150:A:TYR:HE1  | 1:209:A:VAL:HG12 | 7        | 0.89          |
| (1,2758) | 1:150:A:TYR:HE1  | 1:209:A:VAL:HG13 | 7        | 0.89          |
| (1,2758) | 1:150:A:TYR:HE2  | 1:209:A:VAL:HG11 | 7        | 0.89          |
| (1,2758) | 1:150:A:TYR:HE2  | 1:209:A:VAL:HG12 | 7        | 0.89          |
| (1,2758) | 1:150:A:TYR:HE2  | 1:209:A:VAL:HG13 | 7        | 0.89          |
| (1,2735) | 1:186:A:GLN:HB3  | 1:187:A:HIS:HD2  | 10       | 0.89          |
| (1,2681) | 1:141:A:PHE:HZ   | 1:208:A:ARG:HB3  | 10       | 0.89          |
| (1,2615) | 1:141:A:PHE:HD1  | 1:147:A:ASP:HB3  | 8        | 0.89          |
| (1,2615) | 1:141:A:PHE:HD2  | 1:147:A:ASP:HB3  | 8        | 0.89          |
| (1,2615) | 1:141:A:PHE:HD1  | 1:147:A:ASP:HB3  | 18       | 0.89          |
| (1,2615) | 1:141:A:PHE:HD2  | 1:147:A:ASP:HB3  | 18       | 0.89          |
| (1,2492) | 1:139:A:ILE:HG12 | 1:150:A:TYR:HD1  | 4        | 0.89          |
| (1,2492) | 1:139:A:ILE:HG12 | 1:150:A:TYR:HD2  | 4        | 0.89          |
| (1,2492) | 1:139:A:ILE:HG12 | 1:150:A:TYR:HD1  | 10       | 0.89          |
| (1,2492) | 1:139:A:ILE:HG12 | 1:150:A:TYR:HD2  | 10       | 0.89          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2347) | 1:139:A:ILE:HG13 | 1:212:A:GLN:HE22 | 20       | 0.89          |
| (1,2250) | 1:217:A:GLN:HE21 | 1:218:A:TYR:HA   | 12       | 0.89          |
| (1,1231) | 1:209:A:VAL:HG21 | 1:213:A:MET:HG3  | 11       | 0.89          |
| (1,1231) | 1:209:A:VAL:HG22 | 1:213:A:MET:HG3  | 11       | 0.89          |
| (1,1231) | 1:209:A:VAL:HG23 | 1:213:A:MET:HG3  | 11       | 0.89          |
| (1,637)  | 1:147:A:ASP:HB2  | 1:148:A:ARG:HG2  | 5        | 0.89          |
| (1,314)  | 1:166:A:VAL:HG21 | 1:169:A:TYR:HB3  | 3        | 0.89          |
| (1,314)  | 1:166:A:VAL:HG22 | 1:169:A:TYR:HB3  | 3        | 0.89          |
| (1,314)  | 1:166:A:VAL:HG23 | 1:169:A:TYR:HB3  | 3        | 0.89          |
| (1,155)  | 1:125:A:LEU:HB3  | 1:126:A:GLY:HA3  | 4        | 0.89          |
| (1,98)   | 1:139:A:ILE:HG21 | 1:209:A:VAL:HG11 | 7        | 0.89          |
| (1,98)   | 1:139:A:ILE:HG21 | 1:209:A:VAL:HG12 | 7        | 0.89          |
| (1,98)   | 1:139:A:ILE:HG21 | 1:209:A:VAL:HG13 | 7        | 0.89          |
| (1,98)   | 1:139:A:ILE:HG22 | 1:209:A:VAL:HG11 | 7        | 0.89          |
| (1,98)   | 1:139:A:ILE:HG22 | 1:209:A:VAL:HG12 | 7        | 0.89          |
| (1,98)   | 1:139:A:ILE:HG22 | 1:209:A:VAL:HG13 | 7        | 0.89          |
| (1,98)   | 1:139:A:ILE:HG23 | 1:209:A:VAL:HG11 | 7        | 0.89          |
| (1,98)   | 1:139:A:ILE:HG23 | 1:209:A:VAL:HG12 | 7        | 0.89          |
| (1,98)   | 1:139:A:ILE:HG23 | 1:209:A:VAL:HG13 | 7        | 0.89          |
| (1,89)   | 1:206:A:MET:HB3  | 1:210:A:VAL:HG21 | 9        | 0.89          |
| (1,89)   | 1:206:A:MET:HB3  | 1:210:A:VAL:HG22 | 9        | 0.89          |
| (1,89)   | 1:206:A:MET:HB3  | 1:210:A:VAL:HG23 | 9        | 0.89          |
| (1,2821) | 1:129:A:MET:HB3  | 1:163:A:TYR:HE1  | 7        | 0.88          |
| (1,2821) | 1:129:A:MET:HB3  | 1:163:A:TYR:HE2  | 7        | 0.88          |
| (1,2821) | 1:129:A:MET:HB3  | 1:163:A:TYR:HE1  | 10       | 0.88          |
| (1,2821) | 1:129:A:MET:HB3  | 1:163:A:TYR:HE2  | 10       | 0.88          |
| (1,2758) | 1:150:A:TYR:HE1  | 1:209:A:VAL:HG11 | 8        | 0.88          |
| (1,2758) | 1:150:A:TYR:HE1  | 1:209:A:VAL:HG12 | 8        | 0.88          |
| (1,2758) | 1:150:A:TYR:HE1  | 1:209:A:VAL:HG13 | 8        | 0.88          |
| (1,2758) | 1:150:A:TYR:HE2  | 1:209:A:VAL:HG11 | 8        | 0.88          |
| (1,2758) | 1:150:A:TYR:HE2  | 1:209:A:VAL:HG12 | 8        | 0.88          |
| (1,2758) | 1:150:A:TYR:HE2  | 1:209:A:VAL:HG13 | 8        | 0.88          |
| (1,2735) | 1:186:A:GLN:HB3  | 1:187:A:HIS:HD2  | 6        | 0.88          |
| (1,2650) | 1:139:A:ILE:HG12 | 1:141:A:PHE:HE1  | 3        | 0.88          |
| (1,2650) | 1:139:A:ILE:HG12 | 1:141:A:PHE:HE2  | 3        | 0.88          |
| (1,2650) | 1:139:A:ILE:HG12 | 1:141:A:PHE:HE1  | 16       | 0.88          |
| (1,2650) | 1:139:A:ILE:HG12 | 1:141:A:PHE:HE2  | 16       | 0.88          |
| (1,1752) | 1:166:A:VAL:HG11 | 1:223:A:GLN:H    | 3        | 0.88          |
| (1,1752) | 1:166:A:VAL:HG12 | 1:223:A:GLN:H    | 3        | 0.88          |
| (1,1752) | 1:166:A:VAL:HG13 | 1:223:A:GLN:H    | 3        | 0.88          |
| (1,1089) | 1:182:A:ILE:HD11 | 1:186:A:GLN:HE21 | 4        | 0.88          |
| (1,1089) | 1:182:A:ILE:HD12 | 1:186:A:GLN:HE21 | 4        | 0.88          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1089) | 1:182:A:ILE:HD13 | 1:186:A:GLN:HE21 | 4        | 0.88          |
| (1,752)  | 1:138:A:MET:HE1  | 1:139:A:ILE:HG12 | 6        | 0.88          |
| (1,752)  | 1:138:A:MET:HE2  | 1:139:A:ILE:HG12 | 6        | 0.88          |
| (1,752)  | 1:138:A:MET:HE3  | 1:139:A:ILE:HG12 | 6        | 0.88          |
| (1,752)  | 1:138:A:MET:HE1  | 1:139:A:ILE:HG12 | 13       | 0.88          |
| (1,752)  | 1:138:A:MET:HE2  | 1:139:A:ILE:HG12 | 13       | 0.88          |
| (1,752)  | 1:138:A:MET:HE3  | 1:139:A:ILE:HG12 | 13       | 0.88          |
| (1,751)  | 1:222:A:SER:HB2  | 1:223:A:GLN:HA   | 16       | 0.88          |
| (1,733)  | 1:222:A:SER:HB2  | 1:226:A:TYR:HD1  | 10       | 0.88          |
| (1,733)  | 1:222:A:SER:HB2  | 1:226:A:TYR:HD2  | 10       | 0.88          |
| (1,637)  | 1:147:A:ASP:HB2  | 1:148:A:ARG:HG2  | 17       | 0.88          |
| (1,323)  | 1:209:A:VAL:HG21 | 1:212:A:GLN:HB3  | 4        | 0.88          |
| (1,323)  | 1:209:A:VAL:HG22 | 1:212:A:GLN:HB3  | 4        | 0.88          |
| (1,323)  | 1:209:A:VAL:HG23 | 1:212:A:GLN:HB3  | 4        | 0.88          |
| (1,322)  | 1:158:A:PRO:HD3  | 1:209:A:VAL:HG21 | 7        | 0.88          |
| (1,322)  | 1:158:A:PRO:HD3  | 1:209:A:VAL:HG22 | 7        | 0.88          |
| (1,322)  | 1:158:A:PRO:HD3  | 1:209:A:VAL:HG23 | 7        | 0.88          |
| (1,155)  | 1:125:A:LEU:HB3  | 1:126:A:GLY:HA3  | 10       | 0.88          |
| (1,104)  | 1:213:A:MET:HA   | 1:215:A:VAL:HG11 | 4        | 0.88          |
| (1,104)  | 1:213:A:MET:HA   | 1:215:A:VAL:HG12 | 4        | 0.88          |
| (1,104)  | 1:213:A:MET:HA   | 1:215:A:VAL:HG13 | 4        | 0.88          |
| (1,2847) | 1:157:A:TYR:HE1  | 1:209:A:VAL:HG11 | 2        | 0.87          |
| (1,2847) | 1:157:A:TYR:HE1  | 1:209:A:VAL:HG12 | 2        | 0.87          |
| (1,2847) | 1:157:A:TYR:HE1  | 1:209:A:VAL:HG13 | 2        | 0.87          |
| (1,2847) | 1:157:A:TYR:HE2  | 1:209:A:VAL:HG11 | 2        | 0.87          |
| (1,2847) | 1:157:A:TYR:HE2  | 1:209:A:VAL:HG12 | 2        | 0.87          |
| (1,2847) | 1:157:A:TYR:HE2  | 1:209:A:VAL:HG13 | 2        | 0.87          |
| (1,2794) | 1:128:A:TYR:HE1  | 1:164:A:ARG:HG2  | 12       | 0.87          |
| (1,2794) | 1:128:A:TYR:HE2  | 1:164:A:ARG:HG2  | 12       | 0.87          |
| (1,2782) | 1:150:A:TYR:HE1  | 1:154:A:MET:HG3  | 19       | 0.87          |
| (1,2782) | 1:150:A:TYR:HE2  | 1:154:A:MET:HG3  | 19       | 0.87          |
| (1,2711) | 1:145:A:TRP:HZ3  | 1:146:A:GLU:HG3  | 14       | 0.87          |
| (1,2492) | 1:139:A:ILE:HG12 | 1:150:A:TYR:HD1  | 16       | 0.87          |
| (1,2492) | 1:139:A:ILE:HG12 | 1:150:A:TYR:HD2  | 16       | 0.87          |
| (1,2414) | 1:136:A:ARG:HB3  | 1:159:A:ASN:HD21 | 4        | 0.87          |
| (1,1575) | 1:136:A:ARG:H    | 1:136:A:ARG:HD3  | 4        | 0.87          |
| (1,1523) | 1:162:A:TYR:HB3  | 1:182:A:ILE:HG12 | 15       | 0.87          |
| (1,1523) | 1:162:A:TYR:HB3  | 1:182:A:ILE:HG13 | 15       | 0.87          |
| (1,1197) | 1:160:A:GLN:HB2  | 1:183:A:THR:HG21 | 2        | 0.87          |
| (1,1197) | 1:160:A:GLN:HB2  | 1:183:A:THR:HG22 | 2        | 0.87          |
| (1,1197) | 1:160:A:GLN:HB2  | 1:183:A:THR:HG23 | 2        | 0.87          |
| (1,1164) | 1:215:A:VAL:HG21 | 1:219:A:GLN:HG2  | 13       | 0.87          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1164) | 1:215:A:VAL:HG22 | 1:219:A:GLN:HG2  | 13       | 0.87          |
| (1,1164) | 1:215:A:VAL:HG23 | 1:219:A:GLN:HG2  | 13       | 0.87          |
| (1,637)  | 1:147:A:ASP:HB2  | 1:148:A:ARG:HG2  | 15       | 0.87          |
| (1,567)  | 1:230:A:ARG:HB2  | 1:231:A:SER:HB3  | 8        | 0.87          |
| (1,107)  | 1:211:A:GLU:HG3  | 1:215:A:VAL:HG11 | 9        | 0.87          |
| (1,107)  | 1:211:A:GLU:HG3  | 1:215:A:VAL:HG12 | 9        | 0.87          |
| (1,107)  | 1:211:A:GLU:HG3  | 1:215:A:VAL:HG13 | 9        | 0.87          |
| (1,76)   | 1:139:A:ILE:HG12 | 1:209:A:VAL:HG11 | 18       | 0.87          |
| (1,76)   | 1:139:A:ILE:HG12 | 1:209:A:VAL:HG12 | 18       | 0.87          |
| (1,76)   | 1:139:A:ILE:HG12 | 1:209:A:VAL:HG13 | 18       | 0.87          |
| (1,2851) | 1:184:A:ILE:HG13 | 1:187:A:HIS:HE1  | 5        | 0.86          |
| (1,2847) | 1:157:A:TYR:HE1  | 1:209:A:VAL:HG11 | 20       | 0.86          |
| (1,2847) | 1:157:A:TYR:HE1  | 1:209:A:VAL:HG12 | 20       | 0.86          |
| (1,2847) | 1:157:A:TYR:HE1  | 1:209:A:VAL:HG13 | 20       | 0.86          |
| (1,2847) | 1:157:A:TYR:HE2  | 1:209:A:VAL:HG11 | 20       | 0.86          |
| (1,2847) | 1:157:A:TYR:HE2  | 1:209:A:VAL:HG12 | 20       | 0.86          |
| (1,2847) | 1:157:A:TYR:HE2  | 1:209:A:VAL:HG13 | 20       | 0.86          |
| (1,2758) | 1:150:A:TYR:HE1  | 1:209:A:VAL:HG11 | 4        | 0.86          |
| (1,2758) | 1:150:A:TYR:HE1  | 1:209:A:VAL:HG12 | 4        | 0.86          |
| (1,2758) | 1:150:A:TYR:HE1  | 1:209:A:VAL:HG13 | 4        | 0.86          |
| (1,2758) | 1:150:A:TYR:HE2  | 1:209:A:VAL:HG11 | 4        | 0.86          |
| (1,2758) | 1:150:A:TYR:HE2  | 1:209:A:VAL:HG12 | 4        | 0.86          |
| (1,2758) | 1:150:A:TYR:HE2  | 1:209:A:VAL:HG13 | 4        | 0.86          |
| (1,2735) | 1:186:A:GLN:HB3  | 1:187:A:HIS:HD2  | 9        | 0.86          |
| (1,2711) | 1:145:A:TRP:HZ3  | 1:146:A:GLU:HG3  | 2        | 0.86          |
| (1,2657) | 1:141:A:PHE:HE1  | 1:208:A:ARG:HB3  | 20       | 0.86          |
| (1,2657) | 1:141:A:PHE:HE2  | 1:208:A:ARG:HB3  | 20       | 0.86          |
| (1,2559) | 1:128:A:TYR:HD1  | 1:164:A:ARG:HD3  | 16       | 0.86          |
| (1,2559) | 1:128:A:TYR:HD2  | 1:164:A:ARG:HD3  | 16       | 0.86          |
| (1,2356) | 1:169:A:TYR:HB2  | 1:174:A:ASN:HD21 | 19       | 0.86          |
| (1,2123) | 1:199:A:THR:H    | 1:203:A:VAL:HG11 | 8        | 0.86          |
| (1,2123) | 1:199:A:THR:H    | 1:203:A:VAL:HG12 | 8        | 0.86          |
| (1,2123) | 1:199:A:THR:H    | 1:203:A:VAL:HG13 | 8        | 0.86          |
| (1,1914) | 1:209:A:VAL:HG21 | 1:213:A:MET:H    | 19       | 0.86          |
| (1,1914) | 1:209:A:VAL:HG22 | 1:213:A:MET:H    | 19       | 0.86          |
| (1,1914) | 1:209:A:VAL:HG23 | 1:213:A:MET:H    | 19       | 0.86          |
| (1,1497) | 1:139:A:ILE:HD11 | 1:212:A:GLN:HB3  | 8        | 0.86          |
| (1,1497) | 1:139:A:ILE:HD12 | 1:212:A:GLN:HB3  | 8        | 0.86          |
| (1,1497) | 1:139:A:ILE:HD13 | 1:212:A:GLN:HB3  | 8        | 0.86          |
| (1,1256) | 1:184:A:ILE:HG13 | 1:206:A:MET:HG3  | 19       | 0.86          |
| (1,1131) | 1:223:A:GLN:HG2  | 1:226:A:TYR:H    | 5        | 0.86          |
| (1,1131) | 1:223:A:GLN:HG2  | 1:226:A:TYR:H    | 12       | 0.86          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1104) | 1:213:A:MET:HB3  | 1:214:A:CYS:HA   | 6        | 0.86          |
| (1,1085) | 1:129:A:MET:HB2  | 1:164:A:ARG:HA   | 1        | 0.86          |
| (1,893)  | 1:162:A:TYR:HB3  | 1:182:A:ILE:HB   | 8        | 0.86          |
| (1,873)  | 1:146:A:GLU:HA   | 1:150:A:TYR:HB3  | 7        | 0.86          |
| (1,396)  | 1:210:A:VAL:HA   | 1:213:A:MET:HB3  | 12       | 0.86          |
| (1,323)  | 1:209:A:VAL:HG21 | 1:212:A:GLN:HB3  | 11       | 0.86          |
| (1,323)  | 1:209:A:VAL:HG22 | 1:212:A:GLN:HB3  | 11       | 0.86          |
| (1,323)  | 1:209:A:VAL:HG23 | 1:212:A:GLN:HB3  | 11       | 0.86          |
| (1,240)  | 1:166:A:VAL:HG21 | 1:169:A:TYR:HB2  | 1        | 0.86          |
| (1,240)  | 1:166:A:VAL:HG22 | 1:169:A:TYR:HB2  | 1        | 0.86          |
| (1,240)  | 1:166:A:VAL:HG23 | 1:169:A:TYR:HB2  | 1        | 0.86          |
| (1,98)   | 1:139:A:ILE:HG21 | 1:209:A:VAL:HG11 | 4        | 0.86          |
| (1,98)   | 1:139:A:ILE:HG21 | 1:209:A:VAL:HG12 | 4        | 0.86          |
| (1,98)   | 1:139:A:ILE:HG21 | 1:209:A:VAL:HG13 | 4        | 0.86          |
| (1,98)   | 1:139:A:ILE:HG22 | 1:209:A:VAL:HG11 | 4        | 0.86          |
| (1,98)   | 1:139:A:ILE:HG22 | 1:209:A:VAL:HG12 | 4        | 0.86          |
| (1,98)   | 1:139:A:ILE:HG22 | 1:209:A:VAL:HG13 | 4        | 0.86          |
| (1,98)   | 1:139:A:ILE:HG23 | 1:209:A:VAL:HG11 | 4        | 0.86          |
| (1,98)   | 1:139:A:ILE:HG23 | 1:209:A:VAL:HG12 | 4        | 0.86          |
| (1,98)   | 1:139:A:ILE:HG23 | 1:209:A:VAL:HG13 | 4        | 0.86          |
| (1,98)   | 1:139:A:ILE:HG21 | 1:209:A:VAL:HG11 | 19       | 0.86          |
| (1,98)   | 1:139:A:ILE:HG21 | 1:209:A:VAL:HG12 | 19       | 0.86          |
| (1,98)   | 1:139:A:ILE:HG21 | 1:209:A:VAL:HG13 | 19       | 0.86          |
| (1,98)   | 1:139:A:ILE:HG22 | 1:209:A:VAL:HG11 | 19       | 0.86          |
| (1,98)   | 1:139:A:ILE:HG22 | 1:209:A:VAL:HG12 | 19       | 0.86          |
| (1,98)   | 1:139:A:ILE:HG22 | 1:209:A:VAL:HG13 | 19       | 0.86          |
| (1,98)   | 1:139:A:ILE:HG23 | 1:209:A:VAL:HG11 | 19       | 0.86          |
| (1,98)   | 1:139:A:ILE:HG23 | 1:209:A:VAL:HG12 | 19       | 0.86          |
| (1,98)   | 1:139:A:ILE:HG23 | 1:209:A:VAL:HG13 | 19       | 0.86          |
| (1,2847) | 1:157:A:TYR:HE1  | 1:209:A:VAL:HG11 | 17       | 0.85          |
| (1,2847) | 1:157:A:TYR:HE1  | 1:209:A:VAL:HG12 | 17       | 0.85          |
| (1,2847) | 1:157:A:TYR:HE1  | 1:209:A:VAL:HG13 | 17       | 0.85          |
| (1,2847) | 1:157:A:TYR:HE2  | 1:209:A:VAL:HG11 | 17       | 0.85          |
| (1,2847) | 1:157:A:TYR:HE2  | 1:209:A:VAL:HG12 | 17       | 0.85          |
| (1,2847) | 1:157:A:TYR:HE2  | 1:209:A:VAL:HG13 | 17       | 0.85          |
| (1,2482) | 1:163:A:TYR:HD1  | 1:221:A:GLU:HG2  | 16       | 0.85          |
| (1,2482) | 1:163:A:TYR:HD2  | 1:221:A:GLU:HG2  | 16       | 0.85          |
| (1,1914) | 1:209:A:VAL:HG21 | 1:213:A:MET:H    | 7        | 0.85          |
| (1,1914) | 1:209:A:VAL:HG22 | 1:213:A:MET:H    | 7        | 0.85          |
| (1,1914) | 1:209:A:VAL:HG23 | 1:213:A:MET:H    | 7        | 0.85          |
| (1,1914) | 1:209:A:VAL:HG21 | 1:213:A:MET:H    | 13       | 0.85          |
| (1,1914) | 1:209:A:VAL:HG22 | 1:213:A:MET:H    | 13       | 0.85          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1914) | 1:209:A:VAL:HG23 | 1:213:A:MET:H    | 13       | 0.85          |
| (1,1914) | 1:209:A:VAL:HG21 | 1:213:A:MET:H    | 16       | 0.85          |
| (1,1914) | 1:209:A:VAL:HG22 | 1:213:A:MET:H    | 16       | 0.85          |
| (1,1914) | 1:209:A:VAL:HG23 | 1:213:A:MET:H    | 16       | 0.85          |
| (1,1914) | 1:209:A:VAL:HG21 | 1:213:A:MET:H    | 18       | 0.85          |
| (1,1914) | 1:209:A:VAL:HG22 | 1:213:A:MET:H    | 18       | 0.85          |
| (1,1914) | 1:209:A:VAL:HG23 | 1:213:A:MET:H    | 18       | 0.85          |
| (1,1575) | 1:136:A:ARG:H    | 1:136:A:ARG:HD3  | 17       | 0.85          |
| (1,1104) | 1:213:A:MET:HB3  | 1:214:A:CYS:HA   | 10       | 0.85          |
| (1,1055) | 1:203:A:VAL:HG21 | 1:207:A:GLU:HG2  | 5        | 0.85          |
| (1,1055) | 1:203:A:VAL:HG22 | 1:207:A:GLU:HG2  | 5        | 0.85          |
| (1,1055) | 1:203:A:VAL:HG23 | 1:207:A:GLU:HG2  | 5        | 0.85          |
| (1,1055) | 1:203:A:VAL:HG21 | 1:207:A:GLU:HG2  | 7        | 0.85          |
| (1,1055) | 1:203:A:VAL:HG22 | 1:207:A:GLU:HG2  | 7        | 0.85          |
| (1,1055) | 1:203:A:VAL:HG23 | 1:207:A:GLU:HG2  | 7        | 0.85          |
| (1,921)  | 1:167:A:SER:HA   | 1:168:A:GLN:HG3  | 7        | 0.85          |
| (1,921)  | 1:167:A:SER:HA   | 1:168:A:GLN:HG3  | 20       | 0.85          |
| (1,189)  | 1:123:A:GLY:HA2  | 1:125:A:LEU:HD21 | 6        | 0.85          |
| (1,189)  | 1:123:A:GLY:HA2  | 1:125:A:LEU:HD22 | 6        | 0.85          |
| (1,189)  | 1:123:A:GLY:HA2  | 1:125:A:LEU:HD23 | 6        | 0.85          |
| (1,189)  | 1:123:A:GLY:HA3  | 1:125:A:LEU:HD21 | 6        | 0.85          |
| (1,189)  | 1:123:A:GLY:HA3  | 1:125:A:LEU:HD22 | 6        | 0.85          |
| (1,189)  | 1:123:A:GLY:HA3  | 1:125:A:LEU:HD23 | 6        | 0.85          |
| (1,127)  | 1:161:A:VAL:HG11 | 1:210:A:VAL:HA   | 10       | 0.85          |
| (1,127)  | 1:161:A:VAL:HG12 | 1:210:A:VAL:HA   | 10       | 0.85          |
| (1,127)  | 1:161:A:VAL:HG13 | 1:210:A:VAL:HA   | 10       | 0.85          |
| (1,98)   | 1:139:A:ILE:HG21 | 1:209:A:VAL:HG11 | 12       | 0.85          |
| (1,98)   | 1:139:A:ILE:HG21 | 1:209:A:VAL:HG12 | 12       | 0.85          |
| (1,98)   | 1:139:A:ILE:HG21 | 1:209:A:VAL:HG13 | 12       | 0.85          |
| (1,98)   | 1:139:A:ILE:HG22 | 1:209:A:VAL:HG11 | 12       | 0.85          |
| (1,98)   | 1:139:A:ILE:HG22 | 1:209:A:VAL:HG12 | 12       | 0.85          |
| (1,98)   | 1:139:A:ILE:HG22 | 1:209:A:VAL:HG13 | 12       | 0.85          |
| (1,98)   | 1:139:A:ILE:HG23 | 1:209:A:VAL:HG11 | 12       | 0.85          |
| (1,98)   | 1:139:A:ILE:HG23 | 1:209:A:VAL:HG12 | 12       | 0.85          |
| (1,98)   | 1:139:A:ILE:HG23 | 1:209:A:VAL:HG13 | 12       | 0.85          |
| (1,2831) | 1:166:A:VAL:HG21 | 1:218:A:TYR:HE1  | 1        | 0.84          |
| (1,2831) | 1:166:A:VAL:HG21 | 1:218:A:TYR:HE2  | 1        | 0.84          |
| (1,2831) | 1:166:A:VAL:HG22 | 1:218:A:TYR:HE1  | 1        | 0.84          |
| (1,2831) | 1:166:A:VAL:HG22 | 1:218:A:TYR:HE2  | 1        | 0.84          |
| (1,2831) | 1:166:A:VAL:HG23 | 1:218:A:TYR:HE1  | 1        | 0.84          |
| (1,2831) | 1:166:A:VAL:HG23 | 1:218:A:TYR:HE2  | 1        | 0.84          |
| (1,2821) | 1:129:A:MET:HB3  | 1:163:A:TYR:HE1  | 1        | 0.84          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2821) | 1:129:A:MET:HB3  | 1:163:A:TYR:HE2  | 1        | 0.84          |
| (1,2699) | 1:141:A:PHE:HZ   | 1:150:A:TYR:HB3  | 11       | 0.84          |
| (1,2615) | 1:141:A:PHE:HD1  | 1:147:A:ASP:HB3  | 6        | 0.84          |
| (1,2615) | 1:141:A:PHE:HD2  | 1:147:A:ASP:HB3  | 6        | 0.84          |
| (1,2518) | 1:155:A:TYR:HD1  | 1:156:A:ARG:HD2  | 12       | 0.84          |
| (1,2518) | 1:155:A:TYR:HD2  | 1:156:A:ARG:HD2  | 12       | 0.84          |
| (1,2492) | 1:139:A:ILE:HG12 | 1:150:A:TYR:HD1  | 2        | 0.84          |
| (1,2492) | 1:139:A:ILE:HG12 | 1:150:A:TYR:HD2  | 2        | 0.84          |
| (1,2346) | 1:212:A:GLN:HE22 | 1:215:A:VAL:HG21 | 18       | 0.84          |
| (1,2346) | 1:212:A:GLN:HE22 | 1:215:A:VAL:HG22 | 18       | 0.84          |
| (1,2346) | 1:212:A:GLN:HE22 | 1:215:A:VAL:HG23 | 18       | 0.84          |
| (1,1575) | 1:136:A:ARG:H    | 1:136:A:ARG:HD3  | 13       | 0.84          |
| (1,1297) | 1:173:A:LYS:HG2  | 1:176:A:VAL:HB   | 17       | 0.84          |
| (1,1131) | 1:223:A:GLN:HG2  | 1:226:A:TYR:H    | 6        | 0.84          |
| (1,1104) | 1:213:A:MET:HB3  | 1:214:A:CYS:HA   | 13       | 0.84          |
| (1,1104) | 1:213:A:MET:HB3  | 1:214:A:CYS:HA   | 15       | 0.84          |
| (1,1058) | 1:203:A:VAL:HG21 | 1:207:A:GLU:HG3  | 2        | 0.84          |
| (1,1058) | 1:203:A:VAL:HG22 | 1:207:A:GLU:HG3  | 2        | 0.84          |
| (1,1058) | 1:203:A:VAL:HG23 | 1:207:A:GLU:HG3  | 2        | 0.84          |
| (1,864)  | 1:134:A:MET:HB3  | 1:135:A:SER:HB2  | 2        | 0.84          |
| (1,862)  | 1:143:A:ASN:HD22 | 1:146:A:GLU:HG2  | 7        | 0.84          |
| (1,733)  | 1:222:A:SER:HB2  | 1:226:A:TYR:HD1  | 5        | 0.84          |
| (1,733)  | 1:222:A:SER:HB2  | 1:226:A:TYR:HD2  | 5        | 0.84          |
| (1,733)  | 1:222:A:SER:HB2  | 1:226:A:TYR:HD1  | 13       | 0.84          |
| (1,733)  | 1:222:A:SER:HB2  | 1:226:A:TYR:HD2  | 13       | 0.84          |
| (1,634)  | 1:192:A:THR:HA   | 1:195:A:GLY:HA3  | 8        | 0.84          |
| (1,502)  | 1:162:A:TYR:HB3  | 1:183:A:THR:HA   | 12       | 0.84          |
| (1,476)  | 1:203:A:VAL:HG21 | 1:204:A:LYS:HE2  | 2        | 0.84          |
| (1,476)  | 1:203:A:VAL:HG21 | 1:204:A:LYS:HE3  | 2        | 0.84          |
| (1,476)  | 1:203:A:VAL:HG22 | 1:204:A:LYS:HE2  | 2        | 0.84          |
| (1,476)  | 1:203:A:VAL:HG22 | 1:204:A:LYS:HE3  | 2        | 0.84          |
| (1,476)  | 1:203:A:VAL:HG23 | 1:204:A:LYS:HE2  | 2        | 0.84          |
| (1,476)  | 1:203:A:VAL:HG23 | 1:204:A:LYS:HE3  | 2        | 0.84          |
| (1,429)  | 1:122:A:VAL:HG11 | 1:186:A:GLN:HA   | 19       | 0.84          |
| (1,429)  | 1:122:A:VAL:HG12 | 1:186:A:GLN:HA   | 19       | 0.84          |
| (1,429)  | 1:122:A:VAL:HG13 | 1:186:A:GLN:HA   | 19       | 0.84          |
| (1,392)  | 1:122:A:VAL:HG11 | 1:190:A:THR:HB   | 19       | 0.84          |
| (1,392)  | 1:122:A:VAL:HG12 | 1:190:A:THR:HB   | 19       | 0.84          |
| (1,392)  | 1:122:A:VAL:HG13 | 1:190:A:THR:HB   | 19       | 0.84          |
| (1,323)  | 1:209:A:VAL:HG21 | 1:212:A:GLN:HB3  | 5        | 0.84          |
| (1,323)  | 1:209:A:VAL:HG22 | 1:212:A:GLN:HB3  | 5        | 0.84          |
| (1,323)  | 1:209:A:VAL:HG23 | 1:212:A:GLN:HB3  | 5        | 0.84          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,258)  | 1:122:A:VAL:HG11 | 1:190:A:THR:HG21 | 12       | 0.84          |
| (1,258)  | 1:122:A:VAL:HG11 | 1:190:A:THR:HG22 | 12       | 0.84          |
| (1,258)  | 1:122:A:VAL:HG11 | 1:190:A:THR:HG23 | 12       | 0.84          |
| (1,258)  | 1:122:A:VAL:HG12 | 1:190:A:THR:HG21 | 12       | 0.84          |
| (1,258)  | 1:122:A:VAL:HG12 | 1:190:A:THR:HG22 | 12       | 0.84          |
| (1,258)  | 1:122:A:VAL:HG12 | 1:190:A:THR:HG23 | 12       | 0.84          |
| (1,258)  | 1:122:A:VAL:HG13 | 1:190:A:THR:HG21 | 12       | 0.84          |
| (1,258)  | 1:122:A:VAL:HG13 | 1:190:A:THR:HG22 | 12       | 0.84          |
| (1,258)  | 1:122:A:VAL:HG13 | 1:190:A:THR:HG23 | 12       | 0.84          |
| (1,2821) | 1:129:A:MET:HB3  | 1:163:A:TYR:HE1  | 16       | 0.83          |
| (1,2821) | 1:129:A:MET:HB3  | 1:163:A:TYR:HE2  | 16       | 0.83          |
| (1,2681) | 1:141:A:PHE:HZ   | 1:208:A:ARG:HB3  | 20       | 0.83          |
| (1,2650) | 1:139:A:ILE:HG12 | 1:141:A:PHE:HE1  | 9        | 0.83          |
| (1,2650) | 1:139:A:ILE:HG12 | 1:141:A:PHE:HE2  | 9        | 0.83          |
| (1,2615) | 1:141:A:PHE:HD1  | 1:147:A:ASP:HB3  | 19       | 0.83          |
| (1,2615) | 1:141:A:PHE:HD2  | 1:147:A:ASP:HB3  | 19       | 0.83          |
| (1,2414) | 1:136:A:ARG:HB3  | 1:159:A:ASN:HD21 | 14       | 0.83          |
| (1,1523) | 1:162:A:TYR:HB3  | 1:182:A:ILE:HG12 | 2        | 0.83          |
| (1,1523) | 1:162:A:TYR:HB3  | 1:182:A:ILE:HG13 | 2        | 0.83          |
| (1,1303) | 1:137:A:PRO:HB2  | 1:213:A:MET:HG2  | 9        | 0.83          |
| (1,1131) | 1:223:A:GLN:HG2  | 1:226:A:TYR:H    | 13       | 0.83          |
| (1,1095) | 1:165:A:PRO:HA   | 1:168:A:GLN:HG2  | 4        | 0.83          |
| (1,862)  | 1:143:A:ASN:HD22 | 1:146:A:GLU:HG2  | 17       | 0.83          |
| (1,637)  | 1:147:A:ASP:HB2  | 1:148:A:ARG:HG2  | 3        | 0.83          |
| (1,470)  | 1:122:A:VAL:HG21 | 1:125:A:LEU:HB2  | 16       | 0.83          |
| (1,470)  | 1:122:A:VAL:HG22 | 1:125:A:LEU:HB2  | 16       | 0.83          |
| (1,470)  | 1:122:A:VAL:HG23 | 1:125:A:LEU:HB2  | 16       | 0.83          |
| (1,323)  | 1:209:A:VAL:HG21 | 1:212:A:GLN:HB3  | 9        | 0.83          |
| (1,323)  | 1:209:A:VAL:HG22 | 1:212:A:GLN:HB3  | 9        | 0.83          |
| (1,323)  | 1:209:A:VAL:HG23 | 1:212:A:GLN:HB3  | 9        | 0.83          |
| (1,55)   | 1:125:A:LEU:HD11 | 1:162:A:TYR:HB2  | 1        | 0.83          |
| (1,55)   | 1:125:A:LEU:HD12 | 1:162:A:TYR:HB2  | 1        | 0.83          |
| (1,55)   | 1:125:A:LEU:HD13 | 1:162:A:TYR:HB2  | 1        | 0.83          |
| (1,2821) | 1:129:A:MET:HB3  | 1:163:A:TYR:HE1  | 15       | 0.82          |
| (1,2821) | 1:129:A:MET:HB3  | 1:163:A:TYR:HE2  | 15       | 0.82          |
| (1,2711) | 1:145:A:TRP:HZ3  | 1:146:A:GLU:HG3  | 11       | 0.82          |
| (1,2593) | 1:175:A:PHE:HE1  | 1:221:A:GLU:HG2  | 7        | 0.82          |
| (1,2593) | 1:175:A:PHE:HE2  | 1:221:A:GLU:HG2  | 7        | 0.82          |
| (1,2320) | 1:160:A:GLN:HE22 | 1:213:A:MET:HB2  | 18       | 0.82          |
| (1,1937) | 1:220:A:LYS:H    | 1:221:A:GLU:HG3  | 20       | 0.82          |
| (1,1089) | 1:182:A:ILE:HD11 | 1:186:A:GLN:HE21 | 18       | 0.82          |
| (1,1089) | 1:182:A:ILE:HD12 | 1:186:A:GLN:HE21 | 18       | 0.82          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1089) | 1:182:A:ILE:HD13 | 1:186:A:GLN:HE21 | 18       | 0.82          |
| (1,1089) | 1:182:A:ILE:HD11 | 1:186:A:GLN:HE21 | 20       | 0.82          |
| (1,1089) | 1:182:A:ILE:HD12 | 1:186:A:GLN:HE21 | 20       | 0.82          |
| (1,1089) | 1:182:A:ILE:HD13 | 1:186:A:GLN:HE21 | 20       | 0.82          |
| (1,931)  | 1:166:A:VAL:HG11 | 1:221:A:GLU:HG3  | 3        | 0.82          |
| (1,931)  | 1:166:A:VAL:HG12 | 1:221:A:GLU:HG3  | 3        | 0.82          |
| (1,931)  | 1:166:A:VAL:HG13 | 1:221:A:GLU:HG3  | 3        | 0.82          |
| (1,445)  | 1:180:A:VAL:HA   | 1:184:A:ILE:HG12 | 4        | 0.82          |
| (1,389)  | 1:121:A:VAL:HA   | 1:122:A:VAL:HG11 | 6        | 0.82          |
| (1,389)  | 1:121:A:VAL:HA   | 1:122:A:VAL:HG12 | 6        | 0.82          |
| (1,389)  | 1:121:A:VAL:HA   | 1:122:A:VAL:HG13 | 6        | 0.82          |
| (1,2847) | 1:157:A:TYR:HE1  | 1:209:A:VAL:HG11 | 19       | 0.81          |
| (1,2847) | 1:157:A:TYR:HE1  | 1:209:A:VAL:HG12 | 19       | 0.81          |
| (1,2847) | 1:157:A:TYR:HE1  | 1:209:A:VAL:HG13 | 19       | 0.81          |
| (1,2847) | 1:157:A:TYR:HE2  | 1:209:A:VAL:HG11 | 19       | 0.81          |
| (1,2847) | 1:157:A:TYR:HE2  | 1:209:A:VAL:HG12 | 19       | 0.81          |
| (1,2847) | 1:157:A:TYR:HE2  | 1:209:A:VAL:HG13 | 19       | 0.81          |
| (1,2758) | 1:150:A:TYR:HE1  | 1:209:A:VAL:HG11 | 11       | 0.81          |
| (1,2758) | 1:150:A:TYR:HE1  | 1:209:A:VAL:HG12 | 11       | 0.81          |
| (1,2758) | 1:150:A:TYR:HE1  | 1:209:A:VAL:HG13 | 11       | 0.81          |
| (1,2758) | 1:150:A:TYR:HE2  | 1:209:A:VAL:HG11 | 11       | 0.81          |
| (1,2758) | 1:150:A:TYR:HE2  | 1:209:A:VAL:HG12 | 11       | 0.81          |
| (1,2758) | 1:150:A:TYR:HE2  | 1:209:A:VAL:HG13 | 11       | 0.81          |
| (1,2650) | 1:139:A:ILE:HG12 | 1:141:A:PHE:HE1  | 5        | 0.81          |
| (1,2650) | 1:139:A:ILE:HG12 | 1:141:A:PHE:HE2  | 5        | 0.81          |
| (1,2615) | 1:141:A:PHE:HD1  | 1:147:A:ASP:HB3  | 20       | 0.81          |
| (1,2615) | 1:141:A:PHE:HD2  | 1:147:A:ASP:HB3  | 20       | 0.81          |
| (1,2177) | 1:212:A:GLN:H    | 1:213:A:MET:HG2  | 1        | 0.81          |
| (1,1914) | 1:209:A:VAL:HG21 | 1:213:A:MET:H    | 11       | 0.81          |
| (1,1914) | 1:209:A:VAL:HG22 | 1:213:A:MET:H    | 11       | 0.81          |
| (1,1914) | 1:209:A:VAL:HG23 | 1:213:A:MET:H    | 11       | 0.81          |
| (1,1407) | 1:134:A:MET:HB3  | 1:220:A:LYS:HD2  | 6        | 0.81          |
| (1,1407) | 1:134:A:MET:HB3  | 1:220:A:LYS:HD3  | 6        | 0.81          |
| (1,1164) | 1:215:A:VAL:HG21 | 1:219:A:GLN:HG2  | 2        | 0.81          |
| (1,1164) | 1:215:A:VAL:HG22 | 1:219:A:GLN:HG2  | 2        | 0.81          |
| (1,1164) | 1:215:A:VAL:HG23 | 1:219:A:GLN:HG2  | 2        | 0.81          |
| (1,993)  | 1:211:A:GLU:HG3  | 1:215:A:VAL:H    | 15       | 0.81          |
| (1,634)  | 1:192:A:THR:HA   | 1:195:A:GLY:HA3  | 10       | 0.81          |
| (1,634)  | 1:192:A:THR:HA   | 1:195:A:GLY:HA3  | 16       | 0.81          |
| (1,506)  | 1:179:A:CYS:HB2  | 1:214:A:CYS:HB2  | 14       | 0.81          |
| (1,357)  | 1:122:A:VAL:HG21 | 1:125:A:LEU:HG   | 2        | 0.81          |
| (1,357)  | 1:122:A:VAL:HG22 | 1:125:A:LEU:HG   | 2        | 0.81          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,357)  | 1:122:A:VAL:HG23 | 1:125:A:LEU:HG   | 2        | 0.81          |
| (1,339)  | 1:209:A:VAL:HG21 | 1:210:A:VAL:HG21 | 20       | 0.81          |
| (1,339)  | 1:209:A:VAL:HG21 | 1:210:A:VAL:HG22 | 20       | 0.81          |
| (1,339)  | 1:209:A:VAL:HG21 | 1:210:A:VAL:HG23 | 20       | 0.81          |
| (1,339)  | 1:209:A:VAL:HG22 | 1:210:A:VAL:HG21 | 20       | 0.81          |
| (1,339)  | 1:209:A:VAL:HG22 | 1:210:A:VAL:HG22 | 20       | 0.81          |
| (1,339)  | 1:209:A:VAL:HG22 | 1:210:A:VAL:HG23 | 20       | 0.81          |
| (1,339)  | 1:209:A:VAL:HG23 | 1:210:A:VAL:HG21 | 20       | 0.81          |
| (1,339)  | 1:209:A:VAL:HG23 | 1:210:A:VAL:HG22 | 20       | 0.81          |
| (1,339)  | 1:209:A:VAL:HG23 | 1:210:A:VAL:HG23 | 20       | 0.81          |
| (1,330)  | 1:188:A:THR:HA   | 1:189:A:VAL:HG21 | 11       | 0.81          |
| (1,330)  | 1:188:A:THR:HA   | 1:189:A:VAL:HG22 | 11       | 0.81          |
| (1,330)  | 1:188:A:THR:HA   | 1:189:A:VAL:HG23 | 11       | 0.81          |
| (1,159)  | 1:228:A:GLY:HA2  | 1:230:A:ARG:HD2  | 12       | 0.81          |
| (1,159)  | 1:228:A:GLY:HA3  | 1:230:A:ARG:HD2  | 12       | 0.81          |
| (1,2834) | 1:163:A:TYR:HE1  | 1:221:A:GLU:HG2  | 13       | 0.8           |
| (1,2834) | 1:163:A:TYR:HE2  | 1:221:A:GLU:HG2  | 13       | 0.8           |
| (1,2792) | 1:128:A:TYR:HE1  | 1:164:A:ARG:HD3  | 18       | 0.8           |
| (1,2792) | 1:128:A:TYR:HE2  | 1:164:A:ARG:HD3  | 18       | 0.8           |
| (1,2759) | 1:139:A:ILE:HG12 | 1:150:A:TYR:HE1  | 2        | 0.8           |
| (1,2759) | 1:139:A:ILE:HG12 | 1:150:A:TYR:HE2  | 2        | 0.8           |
| (1,2699) | 1:141:A:PHE:HZ   | 1:150:A:TYR:HB3  | 15       | 0.8           |
| (1,2650) | 1:139:A:ILE:HG12 | 1:141:A:PHE:HE1  | 12       | 0.8           |
| (1,2650) | 1:139:A:ILE:HG12 | 1:141:A:PHE:HE2  | 12       | 0.8           |
| (1,2482) | 1:163:A:TYR:HD1  | 1:221:A:GLU:HG2  | 17       | 0.8           |
| (1,2482) | 1:163:A:TYR:HD2  | 1:221:A:GLU:HG2  | 17       | 0.8           |
| (1,1937) | 1:220:A:LYS:H    | 1:221:A:GLU:HG3  | 11       | 0.8           |
| (1,1914) | 1:209:A:VAL:HG21 | 1:213:A:MET:H    | 17       | 0.8           |
| (1,1914) | 1:209:A:VAL:HG22 | 1:213:A:MET:H    | 17       | 0.8           |
| (1,1914) | 1:209:A:VAL:HG23 | 1:213:A:MET:H    | 17       | 0.8           |
| (1,1207) | 1:168:A:GLN:HA   | 1:168:A:GLN:HE22 | 4        | 0.8           |
| (1,704)  | 1:209:A:VAL:HG21 | 1:213:A:MET:HE1  | 12       | 0.8           |
| (1,704)  | 1:209:A:VAL:HG21 | 1:213:A:MET:HE2  | 12       | 0.8           |
| (1,704)  | 1:209:A:VAL:HG21 | 1:213:A:MET:HE3  | 12       | 0.8           |
| (1,704)  | 1:209:A:VAL:HG22 | 1:213:A:MET:HE1  | 12       | 0.8           |
| (1,704)  | 1:209:A:VAL:HG22 | 1:213:A:MET:HE2  | 12       | 0.8           |
| (1,704)  | 1:209:A:VAL:HG22 | 1:213:A:MET:HE3  | 12       | 0.8           |
| (1,704)  | 1:209:A:VAL:HG23 | 1:213:A:MET:HE1  | 12       | 0.8           |
| (1,704)  | 1:209:A:VAL:HG23 | 1:213:A:MET:HE2  | 12       | 0.8           |
| (1,704)  | 1:209:A:VAL:HG23 | 1:213:A:MET:HE3  | 12       | 0.8           |
| (1,502)  | 1:162:A:TYR:HB3  | 1:183:A:THR:HA   | 14       | 0.8           |
| (1,260)  | 1:186:A:GLN:HB2  | 1:190:A:THR:HG21 | 18       | 0.8           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,260)  | 1:186:A:GLN:HB2  | 1:190:A:THR:HG22 | 18       | 0.8           |
| (1,260)  | 1:186:A:GLN:HB2  | 1:190:A:THR:HG23 | 18       | 0.8           |
| (1,2774) | 1:128:A:TYR:HE1  | 1:162:A:TYR:HB3  | 6        | 0.79          |
| (1,2774) | 1:128:A:TYR:HE2  | 1:162:A:TYR:HB3  | 6        | 0.79          |
| (1,2711) | 1:145:A:TRP:HZ3  | 1:146:A:GLU:HG3  | 6        | 0.79          |
| (1,2699) | 1:141:A:PHE:HZ   | 1:150:A:TYR:HB3  | 2        | 0.79          |
| (1,2681) | 1:141:A:PHE:HZ   | 1:208:A:ARG:HB3  | 1        | 0.79          |
| (1,2548) | 1:162:A:TYR:HD1  | 1:186:A:GLN:HB3  | 10       | 0.79          |
| (1,2548) | 1:162:A:TYR:HD2  | 1:186:A:GLN:HB3  | 10       | 0.79          |
| (1,2320) | 1:160:A:GLN:HE22 | 1:213:A:MET:HB2  | 2        | 0.79          |
| (1,2313) | 1:159:A:ASN:HD22 | 1:160:A:GLN:HE21 | 19       | 0.79          |
| (1,1937) | 1:220:A:LYS:H    | 1:221:A:GLU:HG3  | 18       | 0.79          |
| (1,1104) | 1:213:A:MET:HB3  | 1:214:A:CYS:HA   | 9        | 0.79          |
| (1,1089) | 1:182:A:ILE:HD11 | 1:186:A:GLN:HE21 | 16       | 0.79          |
| (1,1089) | 1:182:A:ILE:HD12 | 1:186:A:GLN:HE21 | 16       | 0.79          |
| (1,1089) | 1:182:A:ILE:HD13 | 1:186:A:GLN:HE21 | 16       | 0.79          |
| (1,893)  | 1:162:A:TYR:HB3  | 1:182:A:ILE:HB   | 12       | 0.79          |
| (1,569)  | 1:128:A:TYR:HE1  | 1:179:A:CYS:HB3  | 18       | 0.79          |
| (1,569)  | 1:128:A:TYR:HE2  | 1:179:A:CYS:HB3  | 18       | 0.79          |
| (1,502)  | 1:162:A:TYR:HB3  | 1:183:A:THR:HA   | 11       | 0.79          |
| (1,470)  | 1:122:A:VAL:HG21 | 1:125:A:LEU:HB2  | 9        | 0.79          |
| (1,470)  | 1:122:A:VAL:HG22 | 1:125:A:LEU:HB2  | 9        | 0.79          |
| (1,470)  | 1:122:A:VAL:HG23 | 1:125:A:LEU:HB2  | 9        | 0.79          |
| (1,467)  | 1:122:A:VAL:HG21 | 1:125:A:LEU:HB3  | 19       | 0.79          |
| (1,467)  | 1:122:A:VAL:HG22 | 1:125:A:LEU:HB3  | 19       | 0.79          |
| (1,467)  | 1:122:A:VAL:HG23 | 1:125:A:LEU:HB3  | 19       | 0.79          |
| (1,445)  | 1:180:A:VAL:HA   | 1:184:A:ILE:HG12 | 7        | 0.79          |
| (1,430)  | 1:122:A:VAL:HG11 | 1:186:A:GLN:HG3  | 9        | 0.79          |
| (1,430)  | 1:122:A:VAL:HG12 | 1:186:A:GLN:HG3  | 9        | 0.79          |
| (1,430)  | 1:122:A:VAL:HG13 | 1:186:A:GLN:HG3  | 9        | 0.79          |
| (1,429)  | 1:122:A:VAL:HG11 | 1:186:A:GLN:HA   | 1        | 0.79          |
| (1,429)  | 1:122:A:VAL:HG12 | 1:186:A:GLN:HA   | 1        | 0.79          |
| (1,429)  | 1:122:A:VAL:HG13 | 1:186:A:GLN:HA   | 1        | 0.79          |
| (1,323)  | 1:209:A:VAL:HG21 | 1:212:A:GLN:HB3  | 8        | 0.79          |
| (1,323)  | 1:209:A:VAL:HG22 | 1:212:A:GLN:HB3  | 8        | 0.79          |
| (1,323)  | 1:209:A:VAL:HG23 | 1:212:A:GLN:HB3  | 8        | 0.79          |
| (1,105)  | 1:212:A:GLN:HA   | 1:215:A:VAL:HG11 | 19       | 0.79          |
| (1,105)  | 1:212:A:GLN:HA   | 1:215:A:VAL:HG12 | 19       | 0.79          |
| (1,105)  | 1:212:A:GLN:HA   | 1:215:A:VAL:HG13 | 19       | 0.79          |
| (1,101)  | 1:138:A:MET:HA   | 1:209:A:VAL:HG11 | 8        | 0.79          |
| (1,101)  | 1:138:A:MET:HA   | 1:209:A:VAL:HG12 | 8        | 0.79          |
| (1,101)  | 1:138:A:MET:HA   | 1:209:A:VAL:HG13 | 8        | 0.79          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2774) | 1:128:A:TYR:HE1  | 1:162:A:TYR:HB3  | 8        | 0.78          |
| (1,2774) | 1:128:A:TYR:HE2  | 1:162:A:TYR:HB3  | 8        | 0.78          |
| (1,2758) | 1:150:A:TYR:HE1  | 1:209:A:VAL:HG11 | 1        | 0.78          |
| (1,2758) | 1:150:A:TYR:HE1  | 1:209:A:VAL:HG12 | 1        | 0.78          |
| (1,2758) | 1:150:A:TYR:HE1  | 1:209:A:VAL:HG13 | 1        | 0.78          |
| (1,2758) | 1:150:A:TYR:HE2  | 1:209:A:VAL:HG11 | 1        | 0.78          |
| (1,2758) | 1:150:A:TYR:HE2  | 1:209:A:VAL:HG12 | 1        | 0.78          |
| (1,2758) | 1:150:A:TYR:HE2  | 1:209:A:VAL:HG13 | 1        | 0.78          |
| (1,2756) | 1:150:A:TYR:HE1  | 1:205:A:MET:HG2  | 20       | 0.78          |
| (1,2756) | 1:150:A:TYR:HE2  | 1:205:A:MET:HG2  | 20       | 0.78          |
| (1,2488) | 1:149:A:TYR:HD1  | 1:153:A:ASN:HB3  | 11       | 0.78          |
| (1,2488) | 1:149:A:TYR:HD2  | 1:153:A:ASN:HB3  | 11       | 0.78          |
| (1,2469) | 1:166:A:VAL:HG21 | 1:169:A:TYR:HD1  | 1        | 0.78          |
| (1,2469) | 1:166:A:VAL:HG21 | 1:169:A:TYR:HD2  | 1        | 0.78          |
| (1,2469) | 1:166:A:VAL:HG22 | 1:169:A:TYR:HD1  | 1        | 0.78          |
| (1,2469) | 1:166:A:VAL:HG22 | 1:169:A:TYR:HD2  | 1        | 0.78          |
| (1,2469) | 1:166:A:VAL:HG23 | 1:169:A:TYR:HD1  | 1        | 0.78          |
| (1,2469) | 1:166:A:VAL:HG23 | 1:169:A:TYR:HD2  | 1        | 0.78          |
| (1,2354) | 1:170:A:SER:HB2  | 1:174:A:ASN:HD21 | 13       | 0.78          |
| (1,2045) | 1:230:A:ARG:HG3  | 1:231:A:SER:H    | 10       | 0.78          |
| (1,1497) | 1:139:A:ILE:HD11 | 1:212:A:GLN:HB3  | 5        | 0.78          |
| (1,1497) | 1:139:A:ILE:HD12 | 1:212:A:GLN:HB3  | 5        | 0.78          |
| (1,1497) | 1:139:A:ILE:HD13 | 1:212:A:GLN:HB3  | 5        | 0.78          |
| (1,1104) | 1:213:A:MET:HB3  | 1:214:A:CYS:HA   | 14       | 0.78          |
| (1,1097) | 1:165:A:PRO:HB3  | 1:168:A:GLN:HG2  | 8        | 0.78          |
| (1,637)  | 1:147:A:ASP:HB2  | 1:148:A:ARG:HG2  | 4        | 0.78          |
| (1,423)  | 1:151:A:ARG:HD3  | 1:152:A:GLU:H    | 7        | 0.78          |
| (1,155)  | 1:125:A:LEU:HB3  | 1:126:A:GLY:HA3  | 2        | 0.78          |
| (1,107)  | 1:211:A:GLU:HG3  | 1:215:A:VAL:HG11 | 5        | 0.78          |
| (1,107)  | 1:211:A:GLU:HG3  | 1:215:A:VAL:HG12 | 5        | 0.78          |
| (1,107)  | 1:211:A:GLU:HG3  | 1:215:A:VAL:HG13 | 5        | 0.78          |
| (1,79)   | 1:138:A:MET:H    | 1:209:A:VAL:HG11 | 18       | 0.78          |
| (1,79)   | 1:138:A:MET:H    | 1:209:A:VAL:HG12 | 18       | 0.78          |
| (1,79)   | 1:138:A:MET:H    | 1:209:A:VAL:HG13 | 18       | 0.78          |
| (1,2851) | 1:184:A:ILE:HG13 | 1:187:A:HIS:HE1  | 4        | 0.77          |
| (1,2846) | 1:157:A:TYR:HE1  | 1:206:A:MET:HB2  | 4        | 0.77          |
| (1,2846) | 1:157:A:TYR:HE2  | 1:206:A:MET:HB2  | 4        | 0.77          |
| (1,2721) | 1:177:A:HIS:HD2  | 1:178:A:ASP:HB3  | 15       | 0.77          |
| (1,2650) | 1:139:A:ILE:HG12 | 1:141:A:PHE:HE1  | 15       | 0.77          |
| (1,2650) | 1:139:A:ILE:HG12 | 1:141:A:PHE:HE2  | 15       | 0.77          |
| (1,2579) | 1:218:A:TYR:HD1  | 1:219:A:GLN:HG3  | 19       | 0.77          |
| (1,2579) | 1:218:A:TYR:HD2  | 1:219:A:GLN:HG3  | 19       | 0.77          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2492) | 1:139:A:ILE:HG12 | 1:150:A:TYR:HD1  | 7        | 0.77          |
| (1,2492) | 1:139:A:ILE:HG12 | 1:150:A:TYR:HD2  | 7        | 0.77          |
| (1,2492) | 1:139:A:ILE:HG12 | 1:150:A:TYR:HD1  | 19       | 0.77          |
| (1,2492) | 1:139:A:ILE:HG12 | 1:150:A:TYR:HD2  | 19       | 0.77          |
| (1,2356) | 1:169:A:TYR:HB2  | 1:174:A:ASN:HD21 | 3        | 0.77          |
| (1,1523) | 1:162:A:TYR:HB3  | 1:182:A:ILE:HG12 | 18       | 0.77          |
| (1,1523) | 1:162:A:TYR:HB3  | 1:182:A:ILE:HG13 | 18       | 0.77          |
| (1,1497) | 1:139:A:ILE:HD11 | 1:212:A:GLN:HB3  | 4        | 0.77          |
| (1,1497) | 1:139:A:ILE:HD12 | 1:212:A:GLN:HB3  | 4        | 0.77          |
| (1,1497) | 1:139:A:ILE:HD13 | 1:212:A:GLN:HB3  | 4        | 0.77          |
| (1,1459) | 1:136:A:ARG:HB3  | 1:159:A:ASN:HB3  | 9        | 0.77          |
| (1,1344) | 1:206:A:MET:HB3  | 1:210:A:VAL:HB   | 5        | 0.77          |
| (1,1207) | 1:168:A:GLN:HA   | 1:168:A:GLN:HE22 | 18       | 0.77          |
| (1,1104) | 1:213:A:MET:HB3  | 1:214:A:CYS:HA   | 11       | 0.77          |
| (1,739)  | 1:166:A:VAL:HG11 | 1:222:A:SER:HB3  | 17       | 0.77          |
| (1,739)  | 1:166:A:VAL:HG12 | 1:222:A:SER:HB3  | 17       | 0.77          |
| (1,739)  | 1:166:A:VAL:HG13 | 1:222:A:SER:HB3  | 17       | 0.77          |
| (1,637)  | 1:147:A:ASP:HB2  | 1:148:A:ARG:HG2  | 14       | 0.77          |
| (1,322)  | 1:158:A:PRO:HD3  | 1:209:A:VAL:HG21 | 4        | 0.77          |
| (1,322)  | 1:158:A:PRO:HD3  | 1:209:A:VAL:HG22 | 4        | 0.77          |
| (1,322)  | 1:158:A:PRO:HD3  | 1:209:A:VAL:HG23 | 4        | 0.77          |
| (1,260)  | 1:186:A:GLN:HB2  | 1:190:A:THR:HG21 | 16       | 0.77          |
| (1,260)  | 1:186:A:GLN:HB2  | 1:190:A:THR:HG22 | 16       | 0.77          |
| (1,260)  | 1:186:A:GLN:HB2  | 1:190:A:THR:HG23 | 16       | 0.77          |
| (1,155)  | 1:125:A:LEU:HB3  | 1:126:A:GLY:HA3  | 9        | 0.77          |
| (1,98)   | 1:139:A:ILE:HG21 | 1:209:A:VAL:HG11 | 2        | 0.77          |
| (1,98)   | 1:139:A:ILE:HG21 | 1:209:A:VAL:HG12 | 2        | 0.77          |
| (1,98)   | 1:139:A:ILE:HG21 | 1:209:A:VAL:HG13 | 2        | 0.77          |
| (1,98)   | 1:139:A:ILE:HG22 | 1:209:A:VAL:HG11 | 2        | 0.77          |
| (1,98)   | 1:139:A:ILE:HG22 | 1:209:A:VAL:HG12 | 2        | 0.77          |
| (1,98)   | 1:139:A:ILE:HG22 | 1:209:A:VAL:HG13 | 2        | 0.77          |
| (1,98)   | 1:139:A:ILE:HG23 | 1:209:A:VAL:HG11 | 2        | 0.77          |
| (1,98)   | 1:139:A:ILE:HG23 | 1:209:A:VAL:HG12 | 2        | 0.77          |
| (1,98)   | 1:139:A:ILE:HG23 | 1:209:A:VAL:HG13 | 2        | 0.77          |
| (1,58)   | 1:122:A:VAL:HG21 | 1:125:A:LEU:HD11 | 1        | 0.77          |
| (1,58)   | 1:122:A:VAL:HG21 | 1:125:A:LEU:HD12 | 1        | 0.77          |
| (1,58)   | 1:122:A:VAL:HG21 | 1:125:A:LEU:HD13 | 1        | 0.77          |
| (1,58)   | 1:122:A:VAL:HG22 | 1:125:A:LEU:HD11 | 1        | 0.77          |
| (1,58)   | 1:122:A:VAL:HG22 | 1:125:A:LEU:HD12 | 1        | 0.77          |
| (1,58)   | 1:122:A:VAL:HG22 | 1:125:A:LEU:HD13 | 1        | 0.77          |
| (1,58)   | 1:122:A:VAL:HG23 | 1:125:A:LEU:HD11 | 1        | 0.77          |
| (1,58)   | 1:122:A:VAL:HG23 | 1:125:A:LEU:HD12 | 1        | 0.77          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,58)   | 1:122:A:VAL:HG23 | 1:125:A:LEU:HD13 | 1        | 0.77          |
| (1,2846) | 1:157:A:TYR:HE1  | 1:206:A:MET:HB2  | 5        | 0.76          |
| (1,2846) | 1:157:A:TYR:HE2  | 1:206:A:MET:HB2  | 5        | 0.76          |
| (1,2771) | 1:130:A:LEU:HB3  | 1:162:A:TYR:HE1  | 14       | 0.76          |
| (1,2771) | 1:130:A:LEU:HB3  | 1:162:A:TYR:HE2  | 14       | 0.76          |
| (1,2681) | 1:141:A:PHE:HZ   | 1:208:A:ARG:HB3  | 16       | 0.76          |
| (1,2593) | 1:175:A:PHE:HE1  | 1:221:A:GLU:HG2  | 6        | 0.76          |
| (1,2593) | 1:175:A:PHE:HE2  | 1:221:A:GLU:HG2  | 6        | 0.76          |
| (1,2250) | 1:217:A:GLN:HE21 | 1:218:A:TYR:HA   | 15       | 0.76          |
| (1,1638) | 1:161:A:VAL:HG21 | 1:217:A:GLN:H    | 10       | 0.76          |
| (1,1638) | 1:161:A:VAL:HG22 | 1:217:A:GLN:H    | 10       | 0.76          |
| (1,1638) | 1:161:A:VAL:HG23 | 1:217:A:GLN:H    | 10       | 0.76          |
| (1,1285) | 1:205:A:MET:H    | 1:206:A:MET:HG2  | 2        | 0.76          |
| (1,1283) | 1:206:A:MET:HG2  | 1:207:A:GLU:HG3  | 6        | 0.76          |
| (1,1081) | 1:164:A:ARG:HD2  | 1:168:A:GLN:HG2  | 7        | 0.76          |
| (1,974)  | 1:148:A:ARG:HE   | 1:152:A:GLU:HG2  | 9        | 0.76          |
| (1,893)  | 1:162:A:TYR:HB3  | 1:182:A:ILE:HB   | 6        | 0.76          |
| (1,637)  | 1:147:A:ASP:HB2  | 1:148:A:ARG:HG2  | 16       | 0.76          |
| (1,391)  | 1:122:A:VAL:HG21 | 1:125:A:LEU:HD21 | 15       | 0.76          |
| (1,391)  | 1:122:A:VAL:HG21 | 1:125:A:LEU:HD22 | 15       | 0.76          |
| (1,391)  | 1:122:A:VAL:HG21 | 1:125:A:LEU:HD23 | 15       | 0.76          |
| (1,391)  | 1:122:A:VAL:HG22 | 1:125:A:LEU:HD21 | 15       | 0.76          |
| (1,391)  | 1:122:A:VAL:HG22 | 1:125:A:LEU:HD22 | 15       | 0.76          |
| (1,391)  | 1:122:A:VAL:HG22 | 1:125:A:LEU:HD23 | 15       | 0.76          |
| (1,391)  | 1:122:A:VAL:HG23 | 1:125:A:LEU:HD21 | 15       | 0.76          |
| (1,391)  | 1:122:A:VAL:HG23 | 1:125:A:LEU:HD22 | 15       | 0.76          |
| (1,391)  | 1:122:A:VAL:HG23 | 1:125:A:LEU:HD23 | 15       | 0.76          |
| (1,322)  | 1:158:A:PRO:HD3  | 1:209:A:VAL:HG21 | 11       | 0.76          |
| (1,322)  | 1:158:A:PRO:HD3  | 1:209:A:VAL:HG22 | 11       | 0.76          |
| (1,322)  | 1:158:A:PRO:HD3  | 1:209:A:VAL:HG23 | 11       | 0.76          |
| (1,322)  | 1:158:A:PRO:HD3  | 1:209:A:VAL:HG21 | 13       | 0.76          |
| (1,322)  | 1:158:A:PRO:HD3  | 1:209:A:VAL:HG22 | 13       | 0.76          |
| (1,322)  | 1:158:A:PRO:HD3  | 1:209:A:VAL:HG23 | 13       | 0.76          |
| (1,2774) | 1:128:A:TYR:HE1  | 1:162:A:TYR:HB3  | 2        | 0.75          |
| (1,2774) | 1:128:A:TYR:HE2  | 1:162:A:TYR:HB3  | 2        | 0.75          |
| (1,2562) | 1:125:A:LEU:HD21 | 1:128:A:TYR:HD1  | 11       | 0.75          |
| (1,2562) | 1:125:A:LEU:HD21 | 1:128:A:TYR:HD2  | 11       | 0.75          |
| (1,2562) | 1:125:A:LEU:HD22 | 1:128:A:TYR:HD1  | 11       | 0.75          |
| (1,2562) | 1:125:A:LEU:HD22 | 1:128:A:TYR:HD2  | 11       | 0.75          |
| (1,2562) | 1:125:A:LEU:HD23 | 1:128:A:TYR:HD1  | 11       | 0.75          |
| (1,2562) | 1:125:A:LEU:HD23 | 1:128:A:TYR:HD2  | 11       | 0.75          |
| (1,2421) | 1:127:A:GLY:H    | 1:164:A:ARG:HD3  | 17       | 0.75          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2320) | 1:160:A:GLN:HE22 | 1:213:A:MET:HB2  | 15       | 0.75          |
| (1,1914) | 1:209:A:VAL:HG21 | 1:213:A:MET:H    | 10       | 0.75          |
| (1,1914) | 1:209:A:VAL:HG22 | 1:213:A:MET:H    | 10       | 0.75          |
| (1,1914) | 1:209:A:VAL:HG23 | 1:213:A:MET:H    | 10       | 0.75          |
| (1,1459) | 1:136:A:ARG:HB3  | 1:159:A:ASN:HB3  | 7        | 0.75          |
| (1,1303) | 1:137:A:PRO:HB2  | 1:213:A:MET:HG2  | 11       | 0.75          |
| (1,1283) | 1:206:A:MET:HG2  | 1:207:A:GLU:HG3  | 3        | 0.75          |
| (1,1256) | 1:184:A:ILE:HG13 | 1:206:A:MET:HG3  | 15       | 0.75          |
| (1,1164) | 1:215:A:VAL:HG21 | 1:219:A:GLN:HG2  | 6        | 0.75          |
| (1,1164) | 1:215:A:VAL:HG22 | 1:219:A:GLN:HG2  | 6        | 0.75          |
| (1,1164) | 1:215:A:VAL:HG23 | 1:219:A:GLN:HG2  | 6        | 0.75          |
| (1,1085) | 1:129:A:MET:HB2  | 1:164:A:ARG:HA   | 3        | 0.75          |
| (1,1085) | 1:129:A:MET:HB2  | 1:164:A:ARG:HA   | 16       | 0.75          |
| (1,1015) | 1:152:A:GLU:HG2  | 1:153:A:ASN:HD22 | 2        | 0.75          |
| (1,704)  | 1:209:A:VAL:HG21 | 1:213:A:MET:HE1  | 1        | 0.75          |
| (1,704)  | 1:209:A:VAL:HG21 | 1:213:A:MET:HE2  | 1        | 0.75          |
| (1,704)  | 1:209:A:VAL:HG21 | 1:213:A:MET:HE3  | 1        | 0.75          |
| (1,704)  | 1:209:A:VAL:HG22 | 1:213:A:MET:HE1  | 1        | 0.75          |
| (1,704)  | 1:209:A:VAL:HG22 | 1:213:A:MET:HE2  | 1        | 0.75          |
| (1,704)  | 1:209:A:VAL:HG22 | 1:213:A:MET:HE3  | 1        | 0.75          |
| (1,704)  | 1:209:A:VAL:HG23 | 1:213:A:MET:HE1  | 1        | 0.75          |
| (1,704)  | 1:209:A:VAL:HG23 | 1:213:A:MET:HE2  | 1        | 0.75          |
| (1,704)  | 1:209:A:VAL:HG23 | 1:213:A:MET:HE3  | 1        | 0.75          |
| (1,637)  | 1:147:A:ASP:HB2  | 1:148:A:ARG:HG2  | 1        | 0.75          |
| (1,637)  | 1:147:A:ASP:HB2  | 1:148:A:ARG:HG2  | 10       | 0.75          |
| (1,428)  | 1:127:A:GLY:HA2  | 1:164:A:ARG:HD3  | 14       | 0.75          |
| (1,272)  | 1:166:A:VAL:HG11 | 1:221:A:GLU:HB3  | 12       | 0.75          |
| (1,272)  | 1:166:A:VAL:HG12 | 1:221:A:GLU:HB3  | 12       | 0.75          |
| (1,272)  | 1:166:A:VAL:HG13 | 1:221:A:GLU:HB3  | 12       | 0.75          |
| (1,189)  | 1:123:A:GLY:HA2  | 1:125:A:LEU:HD21 | 15       | 0.75          |
| (1,189)  | 1:123:A:GLY:HA2  | 1:125:A:LEU:HD22 | 15       | 0.75          |
| (1,189)  | 1:123:A:GLY:HA2  | 1:125:A:LEU:HD23 | 15       | 0.75          |
| (1,189)  | 1:123:A:GLY:HA3  | 1:125:A:LEU:HD21 | 15       | 0.75          |
| (1,189)  | 1:123:A:GLY:HA3  | 1:125:A:LEU:HD22 | 15       | 0.75          |
| (1,189)  | 1:123:A:GLY:HA3  | 1:125:A:LEU:HD23 | 15       | 0.75          |
| (1,105)  | 1:212:A:GLN:HA   | 1:215:A:VAL:HG11 | 12       | 0.75          |
| (1,105)  | 1:212:A:GLN:HA   | 1:215:A:VAL:HG12 | 12       | 0.75          |
| (1,105)  | 1:212:A:GLN:HA   | 1:215:A:VAL:HG13 | 12       | 0.75          |
| (1,98)   | 1:139:A:ILE:HG21 | 1:209:A:VAL:HG11 | 16       | 0.75          |
| (1,98)   | 1:139:A:ILE:HG21 | 1:209:A:VAL:HG12 | 16       | 0.75          |
| (1,98)   | 1:139:A:ILE:HG21 | 1:209:A:VAL:HG13 | 16       | 0.75          |
| (1,98)   | 1:139:A:ILE:HG22 | 1:209:A:VAL:HG11 | 16       | 0.75          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,98)   | 1:139:A:ILE:HG22 | 1:209:A:VAL:HG12 | 16       | 0.75          |
| (1,98)   | 1:139:A:ILE:HG22 | 1:209:A:VAL:HG13 | 16       | 0.75          |
| (1,98)   | 1:139:A:ILE:HG23 | 1:209:A:VAL:HG11 | 16       | 0.75          |
| (1,98)   | 1:139:A:ILE:HG23 | 1:209:A:VAL:HG12 | 16       | 0.75          |
| (1,98)   | 1:139:A:ILE:HG23 | 1:209:A:VAL:HG13 | 16       | 0.75          |
| (1,80)   | 1:208:A:ARG:HA   | 1:209:A:VAL:HG11 | 18       | 0.75          |
| (1,80)   | 1:208:A:ARG:HA   | 1:209:A:VAL:HG12 | 18       | 0.75          |
| (1,80)   | 1:208:A:ARG:HA   | 1:209:A:VAL:HG13 | 18       | 0.75          |
| (1,2847) | 1:157:A:TYR:HE1  | 1:209:A:VAL:HG11 | 18       | 0.74          |
| (1,2847) | 1:157:A:TYR:HE1  | 1:209:A:VAL:HG12 | 18       | 0.74          |
| (1,2847) | 1:157:A:TYR:HE1  | 1:209:A:VAL:HG13 | 18       | 0.74          |
| (1,2847) | 1:157:A:TYR:HE2  | 1:209:A:VAL:HG11 | 18       | 0.74          |
| (1,2847) | 1:157:A:TYR:HE2  | 1:209:A:VAL:HG12 | 18       | 0.74          |
| (1,2847) | 1:157:A:TYR:HE2  | 1:209:A:VAL:HG13 | 18       | 0.74          |
| (1,2771) | 1:130:A:LEU:HB3  | 1:162:A:TYR:HE1  | 1        | 0.74          |
| (1,2771) | 1:130:A:LEU:HB3  | 1:162:A:TYR:HE2  | 1        | 0.74          |
| (1,2756) | 1:150:A:TYR:HE1  | 1:205:A:MET:HG2  | 12       | 0.74          |
| (1,2756) | 1:150:A:TYR:HE2  | 1:205:A:MET:HG2  | 12       | 0.74          |
| (1,2735) | 1:186:A:GLN:HB3  | 1:187:A:HIS:HD2  | 15       | 0.74          |
| (1,2650) | 1:139:A:ILE:HG12 | 1:141:A:PHE:HE1  | 10       | 0.74          |
| (1,2650) | 1:139:A:ILE:HG12 | 1:141:A:PHE:HE2  | 10       | 0.74          |
| (1,2615) | 1:141:A:PHE:HD1  | 1:147:A:ASP:HB3  | 7        | 0.74          |
| (1,2615) | 1:141:A:PHE:HD2  | 1:147:A:ASP:HB3  | 7        | 0.74          |
| (1,2615) | 1:141:A:PHE:HD1  | 1:147:A:ASP:HB3  | 10       | 0.74          |
| (1,2615) | 1:141:A:PHE:HD2  | 1:147:A:ASP:HB3  | 10       | 0.74          |
| (1,2482) | 1:163:A:TYR:HD1  | 1:221:A:GLU:HG2  | 18       | 0.74          |
| (1,2482) | 1:163:A:TYR:HD2  | 1:221:A:GLU:HG2  | 18       | 0.74          |
| (1,1303) | 1:137:A:PRO:HB2  | 1:213:A:MET:HG2  | 19       | 0.74          |
| (1,1256) | 1:184:A:ILE:HG13 | 1:206:A:MET:HG3  | 18       | 0.74          |
| (1,634)  | 1:192:A:THR:HA   | 1:195:A:GLY:HA3  | 3        | 0.74          |
| (1,502)  | 1:162:A:TYR:HB3  | 1:183:A:THR:HA   | 17       | 0.74          |
| (1,476)  | 1:203:A:VAL:HG21 | 1:204:A:LYS:HE2  | 18       | 0.74          |
| (1,476)  | 1:203:A:VAL:HG21 | 1:204:A:LYS:HE3  | 18       | 0.74          |
| (1,476)  | 1:203:A:VAL:HG22 | 1:204:A:LYS:HE2  | 18       | 0.74          |
| (1,476)  | 1:203:A:VAL:HG22 | 1:204:A:LYS:HE3  | 18       | 0.74          |
| (1,476)  | 1:203:A:VAL:HG23 | 1:204:A:LYS:HE2  | 18       | 0.74          |
| (1,476)  | 1:203:A:VAL:HG23 | 1:204:A:LYS:HE3  | 18       | 0.74          |
| (1,396)  | 1:210:A:VAL:HA   | 1:213:A:MET:HB3  | 7        | 0.74          |
| (1,339)  | 1:209:A:VAL:HG21 | 1:210:A:VAL:HG21 | 4        | 0.74          |
| (1,339)  | 1:209:A:VAL:HG21 | 1:210:A:VAL:HG22 | 4        | 0.74          |
| (1,339)  | 1:209:A:VAL:HG21 | 1:210:A:VAL:HG23 | 4        | 0.74          |
| (1,339)  | 1:209:A:VAL:HG22 | 1:210:A:VAL:HG21 | 4        | 0.74          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,339)  | 1:209:A:VAL:HG22 | 1:210:A:VAL:HG22 | 4        | 0.74          |
| (1,339)  | 1:209:A:VAL:HG22 | 1:210:A:VAL:HG23 | 4        | 0.74          |
| (1,339)  | 1:209:A:VAL:HG23 | 1:210:A:VAL:HG21 | 4        | 0.74          |
| (1,339)  | 1:209:A:VAL:HG23 | 1:210:A:VAL:HG22 | 4        | 0.74          |
| (1,339)  | 1:209:A:VAL:HG23 | 1:210:A:VAL:HG23 | 4        | 0.74          |
| (1,339)  | 1:209:A:VAL:HG21 | 1:210:A:VAL:HG21 | 7        | 0.74          |
| (1,339)  | 1:209:A:VAL:HG21 | 1:210:A:VAL:HG22 | 7        | 0.74          |
| (1,339)  | 1:209:A:VAL:HG21 | 1:210:A:VAL:HG23 | 7        | 0.74          |
| (1,339)  | 1:209:A:VAL:HG22 | 1:210:A:VAL:HG21 | 7        | 0.74          |
| (1,339)  | 1:209:A:VAL:HG22 | 1:210:A:VAL:HG22 | 7        | 0.74          |
| (1,339)  | 1:209:A:VAL:HG22 | 1:210:A:VAL:HG23 | 7        | 0.74          |
| (1,339)  | 1:209:A:VAL:HG23 | 1:210:A:VAL:HG21 | 7        | 0.74          |
| (1,339)  | 1:209:A:VAL:HG23 | 1:210:A:VAL:HG22 | 7        | 0.74          |
| (1,339)  | 1:209:A:VAL:HG23 | 1:210:A:VAL:HG23 | 7        | 0.74          |
| (1,323)  | 1:209:A:VAL:HG21 | 1:212:A:GLN:HB3  | 1        | 0.74          |
| (1,323)  | 1:209:A:VAL:HG22 | 1:212:A:GLN:HB3  | 1        | 0.74          |
| (1,323)  | 1:209:A:VAL:HG23 | 1:212:A:GLN:HB3  | 1        | 0.74          |
| (1,155)  | 1:125:A:LEU:HB3  | 1:126:A:GLY:HA3  | 15       | 0.74          |
| (1,101)  | 1:138:A:MET:HA   | 1:209:A:VAL:HG11 | 11       | 0.74          |
| (1,101)  | 1:138:A:MET:HA   | 1:209:A:VAL:HG12 | 11       | 0.74          |
| (1,101)  | 1:138:A:MET:HA   | 1:209:A:VAL:HG13 | 11       | 0.74          |
| (1,55)   | 1:125:A:LEU:HD11 | 1:162:A:TYR:HB2  | 15       | 0.74          |
| (1,55)   | 1:125:A:LEU:HD12 | 1:162:A:TYR:HB2  | 15       | 0.74          |
| (1,55)   | 1:125:A:LEU:HD13 | 1:162:A:TYR:HB2  | 15       | 0.74          |
| (1,2846) | 1:157:A:TYR:HE1  | 1:206:A:MET:HB2  | 14       | 0.73          |
| (1,2846) | 1:157:A:TYR:HE2  | 1:206:A:MET:HB2  | 14       | 0.73          |
| (1,2807) | 1:149:A:TYR:HE1  | 1:153:A:ASN:HB3  | 2        | 0.73          |
| (1,2807) | 1:149:A:TYR:HE2  | 1:153:A:ASN:HB3  | 2        | 0.73          |
| (1,2736) | 1:184:A:ILE:HG13 | 1:187:A:HIS:HD2  | 14       | 0.73          |
| (1,2681) | 1:141:A:PHE:HZ   | 1:208:A:ARG:HB3  | 4        | 0.73          |
| (1,2674) | 1:175:A:PHE:HZ   | 1:221:A:GLU:HG2  | 12       | 0.73          |
| (1,2650) | 1:139:A:ILE:HG12 | 1:141:A:PHE:HE1  | 6        | 0.73          |
| (1,2650) | 1:139:A:ILE:HG12 | 1:141:A:PHE:HE2  | 6        | 0.73          |
| (1,2615) | 1:141:A:PHE:HD1  | 1:147:A:ASP:HB3  | 15       | 0.73          |
| (1,2615) | 1:141:A:PHE:HD2  | 1:147:A:ASP:HB3  | 15       | 0.73          |
| (1,2492) | 1:139:A:ILE:HG12 | 1:150:A:TYR:HD1  | 15       | 0.73          |
| (1,2492) | 1:139:A:ILE:HG12 | 1:150:A:TYR:HD2  | 15       | 0.73          |
| (1,2354) | 1:170:A:SER:HB2  | 1:174:A:ASN:HD21 | 16       | 0.73          |
| (1,2347) | 1:139:A:ILE:HG13 | 1:212:A:GLN:HE22 | 16       | 0.73          |
| (1,1523) | 1:162:A:TYR:HB3  | 1:182:A:ILE:HG12 | 9        | 0.73          |
| (1,1523) | 1:162:A:TYR:HB3  | 1:182:A:ILE:HG13 | 9        | 0.73          |
| (1,1497) | 1:139:A:ILE:HD11 | 1:212:A:GLN:HB3  | 15       | 0.73          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1497) | 1:139:A:ILE:HD12 | 1:212:A:GLN:HB3  | 15       | 0.73          |
| (1,1497) | 1:139:A:ILE:HD13 | 1:212:A:GLN:HB3  | 15       | 0.73          |
| (1,1085) | 1:129:A:MET:HB2  | 1:164:A:ARG:HA   | 18       | 0.73          |
| (1,921)  | 1:167:A:SER:HA   | 1:168:A:GLN:HG3  | 15       | 0.73          |
| (1,634)  | 1:192:A:THR:HA   | 1:195:A:GLY:HA3  | 7        | 0.73          |
| (1,634)  | 1:192:A:THR:HA   | 1:195:A:GLY:HA3  | 19       | 0.73          |
| (1,525)  | 1:132:A:SER:HB2  | 1:160:A:GLN:HE21 | 3        | 0.73          |
| (1,357)  | 1:122:A:VAL:HG21 | 1:125:A:LEU:HG   | 18       | 0.73          |
| (1,357)  | 1:122:A:VAL:HG22 | 1:125:A:LEU:HG   | 18       | 0.73          |
| (1,357)  | 1:122:A:VAL:HG23 | 1:125:A:LEU:HG   | 18       | 0.73          |
| (1,101)  | 1:138:A:MET:HA   | 1:209:A:VAL:HG11 | 19       | 0.73          |
| (1,101)  | 1:138:A:MET:HA   | 1:209:A:VAL:HG12 | 19       | 0.73          |
| (1,101)  | 1:138:A:MET:HA   | 1:209:A:VAL:HG13 | 19       | 0.73          |
| (1,2759) | 1:139:A:ILE:HG12 | 1:150:A:TYR:HE1  | 17       | 0.72          |
| (1,2759) | 1:139:A:ILE:HG12 | 1:150:A:TYR:HE2  | 17       | 0.72          |
| (1,2758) | 1:150:A:TYR:HE1  | 1:209:A:VAL:HG11 | 12       | 0.72          |
| (1,2758) | 1:150:A:TYR:HE1  | 1:209:A:VAL:HG12 | 12       | 0.72          |
| (1,2758) | 1:150:A:TYR:HE1  | 1:209:A:VAL:HG13 | 12       | 0.72          |
| (1,2758) | 1:150:A:TYR:HE2  | 1:209:A:VAL:HG11 | 12       | 0.72          |
| (1,2758) | 1:150:A:TYR:HE2  | 1:209:A:VAL:HG12 | 12       | 0.72          |
| (1,2758) | 1:150:A:TYR:HE2  | 1:209:A:VAL:HG13 | 12       | 0.72          |
| (1,2756) | 1:150:A:TYR:HE1  | 1:205:A:MET:HG2  | 4        | 0.72          |
| (1,2756) | 1:150:A:TYR:HE2  | 1:205:A:MET:HG2  | 4        | 0.72          |
| (1,2756) | 1:150:A:TYR:HE1  | 1:205:A:MET:HG2  | 17       | 0.72          |
| (1,2756) | 1:150:A:TYR:HE2  | 1:205:A:MET:HG2  | 17       | 0.72          |
| (1,2650) | 1:139:A:ILE:HG12 | 1:141:A:PHE:HE1  | 4        | 0.72          |
| (1,2650) | 1:139:A:ILE:HG12 | 1:141:A:PHE:HE2  | 4        | 0.72          |
| (1,2492) | 1:139:A:ILE:HG12 | 1:150:A:TYR:HD1  | 13       | 0.72          |
| (1,2492) | 1:139:A:ILE:HG12 | 1:150:A:TYR:HD2  | 13       | 0.72          |
| (1,2492) | 1:139:A:ILE:HG12 | 1:150:A:TYR:HD1  | 14       | 0.72          |
| (1,2492) | 1:139:A:ILE:HG12 | 1:150:A:TYR:HD2  | 14       | 0.72          |
| (1,2488) | 1:149:A:TYR:HD1  | 1:153:A:ASN:HB3  | 8        | 0.72          |
| (1,2488) | 1:149:A:TYR:HD2  | 1:153:A:ASN:HB3  | 8        | 0.72          |
| (1,2488) | 1:149:A:TYR:HD1  | 1:153:A:ASN:HB3  | 16       | 0.72          |
| (1,2488) | 1:149:A:TYR:HD2  | 1:153:A:ASN:HB3  | 16       | 0.72          |
| (1,2045) | 1:230:A:ARG:HG3  | 1:231:A:SER:H    | 7        | 0.72          |
| (1,2045) | 1:230:A:ARG:HG3  | 1:231:A:SER:H    | 13       | 0.72          |
| (1,1752) | 1:166:A:VAL:HG11 | 1:223:A:GLN:H    | 1        | 0.72          |
| (1,1752) | 1:166:A:VAL:HG12 | 1:223:A:GLN:H    | 1        | 0.72          |
| (1,1752) | 1:166:A:VAL:HG13 | 1:223:A:GLN:H    | 1        | 0.72          |
| (1,1679) | 1:122:A:VAL:HG21 | 1:125:A:LEU:H    | 12       | 0.72          |
| (1,1679) | 1:122:A:VAL:HG22 | 1:125:A:LEU:H    | 12       | 0.72          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1679) | 1:122:A:VAL:HG23 | 1:125:A:LEU:H    | 12       | 0.72          |
| (1,1678) | 1:125:A:LEU:H    | 1:125:A:LEU:HB2  | 4        | 0.72          |
| (1,1497) | 1:139:A:ILE:HD11 | 1:212:A:GLN:HB3  | 13       | 0.72          |
| (1,1497) | 1:139:A:ILE:HD12 | 1:212:A:GLN:HB3  | 13       | 0.72          |
| (1,1497) | 1:139:A:ILE:HD13 | 1:212:A:GLN:HB3  | 13       | 0.72          |
| (1,1459) | 1:136:A:ARG:HB3  | 1:159:A:ASN:HB3  | 13       | 0.72          |
| (1,1015) | 1:152:A:GLU:HG2  | 1:153:A:ASN:HD22 | 16       | 0.72          |
| (1,893)  | 1:162:A:TYR:HB3  | 1:182:A:ILE:HB   | 11       | 0.72          |
| (1,739)  | 1:166:A:VAL:HG11 | 1:222:A:SER:HB3  | 12       | 0.72          |
| (1,739)  | 1:166:A:VAL:HG12 | 1:222:A:SER:HB3  | 12       | 0.72          |
| (1,739)  | 1:166:A:VAL:HG13 | 1:222:A:SER:HB3  | 12       | 0.72          |
| (1,630)  | 1:165:A:PRO:HA   | 1:166:A:VAL:HG11 | 12       | 0.72          |
| (1,630)  | 1:165:A:PRO:HA   | 1:166:A:VAL:HG12 | 12       | 0.72          |
| (1,630)  | 1:165:A:PRO:HA   | 1:166:A:VAL:HG13 | 12       | 0.72          |
| (1,348)  | 1:122:A:VAL:HG21 | 1:124:A:GLY:HA2  | 8        | 0.72          |
| (1,348)  | 1:122:A:VAL:HG21 | 1:124:A:GLY:HA3  | 8        | 0.72          |
| (1,348)  | 1:122:A:VAL:HG22 | 1:124:A:GLY:HA2  | 8        | 0.72          |
| (1,348)  | 1:122:A:VAL:HG22 | 1:124:A:GLY:HA3  | 8        | 0.72          |
| (1,348)  | 1:122:A:VAL:HG23 | 1:124:A:GLY:HA2  | 8        | 0.72          |
| (1,348)  | 1:122:A:VAL:HG23 | 1:124:A:GLY:HA3  | 8        | 0.72          |
| (1,240)  | 1:166:A:VAL:HG21 | 1:169:A:TYR:HB2  | 17       | 0.72          |
| (1,240)  | 1:166:A:VAL:HG22 | 1:169:A:TYR:HB2  | 17       | 0.72          |
| (1,240)  | 1:166:A:VAL:HG23 | 1:169:A:TYR:HB2  | 17       | 0.72          |
| (1,220)  | 1:127:A:GLY:HA2  | 1:164:A:ARG:HE   | 15       | 0.72          |
| (1,204)  | 1:161:A:VAL:HG11 | 1:183:A:THR:HG21 | 10       | 0.72          |
| (1,204)  | 1:161:A:VAL:HG11 | 1:183:A:THR:HG22 | 10       | 0.72          |
| (1,204)  | 1:161:A:VAL:HG11 | 1:183:A:THR:HG23 | 10       | 0.72          |
| (1,204)  | 1:161:A:VAL:HG12 | 1:183:A:THR:HG21 | 10       | 0.72          |
| (1,204)  | 1:161:A:VAL:HG12 | 1:183:A:THR:HG22 | 10       | 0.72          |
| (1,204)  | 1:161:A:VAL:HG12 | 1:183:A:THR:HG23 | 10       | 0.72          |
| (1,204)  | 1:161:A:VAL:HG13 | 1:183:A:THR:HG21 | 10       | 0.72          |
| (1,204)  | 1:161:A:VAL:HG13 | 1:183:A:THR:HG22 | 10       | 0.72          |
| (1,204)  | 1:161:A:VAL:HG13 | 1:183:A:THR:HG23 | 10       | 0.72          |
| (1,98)   | 1:139:A:ILE:HG21 | 1:209:A:VAL:HG11 | 17       | 0.72          |
| (1,98)   | 1:139:A:ILE:HG21 | 1:209:A:VAL:HG12 | 17       | 0.72          |
| (1,98)   | 1:139:A:ILE:HG21 | 1:209:A:VAL:HG13 | 17       | 0.72          |
| (1,98)   | 1:139:A:ILE:HG22 | 1:209:A:VAL:HG11 | 17       | 0.72          |
| (1,98)   | 1:139:A:ILE:HG22 | 1:209:A:VAL:HG12 | 17       | 0.72          |
| (1,98)   | 1:139:A:ILE:HG22 | 1:209:A:VAL:HG13 | 17       | 0.72          |
| (1,98)   | 1:139:A:ILE:HG23 | 1:209:A:VAL:HG11 | 17       | 0.72          |
| (1,98)   | 1:139:A:ILE:HG23 | 1:209:A:VAL:HG12 | 17       | 0.72          |
| (1,98)   | 1:139:A:ILE:HG23 | 1:209:A:VAL:HG13 | 17       | 0.72          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2721) | 1:177:A:HIS:HD2  | 1:178:A:ASP:HB3  | 17       | 0.71          |
| (1,2548) | 1:162:A:TYR:HD1  | 1:186:A:GLN:HB3  | 19       | 0.71          |
| (1,2548) | 1:162:A:TYR:HD2  | 1:186:A:GLN:HB3  | 19       | 0.71          |
| (1,2501) | 1:149:A:TYR:HD1  | 1:205:A:MET:HG2  | 16       | 0.71          |
| (1,2501) | 1:149:A:TYR:HD2  | 1:205:A:MET:HG2  | 16       | 0.71          |
| (1,1480) | 1:203:A:VAL:HG21 | 1:207:A:GLU:HB2  | 12       | 0.71          |
| (1,1480) | 1:203:A:VAL:HG22 | 1:207:A:GLU:HB2  | 12       | 0.71          |
| (1,1480) | 1:203:A:VAL:HG23 | 1:207:A:GLU:HB2  | 12       | 0.71          |
| (1,1294) | 1:138:A:MET:HG3  | 1:139:A:ILE:H    | 3        | 0.71          |
| (1,1235) | 1:205:A:MET:HG3  | 1:206:A:MET:HG2  | 11       | 0.71          |
| (1,1131) | 1:223:A:GLN:HG2  | 1:226:A:TYR:H    | 20       | 0.71          |
| (1,1104) | 1:213:A:MET:HB3  | 1:214:A:CYS:HA   | 8        | 0.71          |
| (1,1085) | 1:129:A:MET:HB2  | 1:164:A:ARG:HA   | 10       | 0.71          |
| (1,893)  | 1:162:A:TYR:HB3  | 1:182:A:ILE:HB   | 13       | 0.71          |
| (1,864)  | 1:134:A:MET:HB3  | 1:135:A:SER:HB2  | 11       | 0.71          |
| (1,752)  | 1:138:A:MET:HE1  | 1:139:A:ILE:HG12 | 11       | 0.71          |
| (1,752)  | 1:138:A:MET:HE2  | 1:139:A:ILE:HG12 | 11       | 0.71          |
| (1,752)  | 1:138:A:MET:HE3  | 1:139:A:ILE:HG12 | 11       | 0.71          |
| (1,657)  | 1:213:A:MET:HB3  | 1:213:A:MET:HE1  | 10       | 0.71          |
| (1,657)  | 1:213:A:MET:HB3  | 1:213:A:MET:HE2  | 10       | 0.71          |
| (1,657)  | 1:213:A:MET:HB3  | 1:213:A:MET:HE3  | 10       | 0.71          |
| (1,445)  | 1:180:A:VAL:HA   | 1:184:A:ILE:HG12 | 18       | 0.71          |
| (1,430)  | 1:122:A:VAL:HG11 | 1:186:A:GLN:HG3  | 2        | 0.71          |
| (1,430)  | 1:122:A:VAL:HG12 | 1:186:A:GLN:HG3  | 2        | 0.71          |
| (1,430)  | 1:122:A:VAL:HG13 | 1:186:A:GLN:HG3  | 2        | 0.71          |
| (1,166)  | 1:203:A:VAL:HG11 | 1:206:A:MET:HG2  | 12       | 0.71          |
| (1,166)  | 1:203:A:VAL:HG12 | 1:206:A:MET:HG2  | 12       | 0.71          |
| (1,166)  | 1:203:A:VAL:HG13 | 1:206:A:MET:HG2  | 12       | 0.71          |
| (1,112)  | 1:214:A:CYS:HA   | 1:215:A:VAL:HG11 | 8        | 0.71          |
| (1,112)  | 1:214:A:CYS:HA   | 1:215:A:VAL:HG12 | 8        | 0.71          |
| (1,112)  | 1:214:A:CYS:HA   | 1:215:A:VAL:HG13 | 8        | 0.71          |
| (1,80)   | 1:208:A:ARG:HA   | 1:209:A:VAL:HG11 | 17       | 0.71          |
| (1,80)   | 1:208:A:ARG:HA   | 1:209:A:VAL:HG12 | 17       | 0.71          |
| (1,80)   | 1:208:A:ARG:HA   | 1:209:A:VAL:HG13 | 17       | 0.71          |
| (1,2792) | 1:128:A:TYR:HE1  | 1:164:A:ARG:HD3  | 6        | 0.7           |
| (1,2792) | 1:128:A:TYR:HE2  | 1:164:A:ARG:HD3  | 6        | 0.7           |
| (1,2711) | 1:145:A:TRP:HZ3  | 1:146:A:GLU:HG3  | 3        | 0.7           |
| (1,2657) | 1:141:A:PHE:HE1  | 1:208:A:ARG:HB3  | 16       | 0.7           |
| (1,2657) | 1:141:A:PHE:HE2  | 1:208:A:ARG:HB3  | 16       | 0.7           |
| (1,2657) | 1:141:A:PHE:HE1  | 1:208:A:ARG:HB3  | 19       | 0.7           |
| (1,2657) | 1:141:A:PHE:HE2  | 1:208:A:ARG:HB3  | 19       | 0.7           |
| (1,2650) | 1:139:A:ILE:HG12 | 1:141:A:PHE:HE1  | 11       | 0.7           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2650) | 1:139:A:ILE:HG12 | 1:141:A:PHE:HE2  | 11       | 0.7           |
| (1,2492) | 1:139:A:ILE:HG12 | 1:150:A:TYR:HD1  | 11       | 0.7           |
| (1,2492) | 1:139:A:ILE:HG12 | 1:150:A:TYR:HD2  | 11       | 0.7           |
| (1,2184) | 1:212:A:GLN:H    | 1:212:A:GLN:HB3  | 5        | 0.7           |
| (1,2184) | 1:212:A:GLN:H    | 1:212:A:GLN:HB3  | 6        | 0.7           |
| (1,2184) | 1:212:A:GLN:H    | 1:212:A:GLN:HB3  | 8        | 0.7           |
| (1,2184) | 1:212:A:GLN:H    | 1:212:A:GLN:HB3  | 13       | 0.7           |
| (1,2184) | 1:212:A:GLN:H    | 1:212:A:GLN:HB3  | 14       | 0.7           |
| (1,2184) | 1:212:A:GLN:H    | 1:212:A:GLN:HB3  | 17       | 0.7           |
| (1,1678) | 1:125:A:LEU:H    | 1:125:A:LEU:HB2  | 8        | 0.7           |
| (1,1497) | 1:139:A:ILE:HD11 | 1:212:A:GLN:HB3  | 9        | 0.7           |
| (1,1497) | 1:139:A:ILE:HD12 | 1:212:A:GLN:HB3  | 9        | 0.7           |
| (1,1497) | 1:139:A:ILE:HD13 | 1:212:A:GLN:HB3  | 9        | 0.7           |
| (1,1459) | 1:136:A:ARG:HB3  | 1:159:A:ASN:HB3  | 8        | 0.7           |
| (1,974)  | 1:148:A:ARG:HE   | 1:152:A:GLU:HG2  | 3        | 0.7           |
| (1,921)  | 1:167:A:SER:HA   | 1:168:A:GLN:HG3  | 6        | 0.7           |
| (1,901)  | 1:203:A:VAL:HG21 | 1:204:A:LYS:HA   | 18       | 0.7           |
| (1,901)  | 1:203:A:VAL:HG22 | 1:204:A:LYS:HA   | 18       | 0.7           |
| (1,901)  | 1:203:A:VAL:HG23 | 1:204:A:LYS:HA   | 18       | 0.7           |
| (1,658)  | 1:154:A:MET:HG3  | 1:154:A:MET:HE1  | 17       | 0.7           |
| (1,658)  | 1:154:A:MET:HG3  | 1:154:A:MET:HE2  | 17       | 0.7           |
| (1,658)  | 1:154:A:MET:HG3  | 1:154:A:MET:HE3  | 17       | 0.7           |
| (1,567)  | 1:230:A:ARG:HB2  | 1:231:A:SER:HB3  | 17       | 0.7           |
| (1,506)  | 1:179:A:CYS:HB2  | 1:214:A:CYS:HB2  | 16       | 0.7           |
| (1,257)  | 1:188:A:THR:HG21 | 1:189:A:VAL:HG21 | 11       | 0.7           |
| (1,257)  | 1:188:A:THR:HG21 | 1:189:A:VAL:HG22 | 11       | 0.7           |
| (1,257)  | 1:188:A:THR:HG21 | 1:189:A:VAL:HG23 | 11       | 0.7           |
| (1,257)  | 1:188:A:THR:HG22 | 1:189:A:VAL:HG21 | 11       | 0.7           |
| (1,257)  | 1:188:A:THR:HG22 | 1:189:A:VAL:HG22 | 11       | 0.7           |
| (1,257)  | 1:188:A:THR:HG22 | 1:189:A:VAL:HG23 | 11       | 0.7           |
| (1,257)  | 1:188:A:THR:HG23 | 1:189:A:VAL:HG21 | 11       | 0.7           |
| (1,257)  | 1:188:A:THR:HG23 | 1:189:A:VAL:HG22 | 11       | 0.7           |
| (1,257)  | 1:188:A:THR:HG23 | 1:189:A:VAL:HG23 | 11       | 0.7           |
| (1,98)   | 1:139:A:ILE:HG21 | 1:209:A:VAL:HG11 | 20       | 0.7           |
| (1,98)   | 1:139:A:ILE:HG21 | 1:209:A:VAL:HG12 | 20       | 0.7           |
| (1,98)   | 1:139:A:ILE:HG21 | 1:209:A:VAL:HG13 | 20       | 0.7           |
| (1,98)   | 1:139:A:ILE:HG22 | 1:209:A:VAL:HG11 | 20       | 0.7           |
| (1,98)   | 1:139:A:ILE:HG22 | 1:209:A:VAL:HG12 | 20       | 0.7           |
| (1,98)   | 1:139:A:ILE:HG22 | 1:209:A:VAL:HG13 | 20       | 0.7           |
| (1,98)   | 1:139:A:ILE:HG23 | 1:209:A:VAL:HG11 | 20       | 0.7           |
| (1,98)   | 1:139:A:ILE:HG23 | 1:209:A:VAL:HG12 | 20       | 0.7           |
| (1,98)   | 1:139:A:ILE:HG23 | 1:209:A:VAL:HG13 | 20       | 0.7           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2807) | 1:149:A:TYR:HE1  | 1:153:A:ASN:HB3  | 13       | 0.69          |
| (1,2807) | 1:149:A:TYR:HE2  | 1:153:A:ASN:HB3  | 13       | 0.69          |
| (1,2792) | 1:128:A:TYR:HE1  | 1:164:A:ARG:HD3  | 17       | 0.69          |
| (1,2792) | 1:128:A:TYR:HE2  | 1:164:A:ARG:HD3  | 17       | 0.69          |
| (1,2735) | 1:186:A:GLN:HB3  | 1:187:A:HIS:HD2  | 8        | 0.69          |
| (1,2657) | 1:141:A:PHE:HE1  | 1:208:A:ARG:HB3  | 6        | 0.69          |
| (1,2657) | 1:141:A:PHE:HE2  | 1:208:A:ARG:HB3  | 6        | 0.69          |
| (1,2548) | 1:162:A:TYR:HD1  | 1:186:A:GLN:HB3  | 5        | 0.69          |
| (1,2548) | 1:162:A:TYR:HD2  | 1:186:A:GLN:HB3  | 5        | 0.69          |
| (1,2548) | 1:162:A:TYR:HD1  | 1:186:A:GLN:HB3  | 9        | 0.69          |
| (1,2548) | 1:162:A:TYR:HD2  | 1:186:A:GLN:HB3  | 9        | 0.69          |
| (1,2501) | 1:149:A:TYR:HD1  | 1:205:A:MET:HG2  | 1        | 0.69          |
| (1,2501) | 1:149:A:TYR:HD2  | 1:205:A:MET:HG2  | 1        | 0.69          |
| (1,2492) | 1:139:A:ILE:HG12 | 1:150:A:TYR:HD1  | 3        | 0.69          |
| (1,2492) | 1:139:A:ILE:HG12 | 1:150:A:TYR:HD2  | 3        | 0.69          |
| (1,2364) | 1:171:A:ASN:HD22 | 1:174:A:ASN:HD22 | 18       | 0.69          |
| (1,2184) | 1:212:A:GLN:H    | 1:212:A:GLN:HB3  | 2        | 0.69          |
| (1,2184) | 1:212:A:GLN:H    | 1:212:A:GLN:HB3  | 4        | 0.69          |
| (1,2184) | 1:212:A:GLN:H    | 1:212:A:GLN:HB3  | 9        | 0.69          |
| (1,2184) | 1:212:A:GLN:H    | 1:212:A:GLN:HB3  | 10       | 0.69          |
| (1,2184) | 1:212:A:GLN:H    | 1:212:A:GLN:HB3  | 11       | 0.69          |
| (1,2184) | 1:212:A:GLN:H    | 1:212:A:GLN:HB3  | 12       | 0.69          |
| (1,2184) | 1:212:A:GLN:H    | 1:212:A:GLN:HB3  | 15       | 0.69          |
| (1,2184) | 1:212:A:GLN:H    | 1:212:A:GLN:HB3  | 18       | 0.69          |
| (1,2184) | 1:212:A:GLN:H    | 1:212:A:GLN:HB3  | 19       | 0.69          |
| (1,2184) | 1:212:A:GLN:H    | 1:212:A:GLN:HB3  | 20       | 0.69          |
| (1,1678) | 1:125:A:LEU:H    | 1:125:A:LEU:HB2  | 7        | 0.69          |
| (1,1497) | 1:139:A:ILE:HD11 | 1:212:A:GLN:HB3  | 14       | 0.69          |
| (1,1497) | 1:139:A:ILE:HD12 | 1:212:A:GLN:HB3  | 14       | 0.69          |
| (1,1497) | 1:139:A:ILE:HD13 | 1:212:A:GLN:HB3  | 14       | 0.69          |
| (1,1104) | 1:213:A:MET:HB3  | 1:214:A:CYS:HA   | 4        | 0.69          |
| (1,974)  | 1:148:A:ARG:HE   | 1:152:A:GLU:HG2  | 8        | 0.69          |
| (1,921)  | 1:167:A:SER:HA   | 1:168:A:GLN:HG3  | 9        | 0.69          |
| (1,851)  | 1:151:A:ARG:HA   | 1:151:A:ARG:HG2  | 13       | 0.69          |
| (1,657)  | 1:213:A:MET:HB3  | 1:213:A:MET:HE1  | 1        | 0.69          |
| (1,657)  | 1:213:A:MET:HB3  | 1:213:A:MET:HE2  | 1        | 0.69          |
| (1,657)  | 1:213:A:MET:HB3  | 1:213:A:MET:HE3  | 1        | 0.69          |
| (1,657)  | 1:213:A:MET:HB3  | 1:213:A:MET:HE1  | 16       | 0.69          |
| (1,657)  | 1:213:A:MET:HB3  | 1:213:A:MET:HE2  | 16       | 0.69          |
| (1,657)  | 1:213:A:MET:HB3  | 1:213:A:MET:HE3  | 16       | 0.69          |
| (1,656)  | 1:138:A:MET:HG3  | 1:154:A:MET:HE1  | 2        | 0.69          |
| (1,656)  | 1:138:A:MET:HG3  | 1:154:A:MET:HE2  | 2        | 0.69          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,656)  | 1:138:A:MET:HG3  | 1:154:A:MET:HE3  | 2        | 0.69          |
| (1,502)  | 1:162:A:TYR:HB3  | 1:183:A:THR:HA   | 13       | 0.69          |
| (1,155)  | 1:125:A:LEU:HB3  | 1:126:A:GLY:HA3  | 5        | 0.69          |
| (1,155)  | 1:125:A:LEU:HB3  | 1:126:A:GLY:HA3  | 20       | 0.69          |
| (1,138)  | 1:125:A:LEU:HA   | 1:125:A:LEU:HD21 | 1        | 0.69          |
| (1,138)  | 1:125:A:LEU:HA   | 1:125:A:LEU:HD22 | 1        | 0.69          |
| (1,138)  | 1:125:A:LEU:HA   | 1:125:A:LEU:HD23 | 1        | 0.69          |
| (1,112)  | 1:214:A:CYS:HA   | 1:215:A:VAL:HG11 | 4        | 0.69          |
| (1,112)  | 1:214:A:CYS:HA   | 1:215:A:VAL:HG12 | 4        | 0.69          |
| (1,112)  | 1:214:A:CYS:HA   | 1:215:A:VAL:HG13 | 4        | 0.69          |
| (1,101)  | 1:138:A:MET:HA   | 1:209:A:VAL:HG11 | 2        | 0.69          |
| (1,101)  | 1:138:A:MET:HA   | 1:209:A:VAL:HG12 | 2        | 0.69          |
| (1,101)  | 1:138:A:MET:HA   | 1:209:A:VAL:HG13 | 2        | 0.69          |
| (1,80)   | 1:208:A:ARG:HA   | 1:209:A:VAL:HG11 | 7        | 0.69          |
| (1,80)   | 1:208:A:ARG:HA   | 1:209:A:VAL:HG12 | 7        | 0.69          |
| (1,80)   | 1:208:A:ARG:HA   | 1:209:A:VAL:HG13 | 7        | 0.69          |
| (1,80)   | 1:208:A:ARG:HA   | 1:209:A:VAL:HG11 | 19       | 0.69          |
| (1,80)   | 1:208:A:ARG:HA   | 1:209:A:VAL:HG12 | 19       | 0.69          |
| (1,80)   | 1:208:A:ARG:HA   | 1:209:A:VAL:HG13 | 19       | 0.69          |
| (1,55)   | 1:125:A:LEU:HD11 | 1:162:A:TYR:HB2  | 14       | 0.69          |
| (1,55)   | 1:125:A:LEU:HD12 | 1:162:A:TYR:HB2  | 14       | 0.69          |
| (1,55)   | 1:125:A:LEU:HD13 | 1:162:A:TYR:HB2  | 14       | 0.69          |
| (1,2851) | 1:184:A:ILE:HG13 | 1:187:A:HIS:HE1  | 13       | 0.68          |
| (1,2681) | 1:141:A:PHE:HZ   | 1:208:A:ARG:HB3  | 19       | 0.68          |
| (1,2650) | 1:139:A:ILE:HG12 | 1:141:A:PHE:HE1  | 19       | 0.68          |
| (1,2650) | 1:139:A:ILE:HG12 | 1:141:A:PHE:HE2  | 19       | 0.68          |
| (1,2501) | 1:149:A:TYR:HD1  | 1:205:A:MET:HG2  | 7        | 0.68          |
| (1,2501) | 1:149:A:TYR:HD2  | 1:205:A:MET:HG2  | 7        | 0.68          |
| (1,2488) | 1:149:A:TYR:HD1  | 1:153:A:ASN:HB3  | 1        | 0.68          |
| (1,2488) | 1:149:A:TYR:HD2  | 1:153:A:ASN:HB3  | 1        | 0.68          |
| (1,2488) | 1:149:A:TYR:HD1  | 1:153:A:ASN:HB3  | 4        | 0.68          |
| (1,2488) | 1:149:A:TYR:HD2  | 1:153:A:ASN:HB3  | 4        | 0.68          |
| (1,2356) | 1:169:A:TYR:HB2  | 1:174:A:ASN:HD21 | 15       | 0.68          |
| (1,2320) | 1:160:A:GLN:HE22 | 1:213:A:MET:HB2  | 6        | 0.68          |
| (1,2184) | 1:212:A:GLN:H    | 1:212:A:GLN:HB3  | 1        | 0.68          |
| (1,2184) | 1:212:A:GLN:H    | 1:212:A:GLN:HB3  | 7        | 0.68          |
| (1,2184) | 1:212:A:GLN:H    | 1:212:A:GLN:HB3  | 16       | 0.68          |
| (1,1375) | 1:136:A:ARG:HD2  | 1:154:A:MET:HG3  | 5        | 0.68          |
| (1,927)  | 1:212:A:GLN:HA   | 1:213:A:MET:HG2  | 1        | 0.68          |
| (1,658)  | 1:154:A:MET:HG3  | 1:154:A:MET:HE1  | 12       | 0.68          |
| (1,658)  | 1:154:A:MET:HG3  | 1:154:A:MET:HE2  | 12       | 0.68          |
| (1,658)  | 1:154:A:MET:HG3  | 1:154:A:MET:HE3  | 12       | 0.68          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,658)  | 1:154:A:MET:HG3  | 1:154:A:MET:HE1  | 19       | 0.68          |
| (1,658)  | 1:154:A:MET:HG3  | 1:154:A:MET:HE2  | 19       | 0.68          |
| (1,658)  | 1:154:A:MET:HG3  | 1:154:A:MET:HE3  | 19       | 0.68          |
| (1,502)  | 1:162:A:TYR:HB3  | 1:183:A:THR:HA   | 20       | 0.68          |
| (1,408)  | 1:148:A:ARG:HA   | 1:148:A:ARG:HD2  | 9        | 0.68          |
| (1,323)  | 1:209:A:VAL:HG21 | 1:212:A:GLN:HB3  | 2        | 0.68          |
| (1,323)  | 1:209:A:VAL:HG22 | 1:212:A:GLN:HB3  | 2        | 0.68          |
| (1,323)  | 1:209:A:VAL:HG23 | 1:212:A:GLN:HB3  | 2        | 0.68          |
| (1,138)  | 1:125:A:LEU:HA   | 1:125:A:LEU:HD21 | 14       | 0.68          |
| (1,138)  | 1:125:A:LEU:HA   | 1:125:A:LEU:HD22 | 14       | 0.68          |
| (1,138)  | 1:125:A:LEU:HA   | 1:125:A:LEU:HD23 | 14       | 0.68          |
| (1,107)  | 1:211:A:GLU:HG3  | 1:215:A:VAL:HG11 | 1        | 0.68          |
| (1,107)  | 1:211:A:GLU:HG3  | 1:215:A:VAL:HG12 | 1        | 0.68          |
| (1,107)  | 1:211:A:GLU:HG3  | 1:215:A:VAL:HG13 | 1        | 0.68          |
| (1,2721) | 1:177:A:HIS:HD2  | 1:178:A:ASP:HB3  | 7        | 0.67          |
| (1,2674) | 1:175:A:PHE:HZ   | 1:221:A:GLU:HG2  | 6        | 0.67          |
| (1,2237) | 1:166:A:VAL:HG11 | 1:222:A:SER:H    | 17       | 0.67          |
| (1,2237) | 1:166:A:VAL:HG12 | 1:222:A:SER:H    | 17       | 0.67          |
| (1,2237) | 1:166:A:VAL:HG13 | 1:222:A:SER:H    | 17       | 0.67          |
| (1,2184) | 1:212:A:GLN:H    | 1:212:A:GLN:HB3  | 3        | 0.67          |
| (1,1523) | 1:162:A:TYR:HB3  | 1:182:A:ILE:HG12 | 7        | 0.67          |
| (1,1523) | 1:162:A:TYR:HB3  | 1:182:A:ILE:HG13 | 7        | 0.67          |
| (1,1523) | 1:162:A:TYR:HB3  | 1:182:A:ILE:HG12 | 19       | 0.67          |
| (1,1523) | 1:162:A:TYR:HB3  | 1:182:A:ILE:HG13 | 19       | 0.67          |
| (1,1497) | 1:139:A:ILE:HD11 | 1:212:A:GLN:HB3  | 6        | 0.67          |
| (1,1497) | 1:139:A:ILE:HD12 | 1:212:A:GLN:HB3  | 6        | 0.67          |
| (1,1497) | 1:139:A:ILE:HD13 | 1:212:A:GLN:HB3  | 6        | 0.67          |
| (1,1497) | 1:139:A:ILE:HD11 | 1:212:A:GLN:HB3  | 11       | 0.67          |
| (1,1497) | 1:139:A:ILE:HD12 | 1:212:A:GLN:HB3  | 11       | 0.67          |
| (1,1497) | 1:139:A:ILE:HD13 | 1:212:A:GLN:HB3  | 11       | 0.67          |
| (1,893)  | 1:162:A:TYR:HB3  | 1:182:A:ILE:HB   | 9        | 0.67          |
| (1,528)  | 1:143:A:ASN:HB2  | 1:147:A:ASP:HB3  | 18       | 0.67          |
| (1,528)  | 1:143:A:ASN:HB3  | 1:147:A:ASP:HB3  | 18       | 0.67          |
| (1,423)  | 1:151:A:ARG:HD3  | 1:152:A:GLU:H    | 18       | 0.67          |
| (1,177)  | 1:195:A:GLY:HA3  | 1:197:A:ASN:HD21 | 2        | 0.67          |
| (1,112)  | 1:214:A:CYS:HA   | 1:215:A:VAL:HG11 | 2        | 0.67          |
| (1,112)  | 1:214:A:CYS:HA   | 1:215:A:VAL:HG12 | 2        | 0.67          |
| (1,112)  | 1:214:A:CYS:HA   | 1:215:A:VAL:HG13 | 2        | 0.67          |
| (1,112)  | 1:214:A:CYS:HA   | 1:215:A:VAL:HG11 | 14       | 0.67          |
| (1,112)  | 1:214:A:CYS:HA   | 1:215:A:VAL:HG12 | 14       | 0.67          |
| (1,112)  | 1:214:A:CYS:HA   | 1:215:A:VAL:HG13 | 14       | 0.67          |
| (1,107)  | 1:211:A:GLU:HG3  | 1:215:A:VAL:HG11 | 18       | 0.67          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,107)  | 1:211:A:GLU:HG3  | 1:215:A:VAL:HG12 | 18       | 0.67          |
| (1,107)  | 1:211:A:GLU:HG3  | 1:215:A:VAL:HG13 | 18       | 0.67          |
| (1,80)   | 1:208:A:ARG:HA   | 1:209:A:VAL:HG11 | 1        | 0.67          |
| (1,80)   | 1:208:A:ARG:HA   | 1:209:A:VAL:HG12 | 1        | 0.67          |
| (1,80)   | 1:208:A:ARG:HA   | 1:209:A:VAL:HG13 | 1        | 0.67          |
| (1,2792) | 1:128:A:TYR:HE1  | 1:164:A:ARG:HD3  | 2        | 0.66          |
| (1,2792) | 1:128:A:TYR:HE2  | 1:164:A:ARG:HD3  | 2        | 0.66          |
| (1,2774) | 1:128:A:TYR:HE1  | 1:162:A:TYR:HB3  | 7        | 0.66          |
| (1,2774) | 1:128:A:TYR:HE2  | 1:162:A:TYR:HB3  | 7        | 0.66          |
| (1,2774) | 1:128:A:TYR:HE1  | 1:162:A:TYR:HB3  | 15       | 0.66          |
| (1,2774) | 1:128:A:TYR:HE2  | 1:162:A:TYR:HB3  | 15       | 0.66          |
| (1,2774) | 1:128:A:TYR:HE1  | 1:162:A:TYR:HB3  | 18       | 0.66          |
| (1,2774) | 1:128:A:TYR:HE2  | 1:162:A:TYR:HB3  | 18       | 0.66          |
| (1,2771) | 1:130:A:LEU:HB3  | 1:162:A:TYR:HE1  | 7        | 0.66          |
| (1,2771) | 1:130:A:LEU:HB3  | 1:162:A:TYR:HE2  | 7        | 0.66          |
| (1,2736) | 1:184:A:ILE:HG13 | 1:187:A:HIS:HD2  | 20       | 0.66          |
| (1,2615) | 1:141:A:PHE:HD1  | 1:147:A:ASP:HB3  | 4        | 0.66          |
| (1,2615) | 1:141:A:PHE:HD2  | 1:147:A:ASP:HB3  | 4        | 0.66          |
| (1,2488) | 1:149:A:TYR:HD1  | 1:153:A:ASN:HB3  | 14       | 0.66          |
| (1,2488) | 1:149:A:TYR:HD2  | 1:153:A:ASN:HB3  | 14       | 0.66          |
| (1,2354) | 1:170:A:SER:HB2  | 1:174:A:ASN:HD21 | 9        | 0.66          |
| (1,1678) | 1:125:A:LEU:H    | 1:125:A:LEU:HB2  | 3        | 0.66          |
| (1,1579) | 1:132:A:SER:HB3  | 1:133:A:ALA:H    | 6        | 0.66          |
| (1,1294) | 1:138:A:MET:HG3  | 1:139:A:ILE:H    | 15       | 0.66          |
| (1,1166) | 1:215:A:VAL:HG21 | 1:219:A:GLN:HG3  | 14       | 0.66          |
| (1,1166) | 1:215:A:VAL:HG22 | 1:219:A:GLN:HG3  | 14       | 0.66          |
| (1,1166) | 1:215:A:VAL:HG23 | 1:219:A:GLN:HG3  | 14       | 0.66          |
| (1,1164) | 1:215:A:VAL:HG21 | 1:219:A:GLN:HG2  | 17       | 0.66          |
| (1,1164) | 1:215:A:VAL:HG22 | 1:219:A:GLN:HG2  | 17       | 0.66          |
| (1,1164) | 1:215:A:VAL:HG23 | 1:219:A:GLN:HG2  | 17       | 0.66          |
| (1,1015) | 1:152:A:GLU:HG2  | 1:153:A:ASN:HD22 | 8        | 0.66          |
| (1,999)  | 1:176:A:VAL:HG11 | 1:211:A:GLU:HG3  | 12       | 0.66          |
| (1,999)  | 1:176:A:VAL:HG12 | 1:211:A:GLU:HG3  | 12       | 0.66          |
| (1,999)  | 1:176:A:VAL:HG13 | 1:211:A:GLU:HG3  | 12       | 0.66          |
| (1,974)  | 1:148:A:ARG:HE   | 1:152:A:GLU:HG2  | 13       | 0.66          |
| (1,901)  | 1:203:A:VAL:HG21 | 1:204:A:LYS:HA   | 2        | 0.66          |
| (1,901)  | 1:203:A:VAL:HG22 | 1:204:A:LYS:HA   | 2        | 0.66          |
| (1,901)  | 1:203:A:VAL:HG23 | 1:204:A:LYS:HA   | 2        | 0.66          |
| (1,893)  | 1:162:A:TYR:HB3  | 1:182:A:ILE:HB   | 20       | 0.66          |
| (1,733)  | 1:222:A:SER:HB2  | 1:226:A:TYR:HD1  | 15       | 0.66          |
| (1,733)  | 1:222:A:SER:HB2  | 1:226:A:TYR:HD2  | 15       | 0.66          |
| (1,733)  | 1:222:A:SER:HB2  | 1:226:A:TYR:HD1  | 17       | 0.66          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,733)  | 1:222:A:SER:HB2  | 1:226:A:TYR:HD2  | 17       | 0.66          |
| (1,658)  | 1:154:A:MET:HG3  | 1:154:A:MET:HE1  | 8        | 0.66          |
| (1,658)  | 1:154:A:MET:HG3  | 1:154:A:MET:HE2  | 8        | 0.66          |
| (1,658)  | 1:154:A:MET:HG3  | 1:154:A:MET:HE3  | 8        | 0.66          |
| (1,657)  | 1:213:A:MET:HB3  | 1:213:A:MET:HE1  | 12       | 0.66          |
| (1,657)  | 1:213:A:MET:HB3  | 1:213:A:MET:HE2  | 12       | 0.66          |
| (1,657)  | 1:213:A:MET:HB3  | 1:213:A:MET:HE3  | 12       | 0.66          |
| (1,637)  | 1:147:A:ASP:HB2  | 1:148:A:ARG:HG2  | 19       | 0.66          |
| (1,502)  | 1:162:A:TYR:HB3  | 1:183:A:THR:HA   | 5        | 0.66          |
| (1,80)   | 1:208:A:ARG:HA   | 1:209:A:VAL:HG11 | 4        | 0.66          |
| (1,80)   | 1:208:A:ARG:HA   | 1:209:A:VAL:HG12 | 4        | 0.66          |
| (1,80)   | 1:208:A:ARG:HA   | 1:209:A:VAL:HG13 | 4        | 0.66          |
| (1,2782) | 1:150:A:TYR:HE1  | 1:154:A:MET:HG3  | 17       | 0.65          |
| (1,2782) | 1:150:A:TYR:HE2  | 1:154:A:MET:HG3  | 17       | 0.65          |
| (1,2771) | 1:130:A:LEU:HB3  | 1:162:A:TYR:HE1  | 19       | 0.65          |
| (1,2771) | 1:130:A:LEU:HB3  | 1:162:A:TYR:HE2  | 19       | 0.65          |
| (1,2756) | 1:150:A:TYR:HE1  | 1:205:A:MET:HG2  | 5        | 0.65          |
| (1,2756) | 1:150:A:TYR:HE2  | 1:205:A:MET:HG2  | 5        | 0.65          |
| (1,2721) | 1:177:A:HIS:HD2  | 1:178:A:ASP:HB3  | 1        | 0.65          |
| (1,2615) | 1:141:A:PHE:HD1  | 1:147:A:ASP:HB3  | 16       | 0.65          |
| (1,2615) | 1:141:A:PHE:HD2  | 1:147:A:ASP:HB3  | 16       | 0.65          |
| (1,2501) | 1:149:A:TYR:HD1  | 1:205:A:MET:HG2  | 14       | 0.65          |
| (1,2501) | 1:149:A:TYR:HD2  | 1:205:A:MET:HG2  | 14       | 0.65          |
| (1,2313) | 1:159:A:ASN:HD22 | 1:160:A:GLN:HE21 | 20       | 0.65          |
| (1,1937) | 1:220:A:LYS:H    | 1:221:A:GLU:HG3  | 15       | 0.65          |
| (1,1579) | 1:132:A:SER:HB3  | 1:133:A:ALA:H    | 2        | 0.65          |
| (1,1231) | 1:209:A:VAL:HG21 | 1:213:A:MET:HG3  | 13       | 0.65          |
| (1,1231) | 1:209:A:VAL:HG22 | 1:213:A:MET:HG3  | 13       | 0.65          |
| (1,1231) | 1:209:A:VAL:HG23 | 1:213:A:MET:HG3  | 13       | 0.65          |
| (1,1207) | 1:168:A:GLN:HA   | 1:168:A:GLN:HE22 | 5        | 0.65          |
| (1,1166) | 1:215:A:VAL:HG21 | 1:219:A:GLN:HG3  | 4        | 0.65          |
| (1,1166) | 1:215:A:VAL:HG22 | 1:219:A:GLN:HG3  | 4        | 0.65          |
| (1,1166) | 1:215:A:VAL:HG23 | 1:219:A:GLN:HG3  | 4        | 0.65          |
| (1,1164) | 1:215:A:VAL:HG21 | 1:219:A:GLN:HG2  | 19       | 0.65          |
| (1,1164) | 1:215:A:VAL:HG22 | 1:219:A:GLN:HG2  | 19       | 0.65          |
| (1,1164) | 1:215:A:VAL:HG23 | 1:219:A:GLN:HG2  | 19       | 0.65          |
| (1,1097) | 1:165:A:PRO:HB3  | 1:168:A:GLN:HG2  | 20       | 0.65          |
| (1,1015) | 1:152:A:GLU:HG2  | 1:153:A:ASN:HD22 | 9        | 0.65          |
| (1,957)  | 1:184:A:ILE:HD11 | 1:207:A:GLU:HG3  | 8        | 0.65          |
| (1,957)  | 1:184:A:ILE:HD12 | 1:207:A:GLU:HG3  | 8        | 0.65          |
| (1,957)  | 1:184:A:ILE:HD13 | 1:207:A:GLU:HG3  | 8        | 0.65          |
| (1,893)  | 1:162:A:TYR:HB3  | 1:182:A:ILE:HB   | 15       | 0.65          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,658)  | 1:154:A:MET:HG3  | 1:154:A:MET:HE1  | 3        | 0.65          |
| (1,658)  | 1:154:A:MET:HG3  | 1:154:A:MET:HE2  | 3        | 0.65          |
| (1,658)  | 1:154:A:MET:HG3  | 1:154:A:MET:HE3  | 3        | 0.65          |
| (1,657)  | 1:213:A:MET:HB3  | 1:213:A:MET:HE1  | 3        | 0.65          |
| (1,657)  | 1:213:A:MET:HB3  | 1:213:A:MET:HE2  | 3        | 0.65          |
| (1,657)  | 1:213:A:MET:HB3  | 1:213:A:MET:HE3  | 3        | 0.65          |
| (1,657)  | 1:213:A:MET:HB3  | 1:213:A:MET:HE1  | 15       | 0.65          |
| (1,657)  | 1:213:A:MET:HB3  | 1:213:A:MET:HE2  | 15       | 0.65          |
| (1,657)  | 1:213:A:MET:HB3  | 1:213:A:MET:HE3  | 15       | 0.65          |
| (1,656)  | 1:138:A:MET:HG3  | 1:154:A:MET:HE1  | 20       | 0.65          |
| (1,656)  | 1:138:A:MET:HG3  | 1:154:A:MET:HE2  | 20       | 0.65          |
| (1,656)  | 1:138:A:MET:HG3  | 1:154:A:MET:HE3  | 20       | 0.65          |
| (1,637)  | 1:147:A:ASP:HB2  | 1:148:A:ARG:HG2  | 18       | 0.65          |
| (1,637)  | 1:147:A:ASP:HB2  | 1:148:A:ARG:HG2  | 20       | 0.65          |
| (1,630)  | 1:165:A:PRO:HA   | 1:166:A:VAL:HG11 | 17       | 0.65          |
| (1,630)  | 1:165:A:PRO:HA   | 1:166:A:VAL:HG12 | 17       | 0.65          |
| (1,630)  | 1:165:A:PRO:HA   | 1:166:A:VAL:HG13 | 17       | 0.65          |
| (1,496)  | 1:130:A:LEU:HA   | 1:162:A:TYR:HB2  | 20       | 0.65          |
| (1,437)  | 1:229:A:ARG:HB3  | 1:230:A:ARG:HD3  | 5        | 0.65          |
| (1,437)  | 1:229:A:ARG:HB2  | 1:230:A:ARG:HD3  | 5        | 0.65          |
| (1,362)  | 1:172:A:GLN:HG3  | 1:215:A:VAL:HG21 | 10       | 0.65          |
| (1,362)  | 1:172:A:GLN:HG3  | 1:215:A:VAL:HG22 | 10       | 0.65          |
| (1,362)  | 1:172:A:GLN:HG3  | 1:215:A:VAL:HG23 | 10       | 0.65          |
| (1,289)  | 1:189:A:VAL:HG21 | 1:192:A:THR:HG21 | 11       | 0.65          |
| (1,289)  | 1:189:A:VAL:HG21 | 1:192:A:THR:HG22 | 11       | 0.65          |
| (1,289)  | 1:189:A:VAL:HG21 | 1:192:A:THR:HG23 | 11       | 0.65          |
| (1,289)  | 1:189:A:VAL:HG22 | 1:192:A:THR:HG21 | 11       | 0.65          |
| (1,289)  | 1:189:A:VAL:HG22 | 1:192:A:THR:HG22 | 11       | 0.65          |
| (1,289)  | 1:189:A:VAL:HG22 | 1:192:A:THR:HG23 | 11       | 0.65          |
| (1,289)  | 1:189:A:VAL:HG23 | 1:192:A:THR:HG21 | 11       | 0.65          |
| (1,289)  | 1:189:A:VAL:HG23 | 1:192:A:THR:HG22 | 11       | 0.65          |
| (1,289)  | 1:189:A:VAL:HG23 | 1:192:A:THR:HG23 | 11       | 0.65          |
| (1,2774) | 1:128:A:TYR:HE1  | 1:162:A:TYR:HB3  | 9        | 0.64          |
| (1,2774) | 1:128:A:TYR:HE2  | 1:162:A:TYR:HB3  | 9        | 0.64          |
| (1,2774) | 1:128:A:TYR:HE1  | 1:162:A:TYR:HB3  | 12       | 0.64          |
| (1,2774) | 1:128:A:TYR:HE2  | 1:162:A:TYR:HB3  | 12       | 0.64          |
| (1,2699) | 1:141:A:PHE:HZ   | 1:150:A:TYR:HB3  | 9        | 0.64          |
| (1,2681) | 1:141:A:PHE:HZ   | 1:208:A:ARG:HB3  | 11       | 0.64          |
| (1,2681) | 1:141:A:PHE:HZ   | 1:208:A:ARG:HB3  | 14       | 0.64          |
| (1,2681) | 1:141:A:PHE:HZ   | 1:208:A:ARG:HB3  | 15       | 0.64          |
| (1,2492) | 1:139:A:ILE:HG12 | 1:150:A:TYR:HD1  | 1        | 0.64          |
| (1,2492) | 1:139:A:ILE:HG12 | 1:150:A:TYR:HD2  | 1        | 0.64          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2361) | 1:165:A:PRO:HG3  | 1:168:A:GLN:HE21 | 12       | 0.64          |
| (1,2177) | 1:212:A:GLN:H    | 1:213:A:MET:HG2  | 7        | 0.64          |
| (1,1579) | 1:132:A:SER:HB3  | 1:133:A:ALA:H    | 4        | 0.64          |
| (1,1207) | 1:168:A:GLN:HA   | 1:168:A:GLN:HE22 | 6        | 0.64          |
| (1,1015) | 1:152:A:GLU:HG2  | 1:153:A:ASN:HD22 | 12       | 0.64          |
| (1,927)  | 1:212:A:GLN:HA   | 1:213:A:MET:HG2  | 7        | 0.64          |
| (1,893)  | 1:162:A:TYR:HB3  | 1:182:A:ILE:HB   | 2        | 0.64          |
| (1,677)  | 1:135:A:SER:HB2  | 1:213:A:MET:HA   | 8        | 0.64          |
| (1,657)  | 1:213:A:MET:HB3  | 1:213:A:MET:HE1  | 7        | 0.64          |
| (1,657)  | 1:213:A:MET:HB3  | 1:213:A:MET:HE2  | 7        | 0.64          |
| (1,657)  | 1:213:A:MET:HB3  | 1:213:A:MET:HE3  | 7        | 0.64          |
| (1,657)  | 1:213:A:MET:HB3  | 1:213:A:MET:HE1  | 8        | 0.64          |
| (1,657)  | 1:213:A:MET:HB3  | 1:213:A:MET:HE2  | 8        | 0.64          |
| (1,657)  | 1:213:A:MET:HB3  | 1:213:A:MET:HE3  | 8        | 0.64          |
| (1,634)  | 1:192:A:THR:HA   | 1:195:A:GLY:HA3  | 9        | 0.64          |
| (1,502)  | 1:162:A:TYR:HB3  | 1:183:A:THR:HA   | 2        | 0.64          |
| (1,502)  | 1:162:A:TYR:HB3  | 1:183:A:THR:HA   | 15       | 0.64          |
| (1,467)  | 1:122:A:VAL:HG21 | 1:125:A:LEU:HB3  | 18       | 0.64          |
| (1,467)  | 1:122:A:VAL:HG22 | 1:125:A:LEU:HB3  | 18       | 0.64          |
| (1,467)  | 1:122:A:VAL:HG23 | 1:125:A:LEU:HB3  | 18       | 0.64          |
| (1,436)  | 1:229:A:ARG:HA   | 1:230:A:ARG:HD3  | 3        | 0.64          |
| (1,362)  | 1:172:A:GLN:HG3  | 1:215:A:VAL:HG21 | 9        | 0.64          |
| (1,362)  | 1:172:A:GLN:HG3  | 1:215:A:VAL:HG22 | 9        | 0.64          |
| (1,362)  | 1:172:A:GLN:HG3  | 1:215:A:VAL:HG23 | 9        | 0.64          |
| (1,323)  | 1:209:A:VAL:HG21 | 1:212:A:GLN:HB3  | 3        | 0.64          |
| (1,323)  | 1:209:A:VAL:HG22 | 1:212:A:GLN:HB3  | 3        | 0.64          |
| (1,323)  | 1:209:A:VAL:HG23 | 1:212:A:GLN:HB3  | 3        | 0.64          |
| (1,323)  | 1:209:A:VAL:HG21 | 1:212:A:GLN:HB3  | 6        | 0.64          |
| (1,323)  | 1:209:A:VAL:HG22 | 1:212:A:GLN:HB3  | 6        | 0.64          |
| (1,323)  | 1:209:A:VAL:HG23 | 1:212:A:GLN:HB3  | 6        | 0.64          |
| (1,323)  | 1:209:A:VAL:HG21 | 1:212:A:GLN:HB3  | 13       | 0.64          |
| (1,323)  | 1:209:A:VAL:HG22 | 1:212:A:GLN:HB3  | 13       | 0.64          |
| (1,323)  | 1:209:A:VAL:HG23 | 1:212:A:GLN:HB3  | 13       | 0.64          |
| (1,309)  | 1:186:A:GLN:HE21 | 1:189:A:VAL:HG11 | 17       | 0.64          |
| (1,309)  | 1:186:A:GLN:HE21 | 1:189:A:VAL:HG12 | 17       | 0.64          |
| (1,309)  | 1:186:A:GLN:HE21 | 1:189:A:VAL:HG13 | 17       | 0.64          |
| (1,177)  | 1:195:A:GLY:HA3  | 1:197:A:ASN:HD21 | 12       | 0.64          |
| (1,138)  | 1:125:A:LEU:HA   | 1:125:A:LEU:HD21 | 6        | 0.64          |
| (1,138)  | 1:125:A:LEU:HA   | 1:125:A:LEU:HD22 | 6        | 0.64          |
| (1,138)  | 1:125:A:LEU:HA   | 1:125:A:LEU:HD23 | 6        | 0.64          |
| (1,112)  | 1:214:A:CYS:HA   | 1:215:A:VAL:HG11 | 6        | 0.64          |
| (1,112)  | 1:214:A:CYS:HA   | 1:215:A:VAL:HG12 | 6        | 0.64          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,112)  | 1:214:A:CYS:HA   | 1:215:A:VAL:HG13 | 6        | 0.64          |
| (1,80)   | 1:208:A:ARG:HA   | 1:209:A:VAL:HG11 | 20       | 0.64          |
| (1,80)   | 1:208:A:ARG:HA   | 1:209:A:VAL:HG12 | 20       | 0.64          |
| (1,80)   | 1:208:A:ARG:HA   | 1:209:A:VAL:HG13 | 20       | 0.64          |
| (1,2774) | 1:128:A:TYR:HE1  | 1:162:A:TYR:HB3  | 20       | 0.63          |
| (1,2774) | 1:128:A:TYR:HE2  | 1:162:A:TYR:HB3  | 20       | 0.63          |
| (1,2711) | 1:145:A:TRP:HZ3  | 1:146:A:GLU:HG3  | 7        | 0.63          |
| (1,2711) | 1:145:A:TRP:HZ3  | 1:146:A:GLU:HG3  | 19       | 0.63          |
| (1,2657) | 1:141:A:PHE:HE1  | 1:208:A:ARG:HB3  | 10       | 0.63          |
| (1,2657) | 1:141:A:PHE:HE2  | 1:208:A:ARG:HB3  | 10       | 0.63          |
| (1,2650) | 1:139:A:ILE:HG12 | 1:141:A:PHE:HE1  | 14       | 0.63          |
| (1,2650) | 1:139:A:ILE:HG12 | 1:141:A:PHE:HE2  | 14       | 0.63          |
| (1,2650) | 1:139:A:ILE:HG12 | 1:141:A:PHE:HE1  | 20       | 0.63          |
| (1,2650) | 1:139:A:ILE:HG12 | 1:141:A:PHE:HE2  | 20       | 0.63          |
| (1,2579) | 1:218:A:TYR:HD1  | 1:219:A:GLN:HG3  | 2        | 0.63          |
| (1,2579) | 1:218:A:TYR:HD2  | 1:219:A:GLN:HG3  | 2        | 0.63          |
| (1,2518) | 1:155:A:TYR:HD1  | 1:156:A:ARG:HD2  | 18       | 0.63          |
| (1,2518) | 1:155:A:TYR:HD2  | 1:156:A:ARG:HD2  | 18       | 0.63          |
| (1,2488) | 1:149:A:TYR:HD1  | 1:153:A:ASN:HB3  | 18       | 0.63          |
| (1,2488) | 1:149:A:TYR:HD2  | 1:153:A:ASN:HB3  | 18       | 0.63          |
| (1,2474) | 1:168:A:GLN:HG2  | 1:169:A:TYR:HD1  | 4        | 0.63          |
| (1,2474) | 1:168:A:GLN:HG2  | 1:169:A:TYR:HD2  | 4        | 0.63          |
| (1,2445) | 1:122:A:VAL:HG21 | 1:124:A:GLY:H    | 19       | 0.63          |
| (1,2445) | 1:122:A:VAL:HG22 | 1:124:A:GLY:H    | 19       | 0.63          |
| (1,2445) | 1:122:A:VAL:HG23 | 1:124:A:GLY:H    | 19       | 0.63          |
| (1,2414) | 1:136:A:ARG:HB3  | 1:159:A:ASN:HD21 | 16       | 0.63          |
| (1,1894) | 1:215:A:VAL:HG21 | 1:219:A:GLN:H    | 4        | 0.63          |
| (1,1894) | 1:215:A:VAL:HG22 | 1:219:A:GLN:H    | 4        | 0.63          |
| (1,1894) | 1:215:A:VAL:HG23 | 1:219:A:GLN:H    | 4        | 0.63          |
| (1,1894) | 1:215:A:VAL:HG21 | 1:219:A:GLN:H    | 14       | 0.63          |
| (1,1894) | 1:215:A:VAL:HG22 | 1:219:A:GLN:H    | 14       | 0.63          |
| (1,1894) | 1:215:A:VAL:HG23 | 1:219:A:GLN:H    | 14       | 0.63          |
| (1,1893) | 1:208:A:ARG:HB3  | 1:209:A:VAL:H    | 6        | 0.63          |
| (1,1701) | 1:129:A:MET:H    | 1:129:A:MET:HG3  | 19       | 0.63          |
| (1,1538) | 1:164:A:ARG:HD2  | 1:165:A:PRO:HD3  | 18       | 0.63          |
| (1,1523) | 1:162:A:TYR:HB3  | 1:182:A:ILE:HG12 | 6        | 0.63          |
| (1,1523) | 1:162:A:TYR:HB3  | 1:182:A:ILE:HG13 | 6        | 0.63          |
| (1,1227) | 1:210:A:VAL:HA   | 1:213:A:MET:HG2  | 1        | 0.63          |
| (1,1131) | 1:223:A:GLN:HG2  | 1:226:A:TYR:H    | 2        | 0.63          |
| (1,1097) | 1:165:A:PRO:HB3  | 1:168:A:GLN:HG2  | 9        | 0.63          |
| (1,1097) | 1:165:A:PRO:HB3  | 1:168:A:GLN:HG2  | 15       | 0.63          |
| (1,1060) | 1:207:A:GLU:HG3  | 1:208:A:ARG:H    | 16       | 0.63          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,657)  | 1:213:A:MET:HB3  | 1:213:A:MET:HE1  | 17       | 0.63          |
| (1,657)  | 1:213:A:MET:HB3  | 1:213:A:MET:HE2  | 17       | 0.63          |
| (1,657)  | 1:213:A:MET:HB3  | 1:213:A:MET:HE3  | 17       | 0.63          |
| (1,502)  | 1:162:A:TYR:HB3  | 1:183:A:THR:HA   | 18       | 0.63          |
| (1,476)  | 1:203:A:VAL:HG21 | 1:204:A:LYS:HE2  | 12       | 0.63          |
| (1,476)  | 1:203:A:VAL:HG21 | 1:204:A:LYS:HE3  | 12       | 0.63          |
| (1,476)  | 1:203:A:VAL:HG22 | 1:204:A:LYS:HE2  | 12       | 0.63          |
| (1,476)  | 1:203:A:VAL:HG22 | 1:204:A:LYS:HE3  | 12       | 0.63          |
| (1,476)  | 1:203:A:VAL:HG23 | 1:204:A:LYS:HE2  | 12       | 0.63          |
| (1,476)  | 1:203:A:VAL:HG23 | 1:204:A:LYS:HE3  | 12       | 0.63          |
| (1,436)  | 1:229:A:ARG:HA   | 1:230:A:ARG:HD3  | 4        | 0.63          |
| (1,322)  | 1:158:A:PRO:HD3  | 1:209:A:VAL:HG21 | 10       | 0.63          |
| (1,322)  | 1:158:A:PRO:HD3  | 1:209:A:VAL:HG22 | 10       | 0.63          |
| (1,322)  | 1:158:A:PRO:HD3  | 1:209:A:VAL:HG23 | 10       | 0.63          |
| (1,246)  | 1:176:A:VAL:HG21 | 1:215:A:VAL:HA   | 12       | 0.63          |
| (1,246)  | 1:176:A:VAL:HG22 | 1:215:A:VAL:HA   | 12       | 0.63          |
| (1,246)  | 1:176:A:VAL:HG23 | 1:215:A:VAL:HA   | 12       | 0.63          |
| (1,216)  | 1:216:A:THR:HG21 | 1:220:A:LYS:HG3  | 1        | 0.63          |
| (1,216)  | 1:216:A:THR:HG22 | 1:220:A:LYS:HG3  | 1        | 0.63          |
| (1,216)  | 1:216:A:THR:HG23 | 1:220:A:LYS:HG3  | 1        | 0.63          |
| (1,105)  | 1:212:A:GLN:HA   | 1:215:A:VAL:HG11 | 6        | 0.63          |
| (1,105)  | 1:212:A:GLN:HA   | 1:215:A:VAL:HG12 | 6        | 0.63          |
| (1,105)  | 1:212:A:GLN:HA   | 1:215:A:VAL:HG13 | 6        | 0.63          |
| (1,101)  | 1:138:A:MET:HA   | 1:209:A:VAL:HG11 | 4        | 0.63          |
| (1,101)  | 1:138:A:MET:HA   | 1:209:A:VAL:HG12 | 4        | 0.63          |
| (1,101)  | 1:138:A:MET:HA   | 1:209:A:VAL:HG13 | 4        | 0.63          |
| (1,80)   | 1:208:A:ARG:HA   | 1:209:A:VAL:HG11 | 2        | 0.63          |
| (1,80)   | 1:208:A:ARG:HA   | 1:209:A:VAL:HG12 | 2        | 0.63          |
| (1,80)   | 1:208:A:ARG:HA   | 1:209:A:VAL:HG13 | 2        | 0.63          |
| (1,80)   | 1:208:A:ARG:HA   | 1:209:A:VAL:HG11 | 12       | 0.63          |
| (1,80)   | 1:208:A:ARG:HA   | 1:209:A:VAL:HG12 | 12       | 0.63          |
| (1,80)   | 1:208:A:ARG:HA   | 1:209:A:VAL:HG13 | 12       | 0.63          |
| (1,80)   | 1:208:A:ARG:HA   | 1:209:A:VAL:HG11 | 13       | 0.63          |
| (1,80)   | 1:208:A:ARG:HA   | 1:209:A:VAL:HG12 | 13       | 0.63          |
| (1,80)   | 1:208:A:ARG:HA   | 1:209:A:VAL:HG13 | 13       | 0.63          |
| (1,2846) | 1:157:A:TYR:HE1  | 1:206:A:MET:HB2  | 20       | 0.62          |
| (1,2846) | 1:157:A:TYR:HE2  | 1:206:A:MET:HB2  | 20       | 0.62          |
| (1,2830) | 1:172:A:GLN:HG2  | 1:218:A:TYR:HE1  | 6        | 0.62          |
| (1,2830) | 1:172:A:GLN:HG2  | 1:218:A:TYR:HE2  | 6        | 0.62          |
| (1,2824) | 1:218:A:TYR:HE1  | 1:222:A:SER:HB3  | 16       | 0.62          |
| (1,2824) | 1:218:A:TYR:HE2  | 1:222:A:SER:HB3  | 16       | 0.62          |
| (1,2794) | 1:128:A:TYR:HE1  | 1:164:A:ARG:HG2  | 15       | 0.62          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2794) | 1:128:A:TYR:HE2  | 1:164:A:ARG:HG2  | 15       | 0.62          |
| (1,2771) | 1:130:A:LEU:HB3  | 1:162:A:TYR:HE1  | 12       | 0.62          |
| (1,2771) | 1:130:A:LEU:HB3  | 1:162:A:TYR:HE2  | 12       | 0.62          |
| (1,2756) | 1:150:A:TYR:HE1  | 1:205:A:MET:HG2  | 19       | 0.62          |
| (1,2756) | 1:150:A:TYR:HE2  | 1:205:A:MET:HG2  | 19       | 0.62          |
| (1,2736) | 1:184:A:ILE:HG13 | 1:187:A:HIS:HD2  | 19       | 0.62          |
| (1,2501) | 1:149:A:TYR:HD1  | 1:205:A:MET:HG2  | 10       | 0.62          |
| (1,2501) | 1:149:A:TYR:HD2  | 1:205:A:MET:HG2  | 10       | 0.62          |
| (1,2492) | 1:139:A:ILE:HG12 | 1:150:A:TYR:HD1  | 6        | 0.62          |
| (1,2492) | 1:139:A:ILE:HG12 | 1:150:A:TYR:HD2  | 6        | 0.62          |
| (1,2445) | 1:122:A:VAL:HG21 | 1:124:A:GLY:H    | 1        | 0.62          |
| (1,2445) | 1:122:A:VAL:HG22 | 1:124:A:GLY:H    | 1        | 0.62          |
| (1,2445) | 1:122:A:VAL:HG23 | 1:124:A:GLY:H    | 1        | 0.62          |
| (1,2313) | 1:159:A:ASN:HD22 | 1:160:A:GLN:HE21 | 5        | 0.62          |
| (1,2045) | 1:230:A:ARG:HG3  | 1:231:A:SER:H    | 2        | 0.62          |
| (1,1914) | 1:209:A:VAL:HG21 | 1:213:A:MET:H    | 12       | 0.62          |
| (1,1914) | 1:209:A:VAL:HG22 | 1:213:A:MET:H    | 12       | 0.62          |
| (1,1914) | 1:209:A:VAL:HG23 | 1:213:A:MET:H    | 12       | 0.62          |
| (1,1701) | 1:129:A:MET:H    | 1:129:A:MET:HG3  | 14       | 0.62          |
| (1,1579) | 1:132:A:SER:HB3  | 1:133:A:ALA:H    | 10       | 0.62          |
| (1,1579) | 1:132:A:SER:HB3  | 1:133:A:ALA:H    | 16       | 0.62          |
| (1,1480) | 1:203:A:VAL:HG21 | 1:207:A:GLU:HB2  | 5        | 0.62          |
| (1,1480) | 1:203:A:VAL:HG22 | 1:207:A:GLU:HB2  | 5        | 0.62          |
| (1,1480) | 1:203:A:VAL:HG23 | 1:207:A:GLU:HB2  | 5        | 0.62          |
| (1,1375) | 1:136:A:ARG:HD2  | 1:154:A:MET:HG3  | 4        | 0.62          |
| (1,1235) | 1:205:A:MET:HG3  | 1:206:A:MET:HG2  | 4        | 0.62          |
| (1,1131) | 1:223:A:GLN:HG2  | 1:226:A:TYR:H    | 1        | 0.62          |
| (1,1104) | 1:213:A:MET:HB3  | 1:214:A:CYS:HA   | 19       | 0.62          |
| (1,1095) | 1:165:A:PRO:HA   | 1:168:A:GLN:HG2  | 5        | 0.62          |
| (1,1060) | 1:207:A:GLU:HG3  | 1:208:A:ARG:H    | 17       | 0.62          |
| (1,996)  | 1:176:A:VAL:HA   | 1:211:A:GLU:HG3  | 8        | 0.62          |
| (1,945)  | 1:172:A:GLN:HA   | 1:176:A:VAL:HG21 | 12       | 0.62          |
| (1,945)  | 1:172:A:GLN:HA   | 1:176:A:VAL:HG22 | 12       | 0.62          |
| (1,945)  | 1:172:A:GLN:HA   | 1:176:A:VAL:HG23 | 12       | 0.62          |
| (1,862)  | 1:143:A:ASN:HD22 | 1:146:A:GLU:HG2  | 3        | 0.62          |
| (1,811)  | 1:175:A:PHE:HB2  | 1:176:A:VAL:HG21 | 12       | 0.62          |
| (1,811)  | 1:175:A:PHE:HB2  | 1:176:A:VAL:HG22 | 12       | 0.62          |
| (1,811)  | 1:175:A:PHE:HB2  | 1:176:A:VAL:HG23 | 12       | 0.62          |
| (1,752)  | 1:138:A:MET:HE1  | 1:139:A:ILE:HG12 | 16       | 0.62          |
| (1,752)  | 1:138:A:MET:HE2  | 1:139:A:ILE:HG12 | 16       | 0.62          |
| (1,752)  | 1:138:A:MET:HE3  | 1:139:A:ILE:HG12 | 16       | 0.62          |
| (1,528)  | 1:143:A:ASN:HB2  | 1:147:A:ASP:HB3  | 2        | 0.62          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,528)  | 1:143:A:ASN:HB3  | 1:147:A:ASP:HB3  | 2        | 0.62          |
| (1,339)  | 1:209:A:VAL:HG21 | 1:210:A:VAL:HG21 | 10       | 0.62          |
| (1,339)  | 1:209:A:VAL:HG21 | 1:210:A:VAL:HG22 | 10       | 0.62          |
| (1,339)  | 1:209:A:VAL:HG21 | 1:210:A:VAL:HG23 | 10       | 0.62          |
| (1,339)  | 1:209:A:VAL:HG22 | 1:210:A:VAL:HG21 | 10       | 0.62          |
| (1,339)  | 1:209:A:VAL:HG22 | 1:210:A:VAL:HG22 | 10       | 0.62          |
| (1,339)  | 1:209:A:VAL:HG22 | 1:210:A:VAL:HG23 | 10       | 0.62          |
| (1,339)  | 1:209:A:VAL:HG23 | 1:210:A:VAL:HG21 | 10       | 0.62          |
| (1,339)  | 1:209:A:VAL:HG23 | 1:210:A:VAL:HG22 | 10       | 0.62          |
| (1,339)  | 1:209:A:VAL:HG23 | 1:210:A:VAL:HG23 | 10       | 0.62          |
| (1,323)  | 1:209:A:VAL:HG21 | 1:212:A:GLN:HB3  | 7        | 0.62          |
| (1,323)  | 1:209:A:VAL:HG22 | 1:212:A:GLN:HB3  | 7        | 0.62          |
| (1,323)  | 1:209:A:VAL:HG23 | 1:212:A:GLN:HB3  | 7        | 0.62          |
| (1,314)  | 1:166:A:VAL:HG21 | 1:169:A:TYR:HB3  | 12       | 0.62          |
| (1,314)  | 1:166:A:VAL:HG22 | 1:169:A:TYR:HB3  | 12       | 0.62          |
| (1,314)  | 1:166:A:VAL:HG23 | 1:169:A:TYR:HB3  | 12       | 0.62          |
| (1,224)  | 1:127:A:GLY:HA3  | 1:128:A:TYR:HB2  | 7        | 0.62          |
| (1,105)  | 1:212:A:GLN:HA   | 1:215:A:VAL:HG11 | 14       | 0.62          |
| (1,105)  | 1:212:A:GLN:HA   | 1:215:A:VAL:HG12 | 14       | 0.62          |
| (1,105)  | 1:212:A:GLN:HA   | 1:215:A:VAL:HG13 | 14       | 0.62          |
| (1,80)   | 1:208:A:ARG:HA   | 1:209:A:VAL:HG11 | 11       | 0.62          |
| (1,80)   | 1:208:A:ARG:HA   | 1:209:A:VAL:HG12 | 11       | 0.62          |
| (1,80)   | 1:208:A:ARG:HA   | 1:209:A:VAL:HG13 | 11       | 0.62          |
| (1,80)   | 1:208:A:ARG:HA   | 1:209:A:VAL:HG11 | 14       | 0.62          |
| (1,80)   | 1:208:A:ARG:HA   | 1:209:A:VAL:HG12 | 14       | 0.62          |
| (1,80)   | 1:208:A:ARG:HA   | 1:209:A:VAL:HG13 | 14       | 0.62          |
| (1,79)   | 1:138:A:MET:H    | 1:209:A:VAL:HG11 | 8        | 0.62          |
| (1,79)   | 1:138:A:MET:H    | 1:209:A:VAL:HG12 | 8        | 0.62          |
| (1,79)   | 1:138:A:MET:H    | 1:209:A:VAL:HG13 | 8        | 0.62          |
| (1,2774) | 1:128:A:TYR:HE1  | 1:162:A:TYR:HB3  | 17       | 0.61          |
| (1,2774) | 1:128:A:TYR:HE2  | 1:162:A:TYR:HB3  | 17       | 0.61          |
| (1,2758) | 1:150:A:TYR:HE1  | 1:209:A:VAL:HG11 | 17       | 0.61          |
| (1,2758) | 1:150:A:TYR:HE1  | 1:209:A:VAL:HG12 | 17       | 0.61          |
| (1,2758) | 1:150:A:TYR:HE1  | 1:209:A:VAL:HG13 | 17       | 0.61          |
| (1,2758) | 1:150:A:TYR:HE2  | 1:209:A:VAL:HG11 | 17       | 0.61          |
| (1,2758) | 1:150:A:TYR:HE2  | 1:209:A:VAL:HG12 | 17       | 0.61          |
| (1,2758) | 1:150:A:TYR:HE2  | 1:209:A:VAL:HG13 | 17       | 0.61          |
| (1,2756) | 1:150:A:TYR:HE1  | 1:205:A:MET:HG2  | 11       | 0.61          |
| (1,2756) | 1:150:A:TYR:HE2  | 1:205:A:MET:HG2  | 11       | 0.61          |
| (1,2736) | 1:184:A:ILE:HG13 | 1:187:A:HIS:HD2  | 15       | 0.61          |
| (1,2721) | 1:177:A:HIS:HD2  | 1:178:A:ASP:HB3  | 9        | 0.61          |
| (1,2488) | 1:149:A:TYR:HD1  | 1:153:A:ASN:HB3  | 20       | 0.61          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2488) | 1:149:A:TYR:HD2  | 1:153:A:ASN:HB3  | 20       | 0.61          |
| (1,2320) | 1:160:A:GLN:HE22 | 1:213:A:MET:HB2  | 4        | 0.61          |
| (1,1480) | 1:203:A:VAL:HG21 | 1:207:A:GLU:HB2  | 7        | 0.61          |
| (1,1480) | 1:203:A:VAL:HG22 | 1:207:A:GLU:HB2  | 7        | 0.61          |
| (1,1480) | 1:203:A:VAL:HG23 | 1:207:A:GLU:HB2  | 7        | 0.61          |
| (1,1303) | 1:137:A:PRO:HB2  | 1:213:A:MET:HG2  | 20       | 0.61          |
| (1,1235) | 1:205:A:MET:HG3  | 1:206:A:MET:HG2  | 8        | 0.61          |
| (1,1104) | 1:213:A:MET:HB3  | 1:214:A:CYS:HA   | 5        | 0.61          |
| (1,1015) | 1:152:A:GLU:HG2  | 1:153:A:ASN:HD22 | 14       | 0.61          |
| (1,907)  | 1:226:A:TYR:HA   | 1:229:A:ARG:HB2  | 4        | 0.61          |
| (1,733)  | 1:222:A:SER:HB2  | 1:226:A:TYR:HD1  | 8        | 0.61          |
| (1,733)  | 1:222:A:SER:HB2  | 1:226:A:TYR:HD2  | 8        | 0.61          |
| (1,657)  | 1:213:A:MET:HB3  | 1:213:A:MET:HE1  | 2        | 0.61          |
| (1,657)  | 1:213:A:MET:HB3  | 1:213:A:MET:HE2  | 2        | 0.61          |
| (1,657)  | 1:213:A:MET:HB3  | 1:213:A:MET:HE3  | 2        | 0.61          |
| (1,637)  | 1:147:A:ASP:HB2  | 1:148:A:ARG:HG2  | 11       | 0.61          |
| (1,502)  | 1:162:A:TYR:HB3  | 1:183:A:THR:HA   | 1        | 0.61          |
| (1,339)  | 1:209:A:VAL:HG21 | 1:210:A:VAL:HG21 | 14       | 0.61          |
| (1,339)  | 1:209:A:VAL:HG21 | 1:210:A:VAL:HG22 | 14       | 0.61          |
| (1,339)  | 1:209:A:VAL:HG21 | 1:210:A:VAL:HG23 | 14       | 0.61          |
| (1,339)  | 1:209:A:VAL:HG22 | 1:210:A:VAL:HG21 | 14       | 0.61          |
| (1,339)  | 1:209:A:VAL:HG22 | 1:210:A:VAL:HG22 | 14       | 0.61          |
| (1,339)  | 1:209:A:VAL:HG22 | 1:210:A:VAL:HG23 | 14       | 0.61          |
| (1,339)  | 1:209:A:VAL:HG23 | 1:210:A:VAL:HG21 | 14       | 0.61          |
| (1,339)  | 1:209:A:VAL:HG23 | 1:210:A:VAL:HG22 | 14       | 0.61          |
| (1,339)  | 1:209:A:VAL:HG23 | 1:210:A:VAL:HG23 | 14       | 0.61          |
| (1,309)  | 1:186:A:GLN:HE21 | 1:189:A:VAL:HG11 | 4        | 0.61          |
| (1,309)  | 1:186:A:GLN:HE21 | 1:189:A:VAL:HG12 | 4        | 0.61          |
| (1,309)  | 1:186:A:GLN:HE21 | 1:189:A:VAL:HG13 | 4        | 0.61          |
| (1,166)  | 1:203:A:VAL:HG11 | 1:206:A:MET:HG2  | 2        | 0.61          |
| (1,166)  | 1:203:A:VAL:HG12 | 1:206:A:MET:HG2  | 2        | 0.61          |
| (1,166)  | 1:203:A:VAL:HG13 | 1:206:A:MET:HG2  | 2        | 0.61          |
| (1,155)  | 1:125:A:LEU:HB3  | 1:126:A:GLY:HA3  | 14       | 0.61          |
| (1,112)  | 1:214:A:CYS:HA   | 1:215:A:VAL:HG11 | 12       | 0.61          |
| (1,112)  | 1:214:A:CYS:HA   | 1:215:A:VAL:HG12 | 12       | 0.61          |
| (1,112)  | 1:214:A:CYS:HA   | 1:215:A:VAL:HG13 | 12       | 0.61          |
| (1,112)  | 1:214:A:CYS:HA   | 1:215:A:VAL:HG11 | 13       | 0.61          |
| (1,112)  | 1:214:A:CYS:HA   | 1:215:A:VAL:HG12 | 13       | 0.61          |
| (1,112)  | 1:214:A:CYS:HA   | 1:215:A:VAL:HG13 | 13       | 0.61          |
| (1,2851) | 1:184:A:ILE:HG13 | 1:187:A:HIS:HE1  | 16       | 0.6           |
| (1,2830) | 1:172:A:GLN:HG2  | 1:218:A:TYR:HE1  | 12       | 0.6           |
| (1,2830) | 1:172:A:GLN:HG2  | 1:218:A:TYR:HE2  | 12       | 0.6           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2650) | 1:139:A:ILE:HG12 | 1:141:A:PHE:HE1  | 2        | 0.6           |
| (1,2650) | 1:139:A:ILE:HG12 | 1:141:A:PHE:HE2  | 2        | 0.6           |
| (1,2623) | 1:156:A:ARG:HH21 | 1:198:A:PHE:HD1  | 4        | 0.6           |
| (1,2623) | 1:156:A:ARG:HH21 | 1:198:A:PHE:HD2  | 4        | 0.6           |
| (1,2407) | 1:136:A:ARG:HE   | 1:159:A:ASN:HB3  | 12       | 0.6           |
| (1,1937) | 1:220:A:LYS:H    | 1:221:A:GLU:HG3  | 4        | 0.6           |
| (1,1584) | 1:122:A:VAL:H    | 1:122:A:VAL:HG11 | 4        | 0.6           |
| (1,1584) | 1:122:A:VAL:H    | 1:122:A:VAL:HG12 | 4        | 0.6           |
| (1,1584) | 1:122:A:VAL:H    | 1:122:A:VAL:HG13 | 4        | 0.6           |
| (1,1523) | 1:162:A:TYR:HB3  | 1:182:A:ILE:HG12 | 3        | 0.6           |
| (1,1523) | 1:162:A:TYR:HB3  | 1:182:A:ILE:HG13 | 3        | 0.6           |
| (1,1303) | 1:137:A:PRO:HB2  | 1:213:A:MET:HG2  | 12       | 0.6           |
| (1,1294) | 1:138:A:MET:HG3  | 1:139:A:ILE:H    | 19       | 0.6           |
| (1,1207) | 1:168:A:GLN:HA   | 1:168:A:GLN:HE22 | 7        | 0.6           |
| (1,1207) | 1:168:A:GLN:HA   | 1:168:A:GLN:HE22 | 9        | 0.6           |
| (1,1104) | 1:213:A:MET:HB3  | 1:214:A:CYS:HA   | 17       | 0.6           |
| (1,1015) | 1:152:A:GLU:HG2  | 1:153:A:ASN:HD22 | 11       | 0.6           |
| (1,957)  | 1:184:A:ILE:HD11 | 1:207:A:GLU:HG3  | 2        | 0.6           |
| (1,957)  | 1:184:A:ILE:HD12 | 1:207:A:GLU:HG3  | 2        | 0.6           |
| (1,957)  | 1:184:A:ILE:HD13 | 1:207:A:GLU:HG3  | 2        | 0.6           |
| (1,921)  | 1:167:A:SER:HA   | 1:168:A:GLN:HG3  | 5        | 0.6           |
| (1,881)  | 1:145:A:TRP:HE3  | 1:146:A:GLU:HG3  | 1        | 0.6           |
| (1,758)  | 1:138:A:MET:HG3  | 1:138:A:MET:HE1  | 12       | 0.6           |
| (1,758)  | 1:138:A:MET:HG3  | 1:138:A:MET:HE2  | 12       | 0.6           |
| (1,758)  | 1:138:A:MET:HG3  | 1:138:A:MET:HE3  | 12       | 0.6           |
| (1,733)  | 1:222:A:SER:HB2  | 1:226:A:TYR:HD1  | 12       | 0.6           |
| (1,733)  | 1:222:A:SER:HB2  | 1:226:A:TYR:HD2  | 12       | 0.6           |
| (1,657)  | 1:213:A:MET:HB3  | 1:213:A:MET:HE1  | 6        | 0.6           |
| (1,657)  | 1:213:A:MET:HB3  | 1:213:A:MET:HE2  | 6        | 0.6           |
| (1,657)  | 1:213:A:MET:HB3  | 1:213:A:MET:HE3  | 6        | 0.6           |
| (1,634)  | 1:192:A:THR:HA   | 1:195:A:GLY:HA3  | 14       | 0.6           |
| (1,630)  | 1:165:A:PRO:HA   | 1:166:A:VAL:HG11 | 3        | 0.6           |
| (1,630)  | 1:165:A:PRO:HA   | 1:166:A:VAL:HG12 | 3        | 0.6           |
| (1,630)  | 1:165:A:PRO:HA   | 1:166:A:VAL:HG13 | 3        | 0.6           |
| (1,506)  | 1:179:A:CYS:HB2  | 1:214:A:CYS:HB2  | 10       | 0.6           |
| (1,359)  | 1:122:A:VAL:HG21 | 1:182:A:ILE:HG21 | 4        | 0.6           |
| (1,359)  | 1:122:A:VAL:HG21 | 1:182:A:ILE:HG22 | 4        | 0.6           |
| (1,359)  | 1:122:A:VAL:HG21 | 1:182:A:ILE:HG23 | 4        | 0.6           |
| (1,359)  | 1:122:A:VAL:HG22 | 1:182:A:ILE:HG21 | 4        | 0.6           |
| (1,359)  | 1:122:A:VAL:HG22 | 1:182:A:ILE:HG22 | 4        | 0.6           |
| (1,359)  | 1:122:A:VAL:HG22 | 1:182:A:ILE:HG23 | 4        | 0.6           |
| (1,359)  | 1:122:A:VAL:HG23 | 1:182:A:ILE:HG21 | 4        | 0.6           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,359)  | 1:122:A:VAL:HG23 | 1:182:A:ILE:HG22 | 4        | 0.6           |
| (1,359)  | 1:122:A:VAL:HG23 | 1:182:A:ILE:HG23 | 4        | 0.6           |
| (1,359)  | 1:122:A:VAL:HG21 | 1:182:A:ILE:HG21 | 12       | 0.6           |
| (1,359)  | 1:122:A:VAL:HG21 | 1:182:A:ILE:HG22 | 12       | 0.6           |
| (1,359)  | 1:122:A:VAL:HG21 | 1:182:A:ILE:HG23 | 12       | 0.6           |
| (1,359)  | 1:122:A:VAL:HG22 | 1:182:A:ILE:HG21 | 12       | 0.6           |
| (1,359)  | 1:122:A:VAL:HG22 | 1:182:A:ILE:HG22 | 12       | 0.6           |
| (1,359)  | 1:122:A:VAL:HG22 | 1:182:A:ILE:HG23 | 12       | 0.6           |
| (1,359)  | 1:122:A:VAL:HG23 | 1:182:A:ILE:HG21 | 12       | 0.6           |
| (1,359)  | 1:122:A:VAL:HG23 | 1:182:A:ILE:HG22 | 12       | 0.6           |
| (1,359)  | 1:122:A:VAL:HG23 | 1:182:A:ILE:HG23 | 12       | 0.6           |
| (1,359)  | 1:122:A:VAL:HG21 | 1:182:A:ILE:HG21 | 19       | 0.6           |
| (1,359)  | 1:122:A:VAL:HG21 | 1:182:A:ILE:HG22 | 19       | 0.6           |
| (1,359)  | 1:122:A:VAL:HG21 | 1:182:A:ILE:HG23 | 19       | 0.6           |
| (1,359)  | 1:122:A:VAL:HG22 | 1:182:A:ILE:HG21 | 19       | 0.6           |
| (1,359)  | 1:122:A:VAL:HG22 | 1:182:A:ILE:HG22 | 19       | 0.6           |
| (1,359)  | 1:122:A:VAL:HG22 | 1:182:A:ILE:HG23 | 19       | 0.6           |
| (1,359)  | 1:122:A:VAL:HG23 | 1:182:A:ILE:HG21 | 19       | 0.6           |
| (1,359)  | 1:122:A:VAL:HG23 | 1:182:A:ILE:HG22 | 19       | 0.6           |
| (1,359)  | 1:122:A:VAL:HG23 | 1:182:A:ILE:HG23 | 19       | 0.6           |
| (1,323)  | 1:209:A:VAL:HG21 | 1:212:A:GLN:HB3  | 19       | 0.6           |
| (1,323)  | 1:209:A:VAL:HG22 | 1:212:A:GLN:HB3  | 19       | 0.6           |
| (1,323)  | 1:209:A:VAL:HG23 | 1:212:A:GLN:HB3  | 19       | 0.6           |
| (1,220)  | 1:127:A:GLY:HA2  | 1:164:A:ARG:HE   | 6        | 0.6           |
| (1,112)  | 1:214:A:CYS:HA   | 1:215:A:VAL:HG11 | 17       | 0.6           |
| (1,112)  | 1:214:A:CYS:HA   | 1:215:A:VAL:HG12 | 17       | 0.6           |
| (1,112)  | 1:214:A:CYS:HA   | 1:215:A:VAL:HG13 | 17       | 0.6           |
| (1,112)  | 1:214:A:CYS:HA   | 1:215:A:VAL:HG11 | 19       | 0.6           |
| (1,112)  | 1:214:A:CYS:HA   | 1:215:A:VAL:HG12 | 19       | 0.6           |
| (1,112)  | 1:214:A:CYS:HA   | 1:215:A:VAL:HG13 | 19       | 0.6           |
| (1,105)  | 1:212:A:GLN:HA   | 1:215:A:VAL:HG11 | 17       | 0.6           |
| (1,105)  | 1:212:A:GLN:HA   | 1:215:A:VAL:HG12 | 17       | 0.6           |
| (1,105)  | 1:212:A:GLN:HA   | 1:215:A:VAL:HG13 | 17       | 0.6           |
| (1,2791) | 1:126:A:GLY:HA2  | 1:128:A:TYR:HE1  | 3        | 0.59          |
| (1,2791) | 1:126:A:GLY:HA2  | 1:128:A:TYR:HE2  | 3        | 0.59          |
| (1,2774) | 1:128:A:TYR:HE1  | 1:162:A:TYR:HB3  | 16       | 0.59          |
| (1,2774) | 1:128:A:TYR:HE2  | 1:162:A:TYR:HB3  | 16       | 0.59          |
| (1,2736) | 1:184:A:ILE:HG13 | 1:187:A:HIS:HD2  | 17       | 0.59          |
| (1,2735) | 1:186:A:GLN:HB3  | 1:187:A:HIS:HD2  | 11       | 0.59          |
| (1,2548) | 1:162:A:TYR:HD1  | 1:186:A:GLN:HB3  | 17       | 0.59          |
| (1,2548) | 1:162:A:TYR:HD2  | 1:186:A:GLN:HB3  | 17       | 0.59          |
| (1,2501) | 1:149:A:TYR:HD1  | 1:205:A:MET:HG2  | 4        | 0.59          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2501) | 1:149:A:TYR:HD2  | 1:205:A:MET:HG2  | 4        | 0.59          |
| (1,2501) | 1:149:A:TYR:HD1  | 1:205:A:MET:HG2  | 11       | 0.59          |
| (1,2501) | 1:149:A:TYR:HD2  | 1:205:A:MET:HG2  | 11       | 0.59          |
| (1,2492) | 1:139:A:ILE:HG12 | 1:150:A:TYR:HD1  | 9        | 0.59          |
| (1,2492) | 1:139:A:ILE:HG12 | 1:150:A:TYR:HD2  | 9        | 0.59          |
| (1,2469) | 1:166:A:VAL:HG21 | 1:169:A:TYR:HD1  | 17       | 0.59          |
| (1,2469) | 1:166:A:VAL:HG21 | 1:169:A:TYR:HD2  | 17       | 0.59          |
| (1,2469) | 1:166:A:VAL:HG22 | 1:169:A:TYR:HD1  | 17       | 0.59          |
| (1,2469) | 1:166:A:VAL:HG22 | 1:169:A:TYR:HD2  | 17       | 0.59          |
| (1,2469) | 1:166:A:VAL:HG23 | 1:169:A:TYR:HD1  | 17       | 0.59          |
| (1,2469) | 1:166:A:VAL:HG23 | 1:169:A:TYR:HD2  | 17       | 0.59          |
| (1,1894) | 1:215:A:VAL:HG21 | 1:219:A:GLN:H    | 17       | 0.59          |
| (1,1894) | 1:215:A:VAL:HG22 | 1:219:A:GLN:H    | 17       | 0.59          |
| (1,1894) | 1:215:A:VAL:HG23 | 1:219:A:GLN:H    | 17       | 0.59          |
| (1,1861) | 1:147:A:ASP:HB2  | 1:148:A:ARG:H    | 3        | 0.59          |
| (1,1701) | 1:129:A:MET:H    | 1:129:A:MET:HG3  | 20       | 0.59          |
| (1,1584) | 1:122:A:VAL:H    | 1:122:A:VAL:HG11 | 16       | 0.59          |
| (1,1584) | 1:122:A:VAL:H    | 1:122:A:VAL:HG12 | 16       | 0.59          |
| (1,1584) | 1:122:A:VAL:H    | 1:122:A:VAL:HG13 | 16       | 0.59          |
| (1,1575) | 1:136:A:ARG:H    | 1:136:A:ARG:HD3  | 5        | 0.59          |
| (1,1523) | 1:162:A:TYR:HB3  | 1:182:A:ILE:HG12 | 17       | 0.59          |
| (1,1523) | 1:162:A:TYR:HB3  | 1:182:A:ILE:HG13 | 17       | 0.59          |
| (1,1294) | 1:138:A:MET:HG3  | 1:139:A:ILE:H    | 9        | 0.59          |
| (1,1256) | 1:184:A:ILE:HG13 | 1:206:A:MET:HG3  | 8        | 0.59          |
| (1,1235) | 1:205:A:MET:HG3  | 1:206:A:MET:HG2  | 18       | 0.59          |
| (1,1104) | 1:213:A:MET:HB3  | 1:214:A:CYS:HA   | 16       | 0.59          |
| (1,1104) | 1:213:A:MET:HB3  | 1:214:A:CYS:HA   | 20       | 0.59          |
| (1,1095) | 1:165:A:PRO:HA   | 1:168:A:GLN:HG2  | 16       | 0.59          |
| (1,901)  | 1:203:A:VAL:HG21 | 1:204:A:LYS:HA   | 12       | 0.59          |
| (1,901)  | 1:203:A:VAL:HG22 | 1:204:A:LYS:HA   | 12       | 0.59          |
| (1,901)  | 1:203:A:VAL:HG23 | 1:204:A:LYS:HA   | 12       | 0.59          |
| (1,758)  | 1:138:A:MET:HG3  | 1:138:A:MET:HE1  | 8        | 0.59          |
| (1,758)  | 1:138:A:MET:HG3  | 1:138:A:MET:HE2  | 8        | 0.59          |
| (1,758)  | 1:138:A:MET:HG3  | 1:138:A:MET:HE3  | 8        | 0.59          |
| (1,758)  | 1:138:A:MET:HG3  | 1:138:A:MET:HE1  | 18       | 0.59          |
| (1,758)  | 1:138:A:MET:HG3  | 1:138:A:MET:HE2  | 18       | 0.59          |
| (1,758)  | 1:138:A:MET:HG3  | 1:138:A:MET:HE3  | 18       | 0.59          |
| (1,758)  | 1:138:A:MET:HG3  | 1:138:A:MET:HE1  | 19       | 0.59          |
| (1,758)  | 1:138:A:MET:HG3  | 1:138:A:MET:HE2  | 19       | 0.59          |
| (1,758)  | 1:138:A:MET:HG3  | 1:138:A:MET:HE3  | 19       | 0.59          |
| (1,752)  | 1:138:A:MET:HE1  | 1:139:A:ILE:HG12 | 20       | 0.59          |
| (1,752)  | 1:138:A:MET:HE2  | 1:139:A:ILE:HG12 | 20       | 0.59          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,752)  | 1:138:A:MET:HE3  | 1:139:A:ILE:HG12 | 20       | 0.59          |
| (1,733)  | 1:222:A:SER:HB2  | 1:226:A:TYR:HD1  | 7        | 0.59          |
| (1,733)  | 1:222:A:SER:HB2  | 1:226:A:TYR:HD2  | 7        | 0.59          |
| (1,565)  | 1:129:A:MET:HE1  | 1:132:A:SER:HB2  | 16       | 0.59          |
| (1,565)  | 1:129:A:MET:HE2  | 1:132:A:SER:HB2  | 16       | 0.59          |
| (1,565)  | 1:129:A:MET:HE3  | 1:132:A:SER:HB2  | 16       | 0.59          |
| (1,359)  | 1:122:A:VAL:HG21 | 1:182:A:ILE:HG21 | 18       | 0.59          |
| (1,359)  | 1:122:A:VAL:HG21 | 1:182:A:ILE:HG22 | 18       | 0.59          |
| (1,359)  | 1:122:A:VAL:HG21 | 1:182:A:ILE:HG23 | 18       | 0.59          |
| (1,359)  | 1:122:A:VAL:HG22 | 1:182:A:ILE:HG21 | 18       | 0.59          |
| (1,359)  | 1:122:A:VAL:HG22 | 1:182:A:ILE:HG22 | 18       | 0.59          |
| (1,359)  | 1:122:A:VAL:HG22 | 1:182:A:ILE:HG23 | 18       | 0.59          |
| (1,359)  | 1:122:A:VAL:HG23 | 1:182:A:ILE:HG21 | 18       | 0.59          |
| (1,359)  | 1:122:A:VAL:HG23 | 1:182:A:ILE:HG22 | 18       | 0.59          |
| (1,359)  | 1:122:A:VAL:HG23 | 1:182:A:ILE:HG23 | 18       | 0.59          |
| (1,323)  | 1:209:A:VAL:HG21 | 1:212:A:GLN:HB3  | 14       | 0.59          |
| (1,323)  | 1:209:A:VAL:HG22 | 1:212:A:GLN:HB3  | 14       | 0.59          |
| (1,323)  | 1:209:A:VAL:HG23 | 1:212:A:GLN:HB3  | 14       | 0.59          |
| (1,155)  | 1:125:A:LEU:HB3  | 1:126:A:GLY:HA3  | 13       | 0.59          |
| (1,89)   | 1:206:A:MET:HB3  | 1:210:A:VAL:HG21 | 5        | 0.59          |
| (1,89)   | 1:206:A:MET:HB3  | 1:210:A:VAL:HG22 | 5        | 0.59          |
| (1,89)   | 1:206:A:MET:HB3  | 1:210:A:VAL:HG23 | 5        | 0.59          |
| (1,79)   | 1:138:A:MET:H    | 1:209:A:VAL:HG11 | 11       | 0.59          |
| (1,79)   | 1:138:A:MET:H    | 1:209:A:VAL:HG12 | 11       | 0.59          |
| (1,79)   | 1:138:A:MET:H    | 1:209:A:VAL:HG13 | 11       | 0.59          |
| (1,2771) | 1:130:A:LEU:HB3  | 1:162:A:TYR:HE1  | 2        | 0.58          |
| (1,2771) | 1:130:A:LEU:HB3  | 1:162:A:TYR:HE2  | 2        | 0.58          |
| (1,2771) | 1:130:A:LEU:HB3  | 1:162:A:TYR:HE1  | 3        | 0.58          |
| (1,2771) | 1:130:A:LEU:HB3  | 1:162:A:TYR:HE2  | 3        | 0.58          |
| (1,2771) | 1:130:A:LEU:HB3  | 1:162:A:TYR:HE1  | 17       | 0.58          |
| (1,2771) | 1:130:A:LEU:HB3  | 1:162:A:TYR:HE2  | 17       | 0.58          |
| (1,2650) | 1:139:A:ILE:HG12 | 1:141:A:PHE:HE1  | 13       | 0.58          |
| (1,2650) | 1:139:A:ILE:HG12 | 1:141:A:PHE:HE2  | 13       | 0.58          |
| (1,2439) | 1:229:A:ARG:HE   | 1:230:A:ARG:HB3  | 9        | 0.58          |
| (1,2326) | 1:223:A:GLN:HE21 | 1:228:A:GLY:H    | 8        | 0.58          |
| (1,1937) | 1:220:A:LYS:H    | 1:221:A:GLU:HG3  | 1        | 0.58          |
| (1,1937) | 1:220:A:LYS:H    | 1:221:A:GLU:HG3  | 12       | 0.58          |
| (1,1841) | 1:172:A:GLN:H    | 1:176:A:VAL:HG21 | 12       | 0.58          |
| (1,1841) | 1:172:A:GLN:H    | 1:176:A:VAL:HG22 | 12       | 0.58          |
| (1,1841) | 1:172:A:GLN:H    | 1:176:A:VAL:HG23 | 12       | 0.58          |
| (1,1746) | 1:184:A:ILE:H    | 1:184:A:ILE:HG12 | 11       | 0.58          |
| (1,1459) | 1:136:A:ARG:HB3  | 1:159:A:ASN:HB3  | 20       | 0.58          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1285) | 1:205:A:MET:H    | 1:206:A:MET:HG2  | 10       | 0.58          |
| (1,1207) | 1:168:A:GLN:HA   | 1:168:A:GLN:HE22 | 12       | 0.58          |
| (1,1169) | 1:216:A:THR:HB   | 1:219:A:GLN:HG3  | 17       | 0.58          |
| (1,1168) | 1:223:A:GLN:H    | 1:223:A:GLN:HG2  | 5        | 0.58          |
| (1,1096) | 1:165:A:PRO:HD3  | 1:168:A:GLN:HG2  | 4        | 0.58          |
| (1,1048) | 1:125:A:LEU:HB3  | 1:128:A:TYR:HA   | 6        | 0.58          |
| (1,983)  | 1:149:A:TYR:H    | 1:152:A:GLU:HG2  | 19       | 0.58          |
| (1,758)  | 1:138:A:MET:HG3  | 1:138:A:MET:HE1  | 2        | 0.58          |
| (1,758)  | 1:138:A:MET:HG3  | 1:138:A:MET:HE2  | 2        | 0.58          |
| (1,758)  | 1:138:A:MET:HG3  | 1:138:A:MET:HE3  | 2        | 0.58          |
| (1,758)  | 1:138:A:MET:HG3  | 1:138:A:MET:HE1  | 3        | 0.58          |
| (1,758)  | 1:138:A:MET:HG3  | 1:138:A:MET:HE2  | 3        | 0.58          |
| (1,758)  | 1:138:A:MET:HG3  | 1:138:A:MET:HE3  | 3        | 0.58          |
| (1,758)  | 1:138:A:MET:HG3  | 1:138:A:MET:HE1  | 6        | 0.58          |
| (1,758)  | 1:138:A:MET:HG3  | 1:138:A:MET:HE2  | 6        | 0.58          |
| (1,758)  | 1:138:A:MET:HG3  | 1:138:A:MET:HE3  | 6        | 0.58          |
| (1,752)  | 1:138:A:MET:HE1  | 1:139:A:ILE:HG12 | 9        | 0.58          |
| (1,752)  | 1:138:A:MET:HE2  | 1:139:A:ILE:HG12 | 9        | 0.58          |
| (1,752)  | 1:138:A:MET:HE3  | 1:139:A:ILE:HG12 | 9        | 0.58          |
| (1,658)  | 1:154:A:MET:HG3  | 1:154:A:MET:HE1  | 18       | 0.58          |
| (1,658)  | 1:154:A:MET:HG3  | 1:154:A:MET:HE2  | 18       | 0.58          |
| (1,658)  | 1:154:A:MET:HG3  | 1:154:A:MET:HE3  | 18       | 0.58          |
| (1,657)  | 1:213:A:MET:HB3  | 1:213:A:MET:HE1  | 18       | 0.58          |
| (1,657)  | 1:213:A:MET:HB3  | 1:213:A:MET:HE2  | 18       | 0.58          |
| (1,657)  | 1:213:A:MET:HB3  | 1:213:A:MET:HE3  | 18       | 0.58          |
| (1,592)  | 1:161:A:VAL:H    | 1:161:A:VAL:HG21 | 10       | 0.58          |
| (1,592)  | 1:161:A:VAL:H    | 1:161:A:VAL:HG22 | 10       | 0.58          |
| (1,592)  | 1:161:A:VAL:H    | 1:161:A:VAL:HG23 | 10       | 0.58          |
| (1,559)  | 1:162:A:TYR:HB3  | 1:182:A:ILE:HG21 | 12       | 0.58          |
| (1,559)  | 1:162:A:TYR:HB3  | 1:182:A:ILE:HG22 | 12       | 0.58          |
| (1,559)  | 1:162:A:TYR:HB3  | 1:182:A:ILE:HG23 | 12       | 0.58          |
| (1,496)  | 1:130:A:LEU:HA   | 1:162:A:TYR:HB2  | 1        | 0.58          |
| (1,392)  | 1:122:A:VAL:HG11 | 1:190:A:THR:HB   | 1        | 0.58          |
| (1,392)  | 1:122:A:VAL:HG12 | 1:190:A:THR:HB   | 1        | 0.58          |
| (1,392)  | 1:122:A:VAL:HG13 | 1:190:A:THR:HB   | 1        | 0.58          |
| (1,318)  | 1:153:A:ASN:HB2  | 1:156:A:ARG:HD3  | 16       | 0.58          |
| (1,216)  | 1:216:A:THR:HG21 | 1:220:A:LYS:HG3  | 3        | 0.58          |
| (1,216)  | 1:216:A:THR:HG22 | 1:220:A:LYS:HG3  | 3        | 0.58          |
| (1,216)  | 1:216:A:THR:HG23 | 1:220:A:LYS:HG3  | 3        | 0.58          |
| (1,177)  | 1:195:A:GLY:HA3  | 1:197:A:ASN:HD21 | 9        | 0.58          |
| (1,160)  | 1:223:A:GLN:HE21 | 1:228:A:GLY:HA2  | 14       | 0.58          |
| (1,160)  | 1:223:A:GLN:HE21 | 1:228:A:GLY:HA3  | 14       | 0.58          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,160)  | 1:223:A:GLN:HE21 | 1:228:A:GLY:HA2  | 17       | 0.58          |
| (1,160)  | 1:223:A:GLN:HE21 | 1:228:A:GLY:HA3  | 17       | 0.58          |
| (1,80)   | 1:208:A:ARG:HA   | 1:209:A:VAL:HG11 | 8        | 0.58          |
| (1,80)   | 1:208:A:ARG:HA   | 1:209:A:VAL:HG12 | 8        | 0.58          |
| (1,80)   | 1:208:A:ARG:HA   | 1:209:A:VAL:HG13 | 8        | 0.58          |
| (1,2807) | 1:149:A:TYR:HE1  | 1:153:A:ASN:HB3  | 4        | 0.57          |
| (1,2807) | 1:149:A:TYR:HE2  | 1:153:A:ASN:HB3  | 4        | 0.57          |
| (1,2792) | 1:128:A:TYR:HE1  | 1:164:A:ARG:HD3  | 8        | 0.57          |
| (1,2792) | 1:128:A:TYR:HE2  | 1:164:A:ARG:HD3  | 8        | 0.57          |
| (1,2774) | 1:128:A:TYR:HE1  | 1:162:A:TYR:HB3  | 11       | 0.57          |
| (1,2774) | 1:128:A:TYR:HE2  | 1:162:A:TYR:HB3  | 11       | 0.57          |
| (1,2763) | 1:155:A:TYR:HE1  | 1:156:A:ARG:HD2  | 20       | 0.57          |
| (1,2763) | 1:155:A:TYR:HE2  | 1:156:A:ARG:HD2  | 20       | 0.57          |
| (1,2759) | 1:139:A:ILE:HG12 | 1:150:A:TYR:HE1  | 19       | 0.57          |
| (1,2759) | 1:139:A:ILE:HG12 | 1:150:A:TYR:HE2  | 19       | 0.57          |
| (1,2736) | 1:184:A:ILE:HG13 | 1:187:A:HIS:HD2  | 16       | 0.57          |
| (1,2699) | 1:141:A:PHE:HZ   | 1:150:A:TYR:HB3  | 8        | 0.57          |
| (1,2548) | 1:162:A:TYR:HD1  | 1:186:A:GLN:HB3  | 2        | 0.57          |
| (1,2548) | 1:162:A:TYR:HD2  | 1:186:A:GLN:HB3  | 2        | 0.57          |
| (1,2548) | 1:162:A:TYR:HD1  | 1:186:A:GLN:HB3  | 11       | 0.57          |
| (1,2548) | 1:162:A:TYR:HD2  | 1:186:A:GLN:HB3  | 11       | 0.57          |
| (1,2536) | 1:167:A:SER:HB3  | 1:225:A:TYR:HD1  | 6        | 0.57          |
| (1,2536) | 1:167:A:SER:HB3  | 1:225:A:TYR:HD2  | 6        | 0.57          |
| (1,2326) | 1:223:A:GLN:HE21 | 1:228:A:GLY:H    | 19       | 0.57          |
| (1,2270) | 1:132:A:SER:H    | 1:132:A:SER:HB2  | 3        | 0.57          |
| (1,2250) | 1:217:A:GLN:HE21 | 1:218:A:TYR:HA   | 7        | 0.57          |
| (1,1894) | 1:215:A:VAL:HG21 | 1:219:A:GLN:H    | 2        | 0.57          |
| (1,1894) | 1:215:A:VAL:HG22 | 1:219:A:GLN:H    | 2        | 0.57          |
| (1,1894) | 1:215:A:VAL:HG23 | 1:219:A:GLN:H    | 2        | 0.57          |
| (1,1701) | 1:129:A:MET:H    | 1:129:A:MET:HG3  | 11       | 0.57          |
| (1,1584) | 1:122:A:VAL:H    | 1:122:A:VAL:HG11 | 9        | 0.57          |
| (1,1584) | 1:122:A:VAL:H    | 1:122:A:VAL:HG12 | 9        | 0.57          |
| (1,1584) | 1:122:A:VAL:H    | 1:122:A:VAL:HG13 | 9        | 0.57          |
| (1,1523) | 1:162:A:TYR:HB3  | 1:182:A:ILE:HG12 | 8        | 0.57          |
| (1,1523) | 1:162:A:TYR:HB3  | 1:182:A:ILE:HG13 | 8        | 0.57          |
| (1,1294) | 1:138:A:MET:HG3  | 1:139:A:ILE:H    | 8        | 0.57          |
| (1,1257) | 1:206:A:MET:HG3  | 1:210:A:VAL:HG21 | 10       | 0.57          |
| (1,1257) | 1:206:A:MET:HG3  | 1:210:A:VAL:HG22 | 10       | 0.57          |
| (1,1257) | 1:206:A:MET:HG3  | 1:210:A:VAL:HG23 | 10       | 0.57          |
| (1,1197) | 1:160:A:GLN:HB2  | 1:183:A:THR:HG21 | 18       | 0.57          |
| (1,1197) | 1:160:A:GLN:HB2  | 1:183:A:THR:HG22 | 18       | 0.57          |
| (1,1197) | 1:160:A:GLN:HB2  | 1:183:A:THR:HG23 | 18       | 0.57          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1104) | 1:213:A:MET:HB3  | 1:214:A:CYS:HA   | 3        | 0.57          |
| (1,1098) | 1:213:A:MET:HB2  | 1:216:A:THR:HG21 | 10       | 0.57          |
| (1,1098) | 1:213:A:MET:HB2  | 1:216:A:THR:HG22 | 10       | 0.57          |
| (1,1098) | 1:213:A:MET:HB2  | 1:216:A:THR:HG23 | 10       | 0.57          |
| (1,1098) | 1:213:A:MET:HB2  | 1:216:A:THR:HG21 | 19       | 0.57          |
| (1,1098) | 1:213:A:MET:HB2  | 1:216:A:THR:HG22 | 19       | 0.57          |
| (1,1098) | 1:213:A:MET:HB2  | 1:216:A:THR:HG23 | 19       | 0.57          |
| (1,873)  | 1:146:A:GLU:HA   | 1:150:A:TYR:HB3  | 3        | 0.57          |
| (1,758)  | 1:138:A:MET:HG3  | 1:138:A:MET:HE1  | 9        | 0.57          |
| (1,758)  | 1:138:A:MET:HG3  | 1:138:A:MET:HE2  | 9        | 0.57          |
| (1,758)  | 1:138:A:MET:HG3  | 1:138:A:MET:HE3  | 9        | 0.57          |
| (1,758)  | 1:138:A:MET:HG3  | 1:138:A:MET:HE1  | 11       | 0.57          |
| (1,758)  | 1:138:A:MET:HG3  | 1:138:A:MET:HE2  | 11       | 0.57          |
| (1,758)  | 1:138:A:MET:HG3  | 1:138:A:MET:HE3  | 11       | 0.57          |
| (1,758)  | 1:138:A:MET:HG3  | 1:138:A:MET:HE1  | 17       | 0.57          |
| (1,758)  | 1:138:A:MET:HG3  | 1:138:A:MET:HE2  | 17       | 0.57          |
| (1,758)  | 1:138:A:MET:HG3  | 1:138:A:MET:HE3  | 17       | 0.57          |
| (1,502)  | 1:162:A:TYR:HB3  | 1:183:A:THR:HA   | 16       | 0.57          |
| (1,362)  | 1:172:A:GLN:HG3  | 1:215:A:VAL:HG21 | 18       | 0.57          |
| (1,362)  | 1:172:A:GLN:HG3  | 1:215:A:VAL:HG22 | 18       | 0.57          |
| (1,362)  | 1:172:A:GLN:HG3  | 1:215:A:VAL:HG23 | 18       | 0.57          |
| (1,58)   | 1:122:A:VAL:HG21 | 1:125:A:LEU:HD11 | 12       | 0.57          |
| (1,58)   | 1:122:A:VAL:HG21 | 1:125:A:LEU:HD12 | 12       | 0.57          |
| (1,58)   | 1:122:A:VAL:HG21 | 1:125:A:LEU:HD13 | 12       | 0.57          |
| (1,58)   | 1:122:A:VAL:HG22 | 1:125:A:LEU:HD11 | 12       | 0.57          |
| (1,58)   | 1:122:A:VAL:HG22 | 1:125:A:LEU:HD12 | 12       | 0.57          |
| (1,58)   | 1:122:A:VAL:HG22 | 1:125:A:LEU:HD13 | 12       | 0.57          |
| (1,58)   | 1:122:A:VAL:HG23 | 1:125:A:LEU:HD11 | 12       | 0.57          |
| (1,58)   | 1:122:A:VAL:HG23 | 1:125:A:LEU:HD12 | 12       | 0.57          |
| (1,58)   | 1:122:A:VAL:HG23 | 1:125:A:LEU:HD13 | 12       | 0.57          |
| (1,2830) | 1:172:A:GLN:HG2  | 1:218:A:TYR:HE1  | 15       | 0.56          |
| (1,2830) | 1:172:A:GLN:HG2  | 1:218:A:TYR:HE2  | 15       | 0.56          |
| (1,2759) | 1:139:A:ILE:HG12 | 1:150:A:TYR:HE1  | 16       | 0.56          |
| (1,2759) | 1:139:A:ILE:HG12 | 1:150:A:TYR:HE2  | 16       | 0.56          |
| (1,2699) | 1:141:A:PHE:HZ   | 1:150:A:TYR:HB3  | 14       | 0.56          |
| (1,2657) | 1:141:A:PHE:HE1  | 1:208:A:ARG:HB3  | 15       | 0.56          |
| (1,2657) | 1:141:A:PHE:HE2  | 1:208:A:ARG:HB3  | 15       | 0.56          |
| (1,2553) | 1:126:A:GLY:HA2  | 1:128:A:TYR:HD1  | 3        | 0.56          |
| (1,2553) | 1:126:A:GLY:HA2  | 1:128:A:TYR:HD2  | 3        | 0.56          |
| (1,2492) | 1:139:A:ILE:HG12 | 1:150:A:TYR:HD1  | 5        | 0.56          |
| (1,2492) | 1:139:A:ILE:HG12 | 1:150:A:TYR:HD2  | 5        | 0.56          |
| (1,2040) | 1:128:A:TYR:H    | 1:164:A:ARG:HG3  | 5        | 0.56          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1579) | 1:132:A:SER:HB3  | 1:133:A:ALA:H    | 17       | 0.56          |
| (1,1459) | 1:136:A:ARG:HB3  | 1:159:A:ASN:HB3  | 11       | 0.56          |
| (1,1375) | 1:136:A:ARG:HD2  | 1:154:A:MET:HG3  | 7        | 0.56          |
| (1,1303) | 1:137:A:PRO:HB2  | 1:213:A:MET:HG2  | 16       | 0.56          |
| (1,1166) | 1:215:A:VAL:HG21 | 1:219:A:GLN:HG3  | 8        | 0.56          |
| (1,1166) | 1:215:A:VAL:HG22 | 1:219:A:GLN:HG3  | 8        | 0.56          |
| (1,1166) | 1:215:A:VAL:HG23 | 1:219:A:GLN:HG3  | 8        | 0.56          |
| (1,1098) | 1:213:A:MET:HB2  | 1:216:A:THR:HG21 | 1        | 0.56          |
| (1,1098) | 1:213:A:MET:HB2  | 1:216:A:THR:HG22 | 1        | 0.56          |
| (1,1098) | 1:213:A:MET:HB2  | 1:216:A:THR:HG23 | 1        | 0.56          |
| (1,1098) | 1:213:A:MET:HB2  | 1:216:A:THR:HG21 | 3        | 0.56          |
| (1,1098) | 1:213:A:MET:HB2  | 1:216:A:THR:HG22 | 3        | 0.56          |
| (1,1098) | 1:213:A:MET:HB2  | 1:216:A:THR:HG23 | 3        | 0.56          |
| (1,1098) | 1:213:A:MET:HB2  | 1:216:A:THR:HG21 | 8        | 0.56          |
| (1,1098) | 1:213:A:MET:HB2  | 1:216:A:THR:HG22 | 8        | 0.56          |
| (1,1098) | 1:213:A:MET:HB2  | 1:216:A:THR:HG23 | 8        | 0.56          |
| (1,1098) | 1:213:A:MET:HB2  | 1:216:A:THR:HG21 | 13       | 0.56          |
| (1,1098) | 1:213:A:MET:HB2  | 1:216:A:THR:HG22 | 13       | 0.56          |
| (1,1098) | 1:213:A:MET:HB2  | 1:216:A:THR:HG23 | 13       | 0.56          |
| (1,1098) | 1:213:A:MET:HB2  | 1:216:A:THR:HG21 | 18       | 0.56          |
| (1,1098) | 1:213:A:MET:HB2  | 1:216:A:THR:HG22 | 18       | 0.56          |
| (1,1098) | 1:213:A:MET:HB2  | 1:216:A:THR:HG23 | 18       | 0.56          |
| (1,1098) | 1:213:A:MET:HB2  | 1:216:A:THR:HG21 | 20       | 0.56          |
| (1,1098) | 1:213:A:MET:HB2  | 1:216:A:THR:HG22 | 20       | 0.56          |
| (1,1098) | 1:213:A:MET:HB2  | 1:216:A:THR:HG23 | 20       | 0.56          |
| (1,1095) | 1:165:A:PRO:HA   | 1:168:A:GLN:HG2  | 15       | 0.56          |
| (1,1060) | 1:207:A:GLU:HG3  | 1:208:A:ARG:H    | 4        | 0.56          |
| (1,864)  | 1:134:A:MET:HB3  | 1:135:A:SER:HB2  | 17       | 0.56          |
| (1,758)  | 1:138:A:MET:HG3  | 1:138:A:MET:HE1  | 4        | 0.56          |
| (1,758)  | 1:138:A:MET:HG3  | 1:138:A:MET:HE2  | 4        | 0.56          |
| (1,758)  | 1:138:A:MET:HG3  | 1:138:A:MET:HE3  | 4        | 0.56          |
| (1,758)  | 1:138:A:MET:HG3  | 1:138:A:MET:HE1  | 20       | 0.56          |
| (1,758)  | 1:138:A:MET:HG3  | 1:138:A:MET:HE2  | 20       | 0.56          |
| (1,758)  | 1:138:A:MET:HG3  | 1:138:A:MET:HE3  | 20       | 0.56          |
| (1,752)  | 1:138:A:MET:HE1  | 1:139:A:ILE:HG12 | 7        | 0.56          |
| (1,752)  | 1:138:A:MET:HE2  | 1:139:A:ILE:HG12 | 7        | 0.56          |
| (1,752)  | 1:138:A:MET:HE3  | 1:139:A:ILE:HG12 | 7        | 0.56          |
| (1,634)  | 1:192:A:THR:HA   | 1:195:A:GLY:HA3  | 6        | 0.56          |
| (1,521)  | 1:223:A:GLN:HG3  | 1:224:A:ALA:HB1  | 2        | 0.56          |
| (1,521)  | 1:223:A:GLN:HG3  | 1:224:A:ALA:HB2  | 2        | 0.56          |
| (1,521)  | 1:223:A:GLN:HG3  | 1:224:A:ALA:HB3  | 2        | 0.56          |
| (1,496)  | 1:130:A:LEU:HA   | 1:162:A:TYR:HB2  | 11       | 0.56          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,435)  | 1:230:A:ARG:HA   | 1:230:A:ARG:HD2  | 19       | 0.56          |
| (1,357)  | 1:122:A:VAL:HG21 | 1:125:A:LEU:HG   | 9        | 0.56          |
| (1,357)  | 1:122:A:VAL:HG22 | 1:125:A:LEU:HG   | 9        | 0.56          |
| (1,357)  | 1:122:A:VAL:HG23 | 1:125:A:LEU:HG   | 9        | 0.56          |
| (1,138)  | 1:125:A:LEU:HA   | 1:125:A:LEU:HD21 | 15       | 0.56          |
| (1,138)  | 1:125:A:LEU:HA   | 1:125:A:LEU:HD22 | 15       | 0.56          |
| (1,138)  | 1:125:A:LEU:HA   | 1:125:A:LEU:HD23 | 15       | 0.56          |
| (1,105)  | 1:212:A:GLN:HA   | 1:215:A:VAL:HG11 | 13       | 0.56          |
| (1,105)  | 1:212:A:GLN:HA   | 1:215:A:VAL:HG12 | 13       | 0.56          |
| (1,105)  | 1:212:A:GLN:HA   | 1:215:A:VAL:HG13 | 13       | 0.56          |
| (1,2846) | 1:157:A:TYR:HE1  | 1:206:A:MET:HB2  | 8        | 0.55          |
| (1,2846) | 1:157:A:TYR:HE2  | 1:206:A:MET:HB2  | 8        | 0.55          |
| (1,2792) | 1:128:A:TYR:HE1  | 1:164:A:ARG:HD3  | 20       | 0.55          |
| (1,2792) | 1:128:A:TYR:HE2  | 1:164:A:ARG:HD3  | 20       | 0.55          |
| (1,2774) | 1:128:A:TYR:HE1  | 1:162:A:TYR:HB3  | 13       | 0.55          |
| (1,2774) | 1:128:A:TYR:HE2  | 1:162:A:TYR:HB3  | 13       | 0.55          |
| (1,2771) | 1:130:A:LEU:HB3  | 1:162:A:TYR:HE1  | 18       | 0.55          |
| (1,2771) | 1:130:A:LEU:HB3  | 1:162:A:TYR:HE2  | 18       | 0.55          |
| (1,2771) | 1:130:A:LEU:HB3  | 1:162:A:TYR:HE1  | 20       | 0.55          |
| (1,2771) | 1:130:A:LEU:HB3  | 1:162:A:TYR:HE2  | 20       | 0.55          |
| (1,2758) | 1:150:A:TYR:HE1  | 1:209:A:VAL:HG11 | 19       | 0.55          |
| (1,2758) | 1:150:A:TYR:HE1  | 1:209:A:VAL:HG12 | 19       | 0.55          |
| (1,2758) | 1:150:A:TYR:HE1  | 1:209:A:VAL:HG13 | 19       | 0.55          |
| (1,2758) | 1:150:A:TYR:HE2  | 1:209:A:VAL:HG11 | 19       | 0.55          |
| (1,2758) | 1:150:A:TYR:HE2  | 1:209:A:VAL:HG12 | 19       | 0.55          |
| (1,2758) | 1:150:A:TYR:HE2  | 1:209:A:VAL:HG13 | 19       | 0.55          |
| (1,2681) | 1:141:A:PHE:HZ   | 1:208:A:ARG:HB3  | 3        | 0.55          |
| (1,2681) | 1:141:A:PHE:HZ   | 1:208:A:ARG:HB3  | 7        | 0.55          |
| (1,2553) | 1:126:A:GLY:HA2  | 1:128:A:TYR:HD1  | 8        | 0.55          |
| (1,2553) | 1:126:A:GLY:HA2  | 1:128:A:TYR:HD2  | 8        | 0.55          |
| (1,2536) | 1:167:A:SER:HB3  | 1:225:A:TYR:HD1  | 11       | 0.55          |
| (1,2536) | 1:167:A:SER:HB3  | 1:225:A:TYR:HD2  | 11       | 0.55          |
| (1,2501) | 1:149:A:TYR:HD1  | 1:205:A:MET:HG2  | 3        | 0.55          |
| (1,2501) | 1:149:A:TYR:HD2  | 1:205:A:MET:HG2  | 3        | 0.55          |
| (1,2501) | 1:149:A:TYR:HD1  | 1:205:A:MET:HG2  | 19       | 0.55          |
| (1,2501) | 1:149:A:TYR:HD2  | 1:205:A:MET:HG2  | 19       | 0.55          |
| (1,2488) | 1:149:A:TYR:HD1  | 1:153:A:ASN:HB3  | 3        | 0.55          |
| (1,2488) | 1:149:A:TYR:HD2  | 1:153:A:ASN:HB3  | 3        | 0.55          |
| (1,2488) | 1:149:A:TYR:HD1  | 1:153:A:ASN:HB3  | 17       | 0.55          |
| (1,2488) | 1:149:A:TYR:HD2  | 1:153:A:ASN:HB3  | 17       | 0.55          |
| (1,2320) | 1:160:A:GLN:HE22 | 1:213:A:MET:HB2  | 17       | 0.55          |
| (1,1701) | 1:129:A:MET:H    | 1:129:A:MET:HG3  | 2        | 0.55          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1235) | 1:205:A:MET:HG3  | 1:206:A:MET:HG2  | 7        | 0.55          |
| (1,1231) | 1:209:A:VAL:HG21 | 1:213:A:MET:HG3  | 10       | 0.55          |
| (1,1231) | 1:209:A:VAL:HG22 | 1:213:A:MET:HG3  | 10       | 0.55          |
| (1,1231) | 1:209:A:VAL:HG23 | 1:213:A:MET:HG3  | 10       | 0.55          |
| (1,1098) | 1:213:A:MET:HB2  | 1:216:A:THR:HG21 | 2        | 0.55          |
| (1,1098) | 1:213:A:MET:HB2  | 1:216:A:THR:HG22 | 2        | 0.55          |
| (1,1098) | 1:213:A:MET:HB2  | 1:216:A:THR:HG23 | 2        | 0.55          |
| (1,1098) | 1:213:A:MET:HB2  | 1:216:A:THR:HG21 | 7        | 0.55          |
| (1,1098) | 1:213:A:MET:HB2  | 1:216:A:THR:HG22 | 7        | 0.55          |
| (1,1098) | 1:213:A:MET:HB2  | 1:216:A:THR:HG23 | 7        | 0.55          |
| (1,1098) | 1:213:A:MET:HB2  | 1:216:A:THR:HG21 | 9        | 0.55          |
| (1,1098) | 1:213:A:MET:HB2  | 1:216:A:THR:HG22 | 9        | 0.55          |
| (1,1098) | 1:213:A:MET:HB2  | 1:216:A:THR:HG23 | 9        | 0.55          |
| (1,1098) | 1:213:A:MET:HB2  | 1:216:A:THR:HG21 | 14       | 0.55          |
| (1,1098) | 1:213:A:MET:HB2  | 1:216:A:THR:HG22 | 14       | 0.55          |
| (1,1098) | 1:213:A:MET:HB2  | 1:216:A:THR:HG23 | 14       | 0.55          |
| (1,1098) | 1:213:A:MET:HB2  | 1:216:A:THR:HG21 | 16       | 0.55          |
| (1,1098) | 1:213:A:MET:HB2  | 1:216:A:THR:HG22 | 16       | 0.55          |
| (1,1098) | 1:213:A:MET:HB2  | 1:216:A:THR:HG23 | 16       | 0.55          |
| (1,1098) | 1:213:A:MET:HB2  | 1:216:A:THR:HG21 | 17       | 0.55          |
| (1,1098) | 1:213:A:MET:HB2  | 1:216:A:THR:HG22 | 17       | 0.55          |
| (1,1098) | 1:213:A:MET:HB2  | 1:216:A:THR:HG23 | 17       | 0.55          |
| (1,1095) | 1:165:A:PRO:HA   | 1:168:A:GLN:HG2  | 8        | 0.55          |
| (1,1073) | 1:166:A:VAL:HG11 | 1:221:A:GLU:HA   | 1        | 0.55          |
| (1,1073) | 1:166:A:VAL:HG12 | 1:221:A:GLU:HA   | 1        | 0.55          |
| (1,1073) | 1:166:A:VAL:HG13 | 1:221:A:GLU:HA   | 1        | 0.55          |
| (1,1060) | 1:207:A:GLU:HG3  | 1:208:A:ARG:H    | 9        | 0.55          |
| (1,957)  | 1:184:A:ILE:HD11 | 1:207:A:GLU:HG3  | 14       | 0.55          |
| (1,957)  | 1:184:A:ILE:HD12 | 1:207:A:GLU:HG3  | 14       | 0.55          |
| (1,957)  | 1:184:A:ILE:HD13 | 1:207:A:GLU:HG3  | 14       | 0.55          |
| (1,907)  | 1:226:A:TYR:HA   | 1:229:A:ARG:HB2  | 20       | 0.55          |
| (1,901)  | 1:203:A:VAL:HG21 | 1:204:A:LYS:HA   | 5        | 0.55          |
| (1,901)  | 1:203:A:VAL:HG22 | 1:204:A:LYS:HA   | 5        | 0.55          |
| (1,901)  | 1:203:A:VAL:HG23 | 1:204:A:LYS:HA   | 5        | 0.55          |
| (1,864)  | 1:134:A:MET:HB3  | 1:135:A:SER:HB2  | 3        | 0.55          |
| (1,851)  | 1:151:A:ARG:HA   | 1:151:A:ARG:HG2  | 8        | 0.55          |
| (1,758)  | 1:138:A:MET:HG3  | 1:138:A:MET:HE1  | 5        | 0.55          |
| (1,758)  | 1:138:A:MET:HG3  | 1:138:A:MET:HE2  | 5        | 0.55          |
| (1,758)  | 1:138:A:MET:HG3  | 1:138:A:MET:HE3  | 5        | 0.55          |
| (1,569)  | 1:128:A:TYR:HE1  | 1:179:A:CYS:HB3  | 6        | 0.55          |
| (1,569)  | 1:128:A:TYR:HE2  | 1:179:A:CYS:HB3  | 6        | 0.55          |
| (1,525)  | 1:132:A:SER:HB2  | 1:160:A:GLN:HE21 | 15       | 0.55          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,521)  | 1:223:A:GLN:HG3  | 1:224:A:ALA:HB1  | 15       | 0.55          |
| (1,521)  | 1:223:A:GLN:HG3  | 1:224:A:ALA:HB2  | 15       | 0.55          |
| (1,521)  | 1:223:A:GLN:HG3  | 1:224:A:ALA:HB3  | 15       | 0.55          |
| (1,496)  | 1:130:A:LEU:HA   | 1:162:A:TYR:HB2  | 14       | 0.55          |
| (1,389)  | 1:121:A:VAL:HA   | 1:122:A:VAL:HG11 | 16       | 0.55          |
| (1,389)  | 1:121:A:VAL:HA   | 1:122:A:VAL:HG12 | 16       | 0.55          |
| (1,389)  | 1:121:A:VAL:HA   | 1:122:A:VAL:HG13 | 16       | 0.55          |
| (1,336)  | 1:163:A:TYR:HD1  | 1:166:A:VAL:HG11 | 12       | 0.55          |
| (1,336)  | 1:163:A:TYR:HD1  | 1:166:A:VAL:HG12 | 12       | 0.55          |
| (1,336)  | 1:163:A:TYR:HD1  | 1:166:A:VAL:HG13 | 12       | 0.55          |
| (1,336)  | 1:163:A:TYR:HD2  | 1:166:A:VAL:HG11 | 12       | 0.55          |
| (1,336)  | 1:163:A:TYR:HD2  | 1:166:A:VAL:HG12 | 12       | 0.55          |
| (1,336)  | 1:163:A:TYR:HD2  | 1:166:A:VAL:HG13 | 12       | 0.55          |
| (1,273)  | 1:166:A:VAL:HG11 | 1:225:A:TYR:HB2  | 3        | 0.55          |
| (1,273)  | 1:166:A:VAL:HG12 | 1:225:A:TYR:HB2  | 3        | 0.55          |
| (1,273)  | 1:166:A:VAL:HG13 | 1:225:A:TYR:HB2  | 3        | 0.55          |
| (1,258)  | 1:122:A:VAL:HG11 | 1:190:A:THR:HG21 | 15       | 0.55          |
| (1,258)  | 1:122:A:VAL:HG11 | 1:190:A:THR:HG22 | 15       | 0.55          |
| (1,258)  | 1:122:A:VAL:HG11 | 1:190:A:THR:HG23 | 15       | 0.55          |
| (1,258)  | 1:122:A:VAL:HG12 | 1:190:A:THR:HG21 | 15       | 0.55          |
| (1,258)  | 1:122:A:VAL:HG12 | 1:190:A:THR:HG22 | 15       | 0.55          |
| (1,258)  | 1:122:A:VAL:HG12 | 1:190:A:THR:HG23 | 15       | 0.55          |
| (1,258)  | 1:122:A:VAL:HG13 | 1:190:A:THR:HG21 | 15       | 0.55          |
| (1,258)  | 1:122:A:VAL:HG13 | 1:190:A:THR:HG22 | 15       | 0.55          |
| (1,258)  | 1:122:A:VAL:HG13 | 1:190:A:THR:HG23 | 15       | 0.55          |
| (1,179)  | 1:201:A:THR:HB   | 1:205:A:MET:HG3  | 6        | 0.55          |
| (1,80)   | 1:208:A:ARG:HA   | 1:209:A:VAL:HG11 | 10       | 0.55          |
| (1,80)   | 1:208:A:ARG:HA   | 1:209:A:VAL:HG12 | 10       | 0.55          |
| (1,80)   | 1:208:A:ARG:HA   | 1:209:A:VAL:HG13 | 10       | 0.55          |
| (1,55)   | 1:125:A:LEU:HD11 | 1:162:A:TYR:HB2  | 6        | 0.55          |
| (1,55)   | 1:125:A:LEU:HD12 | 1:162:A:TYR:HB2  | 6        | 0.55          |
| (1,55)   | 1:125:A:LEU:HD13 | 1:162:A:TYR:HB2  | 6        | 0.55          |
| (1,2851) | 1:184:A:ILE:HG13 | 1:187:A:HIS:HE1  | 18       | 0.54          |
| (1,2830) | 1:172:A:GLN:HG2  | 1:218:A:TYR:HE1  | 11       | 0.54          |
| (1,2830) | 1:172:A:GLN:HG2  | 1:218:A:TYR:HE2  | 11       | 0.54          |
| (1,2771) | 1:130:A:LEU:HB3  | 1:162:A:TYR:HE1  | 10       | 0.54          |
| (1,2771) | 1:130:A:LEU:HB3  | 1:162:A:TYR:HE2  | 10       | 0.54          |
| (1,2699) | 1:141:A:PHE:HZ   | 1:150:A:TYR:HB3  | 1        | 0.54          |
| (1,2501) | 1:149:A:TYR:HD1  | 1:205:A:MET:HG2  | 12       | 0.54          |
| (1,2501) | 1:149:A:TYR:HD2  | 1:205:A:MET:HG2  | 12       | 0.54          |
| (1,2414) | 1:136:A:ARG:HB3  | 1:159:A:ASN:HD21 | 3        | 0.54          |
| (1,2326) | 1:223:A:GLN:HE21 | 1:228:A:GLY:H    | 16       | 0.54          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1894) | 1:215:A:VAL:HG21 | 1:219:A:GLN:H    | 12       | 0.54          |
| (1,1894) | 1:215:A:VAL:HG22 | 1:219:A:GLN:H    | 12       | 0.54          |
| (1,1894) | 1:215:A:VAL:HG23 | 1:219:A:GLN:H    | 12       | 0.54          |
| (1,1861) | 1:147:A:ASP:HB2  | 1:148:A:ARG:H    | 6        | 0.54          |
| (1,1579) | 1:132:A:SER:HB3  | 1:133:A:ALA:H    | 19       | 0.54          |
| (1,1523) | 1:162:A:TYR:HB3  | 1:182:A:ILE:HG12 | 4        | 0.54          |
| (1,1523) | 1:162:A:TYR:HB3  | 1:182:A:ILE:HG13 | 4        | 0.54          |
| (1,1523) | 1:162:A:TYR:HB3  | 1:182:A:ILE:HG12 | 16       | 0.54          |
| (1,1523) | 1:162:A:TYR:HB3  | 1:182:A:ILE:HG13 | 16       | 0.54          |
| (1,1480) | 1:203:A:VAL:HG21 | 1:207:A:GLU:HB2  | 8        | 0.54          |
| (1,1480) | 1:203:A:VAL:HG22 | 1:207:A:GLU:HB2  | 8        | 0.54          |
| (1,1480) | 1:203:A:VAL:HG23 | 1:207:A:GLU:HB2  | 8        | 0.54          |
| (1,1294) | 1:138:A:MET:HG3  | 1:139:A:ILE:H    | 11       | 0.54          |
| (1,1212) | 1:184:A:ILE:HD11 | 1:206:A:MET:HB3  | 10       | 0.54          |
| (1,1212) | 1:184:A:ILE:HD12 | 1:206:A:MET:HB3  | 10       | 0.54          |
| (1,1212) | 1:184:A:ILE:HD13 | 1:206:A:MET:HB3  | 10       | 0.54          |
| (1,1207) | 1:168:A:GLN:HA   | 1:168:A:GLN:HE22 | 15       | 0.54          |
| (1,1197) | 1:160:A:GLN:HB2  | 1:183:A:THR:HG21 | 12       | 0.54          |
| (1,1197) | 1:160:A:GLN:HB2  | 1:183:A:THR:HG22 | 12       | 0.54          |
| (1,1197) | 1:160:A:GLN:HB2  | 1:183:A:THR:HG23 | 12       | 0.54          |
| (1,1104) | 1:213:A:MET:HB3  | 1:214:A:CYS:HA   | 7        | 0.54          |
| (1,1098) | 1:213:A:MET:HB2  | 1:216:A:THR:HG21 | 4        | 0.54          |
| (1,1098) | 1:213:A:MET:HB2  | 1:216:A:THR:HG22 | 4        | 0.54          |
| (1,1098) | 1:213:A:MET:HB2  | 1:216:A:THR:HG23 | 4        | 0.54          |
| (1,1098) | 1:213:A:MET:HB2  | 1:216:A:THR:HG21 | 11       | 0.54          |
| (1,1098) | 1:213:A:MET:HB2  | 1:216:A:THR:HG22 | 11       | 0.54          |
| (1,1098) | 1:213:A:MET:HB2  | 1:216:A:THR:HG23 | 11       | 0.54          |
| (1,957)  | 1:184:A:ILE:HD11 | 1:207:A:GLU:HG3  | 16       | 0.54          |
| (1,957)  | 1:184:A:ILE:HD12 | 1:207:A:GLU:HG3  | 16       | 0.54          |
| (1,957)  | 1:184:A:ILE:HD13 | 1:207:A:GLU:HG3  | 16       | 0.54          |
| (1,893)  | 1:162:A:TYR:HB3  | 1:182:A:ILE:HB   | 19       | 0.54          |
| (1,758)  | 1:138:A:MET:HG3  | 1:138:A:MET:HE1  | 15       | 0.54          |
| (1,758)  | 1:138:A:MET:HG3  | 1:138:A:MET:HE2  | 15       | 0.54          |
| (1,758)  | 1:138:A:MET:HG3  | 1:138:A:MET:HE3  | 15       | 0.54          |
| (1,657)  | 1:213:A:MET:HB3  | 1:213:A:MET:HE1  | 4        | 0.54          |
| (1,657)  | 1:213:A:MET:HB3  | 1:213:A:MET:HE2  | 4        | 0.54          |
| (1,657)  | 1:213:A:MET:HB3  | 1:213:A:MET:HE3  | 4        | 0.54          |
| (1,502)  | 1:162:A:TYR:HB3  | 1:183:A:THR:HA   | 19       | 0.54          |
| (1,362)  | 1:172:A:GLN:HG3  | 1:215:A:VAL:HG21 | 16       | 0.54          |
| (1,362)  | 1:172:A:GLN:HG3  | 1:215:A:VAL:HG22 | 16       | 0.54          |
| (1,362)  | 1:172:A:GLN:HG3  | 1:215:A:VAL:HG23 | 16       | 0.54          |
| (1,224)  | 1:127:A:GLY:HA3  | 1:128:A:TYR:HB2  | 4        | 0.54          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,179)  | 1:201:A:THR:HB   | 1:205:A:MET:HG3  | 7        | 0.54          |
| (1,158)  | 1:126:A:GLY:HA2  | 1:164:A:ARG:HD3  | 15       | 0.54          |
| (1,80)   | 1:208:A:ARG:HA   | 1:209:A:VAL:HG11 | 16       | 0.54          |
| (1,80)   | 1:208:A:ARG:HA   | 1:209:A:VAL:HG12 | 16       | 0.54          |
| (1,80)   | 1:208:A:ARG:HA   | 1:209:A:VAL:HG13 | 16       | 0.54          |
| (1,79)   | 1:138:A:MET:H    | 1:209:A:VAL:HG11 | 10       | 0.54          |
| (1,79)   | 1:138:A:MET:H    | 1:209:A:VAL:HG12 | 10       | 0.54          |
| (1,79)   | 1:138:A:MET:H    | 1:209:A:VAL:HG13 | 10       | 0.54          |
| (1,76)   | 1:139:A:ILE:HG12 | 1:209:A:VAL:HG11 | 1        | 0.54          |
| (1,76)   | 1:139:A:ILE:HG12 | 1:209:A:VAL:HG12 | 1        | 0.54          |
| (1,76)   | 1:139:A:ILE:HG12 | 1:209:A:VAL:HG13 | 1        | 0.54          |
| (1,76)   | 1:139:A:ILE:HG12 | 1:209:A:VAL:HG11 | 2        | 0.54          |
| (1,76)   | 1:139:A:ILE:HG12 | 1:209:A:VAL:HG12 | 2        | 0.54          |
| (1,76)   | 1:139:A:ILE:HG12 | 1:209:A:VAL:HG13 | 2        | 0.54          |
| (1,76)   | 1:139:A:ILE:HG12 | 1:209:A:VAL:HG11 | 8        | 0.54          |
| (1,76)   | 1:139:A:ILE:HG12 | 1:209:A:VAL:HG12 | 8        | 0.54          |
| (1,76)   | 1:139:A:ILE:HG12 | 1:209:A:VAL:HG13 | 8        | 0.54          |
| (1,76)   | 1:139:A:ILE:HG12 | 1:209:A:VAL:HG11 | 11       | 0.54          |
| (1,76)   | 1:139:A:ILE:HG12 | 1:209:A:VAL:HG12 | 11       | 0.54          |
| (1,76)   | 1:139:A:ILE:HG12 | 1:209:A:VAL:HG13 | 11       | 0.54          |
| (1,76)   | 1:139:A:ILE:HG12 | 1:209:A:VAL:HG11 | 19       | 0.54          |
| (1,76)   | 1:139:A:ILE:HG12 | 1:209:A:VAL:HG12 | 19       | 0.54          |
| (1,76)   | 1:139:A:ILE:HG12 | 1:209:A:VAL:HG13 | 19       | 0.54          |
| (1,76)   | 1:139:A:ILE:HG12 | 1:209:A:VAL:HG11 | 20       | 0.54          |
| (1,76)   | 1:139:A:ILE:HG12 | 1:209:A:VAL:HG12 | 20       | 0.54          |
| (1,76)   | 1:139:A:ILE:HG12 | 1:209:A:VAL:HG13 | 20       | 0.54          |
| (1,2834) | 1:163:A:TYR:HE1  | 1:221:A:GLU:HG2  | 12       | 0.53          |
| (1,2834) | 1:163:A:TYR:HE2  | 1:221:A:GLU:HG2  | 12       | 0.53          |
| (1,2615) | 1:141:A:PHE:HD1  | 1:147:A:ASP:HB3  | 17       | 0.53          |
| (1,2615) | 1:141:A:PHE:HD2  | 1:147:A:ASP:HB3  | 17       | 0.53          |
| (1,2553) | 1:126:A:GLY:HA2  | 1:128:A:TYR:HD1  | 17       | 0.53          |
| (1,2553) | 1:126:A:GLY:HA2  | 1:128:A:TYR:HD2  | 17       | 0.53          |
| (1,1894) | 1:215:A:VAL:HG21 | 1:219:A:GLN:H    | 13       | 0.53          |
| (1,1894) | 1:215:A:VAL:HG22 | 1:219:A:GLN:H    | 13       | 0.53          |
| (1,1894) | 1:215:A:VAL:HG23 | 1:219:A:GLN:H    | 13       | 0.53          |
| (1,1579) | 1:132:A:SER:HB3  | 1:133:A:ALA:H    | 3        | 0.53          |
| (1,1485) | 1:161:A:VAL:HG21 | 1:217:A:GLN:HB3  | 10       | 0.53          |
| (1,1485) | 1:161:A:VAL:HG22 | 1:217:A:GLN:HB3  | 10       | 0.53          |
| (1,1485) | 1:161:A:VAL:HG23 | 1:217:A:GLN:HB3  | 10       | 0.53          |
| (1,1294) | 1:138:A:MET:HG3  | 1:139:A:ILE:H    | 2        | 0.53          |
| (1,1212) | 1:184:A:ILE:HD11 | 1:206:A:MET:HB3  | 7        | 0.53          |
| (1,1212) | 1:184:A:ILE:HD12 | 1:206:A:MET:HB3  | 7        | 0.53          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1212) | 1:184:A:ILE:HD13 | 1:206:A:MET:HB3  | 7        | 0.53          |
| (1,1098) | 1:213:A:MET:HB2  | 1:216:A:THR:HG21 | 5        | 0.53          |
| (1,1098) | 1:213:A:MET:HB2  | 1:216:A:THR:HG22 | 5        | 0.53          |
| (1,1098) | 1:213:A:MET:HB2  | 1:216:A:THR:HG23 | 5        | 0.53          |
| (1,1098) | 1:213:A:MET:HB2  | 1:216:A:THR:HG21 | 12       | 0.53          |
| (1,1098) | 1:213:A:MET:HB2  | 1:216:A:THR:HG22 | 12       | 0.53          |
| (1,1098) | 1:213:A:MET:HB2  | 1:216:A:THR:HG23 | 12       | 0.53          |
| (1,752)  | 1:138:A:MET:HE1  | 1:139:A:ILE:HG12 | 12       | 0.53          |
| (1,752)  | 1:138:A:MET:HE2  | 1:139:A:ILE:HG12 | 12       | 0.53          |
| (1,752)  | 1:138:A:MET:HE3  | 1:139:A:ILE:HG12 | 12       | 0.53          |
| (1,663)  | 1:223:A:GLN:HG2  | 1:227:A:ASP:HB2  | 7        | 0.53          |
| (1,663)  | 1:223:A:GLN:HG2  | 1:227:A:ASP:HB3  | 7        | 0.53          |
| (1,663)  | 1:223:A:GLN:HG2  | 1:227:A:ASP:HB2  | 10       | 0.53          |
| (1,663)  | 1:223:A:GLN:HG2  | 1:227:A:ASP:HB3  | 10       | 0.53          |
| (1,663)  | 1:223:A:GLN:HG2  | 1:227:A:ASP:HB2  | 12       | 0.53          |
| (1,663)  | 1:223:A:GLN:HG2  | 1:227:A:ASP:HB3  | 12       | 0.53          |
| (1,663)  | 1:223:A:GLN:HG2  | 1:227:A:ASP:HB2  | 13       | 0.53          |
| (1,663)  | 1:223:A:GLN:HG2  | 1:227:A:ASP:HB3  | 13       | 0.53          |
| (1,663)  | 1:223:A:GLN:HG2  | 1:227:A:ASP:HB2  | 17       | 0.53          |
| (1,663)  | 1:223:A:GLN:HG2  | 1:227:A:ASP:HB3  | 17       | 0.53          |
| (1,663)  | 1:223:A:GLN:HG2  | 1:227:A:ASP:HB2  | 19       | 0.53          |
| (1,663)  | 1:223:A:GLN:HG2  | 1:227:A:ASP:HB3  | 19       | 0.53          |
| (1,657)  | 1:213:A:MET:HB3  | 1:213:A:MET:HE1  | 13       | 0.53          |
| (1,657)  | 1:213:A:MET:HB3  | 1:213:A:MET:HE2  | 13       | 0.53          |
| (1,657)  | 1:213:A:MET:HB3  | 1:213:A:MET:HE3  | 13       | 0.53          |
| (1,637)  | 1:147:A:ASP:HB2  | 1:148:A:ARG:HG2  | 2        | 0.53          |
| (1,496)  | 1:130:A:LEU:HA   | 1:162:A:TYR:HB2  | 13       | 0.53          |
| (1,476)  | 1:203:A:VAL:HG21 | 1:204:A:LYS:HE2  | 5        | 0.53          |
| (1,476)  | 1:203:A:VAL:HG21 | 1:204:A:LYS:HE3  | 5        | 0.53          |
| (1,476)  | 1:203:A:VAL:HG22 | 1:204:A:LYS:HE2  | 5        | 0.53          |
| (1,476)  | 1:203:A:VAL:HG22 | 1:204:A:LYS:HE3  | 5        | 0.53          |
| (1,476)  | 1:203:A:VAL:HG23 | 1:204:A:LYS:HE2  | 5        | 0.53          |
| (1,476)  | 1:203:A:VAL:HG23 | 1:204:A:LYS:HE3  | 5        | 0.53          |
| (1,389)  | 1:121:A:VAL:HA   | 1:122:A:VAL:HG11 | 9        | 0.53          |
| (1,389)  | 1:121:A:VAL:HA   | 1:122:A:VAL:HG12 | 9        | 0.53          |
| (1,389)  | 1:121:A:VAL:HA   | 1:122:A:VAL:HG13 | 9        | 0.53          |
| (1,339)  | 1:209:A:VAL:HG21 | 1:210:A:VAL:HG21 | 16       | 0.53          |
| (1,339)  | 1:209:A:VAL:HG21 | 1:210:A:VAL:HG22 | 16       | 0.53          |
| (1,339)  | 1:209:A:VAL:HG21 | 1:210:A:VAL:HG23 | 16       | 0.53          |
| (1,339)  | 1:209:A:VAL:HG22 | 1:210:A:VAL:HG21 | 16       | 0.53          |
| (1,339)  | 1:209:A:VAL:HG22 | 1:210:A:VAL:HG22 | 16       | 0.53          |
| (1,339)  | 1:209:A:VAL:HG22 | 1:210:A:VAL:HG23 | 16       | 0.53          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,339)  | 1:209:A:VAL:HG23 | 1:210:A:VAL:HG21 | 16       | 0.53          |
| (1,339)  | 1:209:A:VAL:HG23 | 1:210:A:VAL:HG22 | 16       | 0.53          |
| (1,339)  | 1:209:A:VAL:HG23 | 1:210:A:VAL:HG23 | 16       | 0.53          |
| (1,179)  | 1:201:A:THR:HB   | 1:205:A:MET:HG3  | 10       | 0.53          |
| (1,76)   | 1:139:A:ILE:HG12 | 1:209:A:VAL:HG11 | 4        | 0.53          |
| (1,76)   | 1:139:A:ILE:HG12 | 1:209:A:VAL:HG12 | 4        | 0.53          |
| (1,76)   | 1:139:A:ILE:HG12 | 1:209:A:VAL:HG13 | 4        | 0.53          |
| (1,76)   | 1:139:A:ILE:HG12 | 1:209:A:VAL:HG11 | 7        | 0.53          |
| (1,76)   | 1:139:A:ILE:HG12 | 1:209:A:VAL:HG12 | 7        | 0.53          |
| (1,76)   | 1:139:A:ILE:HG12 | 1:209:A:VAL:HG13 | 7        | 0.53          |
| (1,76)   | 1:139:A:ILE:HG12 | 1:209:A:VAL:HG11 | 10       | 0.53          |
| (1,76)   | 1:139:A:ILE:HG12 | 1:209:A:VAL:HG12 | 10       | 0.53          |
| (1,76)   | 1:139:A:ILE:HG12 | 1:209:A:VAL:HG13 | 10       | 0.53          |
| (1,76)   | 1:139:A:ILE:HG12 | 1:209:A:VAL:HG11 | 12       | 0.53          |
| (1,76)   | 1:139:A:ILE:HG12 | 1:209:A:VAL:HG12 | 12       | 0.53          |
| (1,76)   | 1:139:A:ILE:HG12 | 1:209:A:VAL:HG13 | 12       | 0.53          |
| (1,76)   | 1:139:A:ILE:HG12 | 1:209:A:VAL:HG11 | 13       | 0.53          |
| (1,76)   | 1:139:A:ILE:HG12 | 1:209:A:VAL:HG12 | 13       | 0.53          |
| (1,76)   | 1:139:A:ILE:HG12 | 1:209:A:VAL:HG13 | 13       | 0.53          |
| (1,76)   | 1:139:A:ILE:HG12 | 1:209:A:VAL:HG11 | 17       | 0.53          |
| (1,76)   | 1:139:A:ILE:HG12 | 1:209:A:VAL:HG12 | 17       | 0.53          |
| (1,76)   | 1:139:A:ILE:HG12 | 1:209:A:VAL:HG13 | 17       | 0.53          |
| (1,2834) | 1:163:A:TYR:HE1  | 1:221:A:GLU:HG2  | 8        | 0.52          |
| (1,2834) | 1:163:A:TYR:HE2  | 1:221:A:GLU:HG2  | 8        | 0.52          |
| (1,2824) | 1:218:A:TYR:HE1  | 1:222:A:SER:HB3  | 20       | 0.52          |
| (1,2824) | 1:218:A:TYR:HE2  | 1:222:A:SER:HB3  | 20       | 0.52          |
| (1,2782) | 1:150:A:TYR:HE1  | 1:154:A:MET:HG3  | 18       | 0.52          |
| (1,2782) | 1:150:A:TYR:HE2  | 1:154:A:MET:HG3  | 18       | 0.52          |
| (1,2774) | 1:128:A:TYR:HE1  | 1:162:A:TYR:HB3  | 10       | 0.52          |
| (1,2774) | 1:128:A:TYR:HE2  | 1:162:A:TYR:HB3  | 10       | 0.52          |
| (1,2758) | 1:150:A:TYR:HE1  | 1:209:A:VAL:HG11 | 2        | 0.52          |
| (1,2758) | 1:150:A:TYR:HE1  | 1:209:A:VAL:HG12 | 2        | 0.52          |
| (1,2758) | 1:150:A:TYR:HE1  | 1:209:A:VAL:HG13 | 2        | 0.52          |
| (1,2758) | 1:150:A:TYR:HE2  | 1:209:A:VAL:HG11 | 2        | 0.52          |
| (1,2758) | 1:150:A:TYR:HE2  | 1:209:A:VAL:HG12 | 2        | 0.52          |
| (1,2758) | 1:150:A:TYR:HE2  | 1:209:A:VAL:HG13 | 2        | 0.52          |
| (1,2721) | 1:177:A:HIS:HD2  | 1:178:A:ASP:HB3  | 19       | 0.52          |
| (1,2699) | 1:141:A:PHE:HZ   | 1:150:A:TYR:HB3  | 6        | 0.52          |
| (1,2699) | 1:141:A:PHE:HZ   | 1:150:A:TYR:HB3  | 7        | 0.52          |
| (1,2579) | 1:218:A:TYR:HD1  | 1:219:A:GLN:HG3  | 17       | 0.52          |
| (1,2579) | 1:218:A:TYR:HD2  | 1:219:A:GLN:HG3  | 17       | 0.52          |
| (1,2548) | 1:162:A:TYR:HD1  | 1:186:A:GLN:HB3  | 13       | 0.52          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2548) | 1:162:A:TYR:HD2  | 1:186:A:GLN:HB3  | 13       | 0.52          |
| (1,2492) | 1:139:A:ILE:HG12 | 1:150:A:TYR:HD1  | 8        | 0.52          |
| (1,2492) | 1:139:A:ILE:HG12 | 1:150:A:TYR:HD2  | 8        | 0.52          |
| (1,2270) | 1:132:A:SER:H    | 1:132:A:SER:HB2  | 17       | 0.52          |
| (1,1861) | 1:147:A:ASP:HB2  | 1:148:A:ARG:H    | 15       | 0.52          |
| (1,1861) | 1:147:A:ASP:HB2  | 1:148:A:ARG:H    | 17       | 0.52          |
| (1,1701) | 1:129:A:MET:H    | 1:129:A:MET:HG3  | 9        | 0.52          |
| (1,1584) | 1:122:A:VAL:H    | 1:122:A:VAL:HG11 | 15       | 0.52          |
| (1,1584) | 1:122:A:VAL:H    | 1:122:A:VAL:HG12 | 15       | 0.52          |
| (1,1584) | 1:122:A:VAL:H    | 1:122:A:VAL:HG13 | 15       | 0.52          |
| (1,1523) | 1:162:A:TYR:HB3  | 1:182:A:ILE:HG12 | 1        | 0.52          |
| (1,1523) | 1:162:A:TYR:HB3  | 1:182:A:ILE:HG13 | 1        | 0.52          |
| (1,1197) | 1:160:A:GLN:HB2  | 1:183:A:THR:HG21 | 7        | 0.52          |
| (1,1197) | 1:160:A:GLN:HB2  | 1:183:A:THR:HG22 | 7        | 0.52          |
| (1,1197) | 1:160:A:GLN:HB2  | 1:183:A:THR:HG23 | 7        | 0.52          |
| (1,1098) | 1:213:A:MET:HB2  | 1:216:A:THR:HG21 | 6        | 0.52          |
| (1,1098) | 1:213:A:MET:HB2  | 1:216:A:THR:HG22 | 6        | 0.52          |
| (1,1098) | 1:213:A:MET:HB2  | 1:216:A:THR:HG23 | 6        | 0.52          |
| (1,1098) | 1:213:A:MET:HB2  | 1:216:A:THR:HG21 | 15       | 0.52          |
| (1,1098) | 1:213:A:MET:HB2  | 1:216:A:THR:HG22 | 15       | 0.52          |
| (1,1098) | 1:213:A:MET:HB2  | 1:216:A:THR:HG23 | 15       | 0.52          |
| (1,987)  | 1:149:A:TYR:HA   | 1:152:A:GLU:HG2  | 13       | 0.52          |
| (1,893)  | 1:162:A:TYR:HB3  | 1:182:A:ILE:HB   | 17       | 0.52          |
| (1,864)  | 1:134:A:MET:HB3  | 1:135:A:SER:HB2  | 12       | 0.52          |
| (1,752)  | 1:138:A:MET:HE1  | 1:139:A:ILE:HG12 | 1        | 0.52          |
| (1,752)  | 1:138:A:MET:HE2  | 1:139:A:ILE:HG12 | 1        | 0.52          |
| (1,752)  | 1:138:A:MET:HE3  | 1:139:A:ILE:HG12 | 1        | 0.52          |
| (1,740)  | 1:197:A:ASN:HB2  | 1:198:A:PHE:H    | 10       | 0.52          |
| (1,663)  | 1:223:A:GLN:HG2  | 1:227:A:ASP:HB2  | 4        | 0.52          |
| (1,663)  | 1:223:A:GLN:HG2  | 1:227:A:ASP:HB3  | 4        | 0.52          |
| (1,563)  | 1:132:A:SER:HB3  | 1:133:A:ALA:HB1  | 4        | 0.52          |
| (1,563)  | 1:132:A:SER:HB3  | 1:133:A:ALA:HB2  | 4        | 0.52          |
| (1,563)  | 1:132:A:SER:HB3  | 1:133:A:ALA:HB3  | 4        | 0.52          |
| (1,528)  | 1:143:A:ASN:HB2  | 1:147:A:ASP:HB3  | 17       | 0.52          |
| (1,528)  | 1:143:A:ASN:HB3  | 1:147:A:ASP:HB3  | 17       | 0.52          |
| (1,423)  | 1:151:A:ARG:HD3  | 1:152:A:GLU:H    | 17       | 0.52          |
| (1,388)  | 1:122:A:VAL:HG11 | 1:186:A:GLN:HE21 | 9        | 0.52          |
| (1,388)  | 1:122:A:VAL:HG12 | 1:186:A:GLN:HE21 | 9        | 0.52          |
| (1,388)  | 1:122:A:VAL:HG13 | 1:186:A:GLN:HE21 | 9        | 0.52          |
| (1,224)  | 1:127:A:GLY:HA3  | 1:128:A:TYR:HB2  | 2        | 0.52          |
| (1,224)  | 1:127:A:GLY:HA3  | 1:128:A:TYR:HB2  | 8        | 0.52          |
| (1,224)  | 1:127:A:GLY:HA3  | 1:128:A:TYR:HB2  | 17       | 0.52          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,224)  | 1:127:A:GLY:HA3  | 1:128:A:TYR:HB2  | 19       | 0.52          |
| (1,174)  | 1:202:A:ASP:HB3  | 1:203:A:VAL:HG11 | 8        | 0.52          |
| (1,174)  | 1:202:A:ASP:HB3  | 1:203:A:VAL:HG12 | 8        | 0.52          |
| (1,174)  | 1:202:A:ASP:HB3  | 1:203:A:VAL:HG13 | 8        | 0.52          |
| (1,155)  | 1:125:A:LEU:HB3  | 1:126:A:GLY:HA3  | 1        | 0.52          |
| (1,79)   | 1:138:A:MET:H    | 1:209:A:VAL:HG11 | 7        | 0.52          |
| (1,79)   | 1:138:A:MET:H    | 1:209:A:VAL:HG12 | 7        | 0.52          |
| (1,79)   | 1:138:A:MET:H    | 1:209:A:VAL:HG13 | 7        | 0.52          |
| (1,76)   | 1:139:A:ILE:HG12 | 1:209:A:VAL:HG11 | 14       | 0.52          |
| (1,76)   | 1:139:A:ILE:HG12 | 1:209:A:VAL:HG12 | 14       | 0.52          |
| (1,76)   | 1:139:A:ILE:HG12 | 1:209:A:VAL:HG13 | 14       | 0.52          |
| (1,76)   | 1:139:A:ILE:HG12 | 1:209:A:VAL:HG11 | 16       | 0.52          |
| (1,76)   | 1:139:A:ILE:HG12 | 1:209:A:VAL:HG12 | 16       | 0.52          |
| (1,76)   | 1:139:A:ILE:HG12 | 1:209:A:VAL:HG13 | 16       | 0.52          |
| (1,2834) | 1:163:A:TYR:HE1  | 1:221:A:GLU:HG2  | 20       | 0.51          |
| (1,2834) | 1:163:A:TYR:HE2  | 1:221:A:GLU:HG2  | 20       | 0.51          |
| (1,2791) | 1:126:A:GLY:HA2  | 1:128:A:TYR:HE1  | 8        | 0.51          |
| (1,2791) | 1:126:A:GLY:HA2  | 1:128:A:TYR:HE2  | 8        | 0.51          |
| (1,2771) | 1:130:A:LEU:HB3  | 1:162:A:TYR:HE1  | 4        | 0.51          |
| (1,2771) | 1:130:A:LEU:HB3  | 1:162:A:TYR:HE2  | 4        | 0.51          |
| (1,2771) | 1:130:A:LEU:HB3  | 1:162:A:TYR:HE1  | 9        | 0.51          |
| (1,2771) | 1:130:A:LEU:HB3  | 1:162:A:TYR:HE2  | 9        | 0.51          |
| (1,2759) | 1:139:A:ILE:HG12 | 1:150:A:TYR:HE1  | 12       | 0.51          |
| (1,2759) | 1:139:A:ILE:HG12 | 1:150:A:TYR:HE2  | 12       | 0.51          |
| (1,2758) | 1:150:A:TYR:HE1  | 1:209:A:VAL:HG11 | 20       | 0.51          |
| (1,2758) | 1:150:A:TYR:HE1  | 1:209:A:VAL:HG12 | 20       | 0.51          |
| (1,2758) | 1:150:A:TYR:HE1  | 1:209:A:VAL:HG13 | 20       | 0.51          |
| (1,2758) | 1:150:A:TYR:HE2  | 1:209:A:VAL:HG11 | 20       | 0.51          |
| (1,2758) | 1:150:A:TYR:HE2  | 1:209:A:VAL:HG12 | 20       | 0.51          |
| (1,2758) | 1:150:A:TYR:HE2  | 1:209:A:VAL:HG13 | 20       | 0.51          |
| (1,2756) | 1:150:A:TYR:HE1  | 1:205:A:MET:HG2  | 9        | 0.51          |
| (1,2756) | 1:150:A:TYR:HE2  | 1:205:A:MET:HG2  | 9        | 0.51          |
| (1,2699) | 1:141:A:PHE:HZ   | 1:150:A:TYR:HB3  | 3        | 0.51          |
| (1,2699) | 1:141:A:PHE:HZ   | 1:150:A:TYR:HB3  | 10       | 0.51          |
| (1,2650) | 1:139:A:ILE:HG12 | 1:141:A:PHE:HE1  | 8        | 0.51          |
| (1,2650) | 1:139:A:ILE:HG12 | 1:141:A:PHE:HE2  | 8        | 0.51          |
| (1,2553) | 1:126:A:GLY:HA2  | 1:128:A:TYR:HD1  | 10       | 0.51          |
| (1,2553) | 1:126:A:GLY:HA2  | 1:128:A:TYR:HD2  | 10       | 0.51          |
| (1,2536) | 1:167:A:SER:HB3  | 1:225:A:TYR:HD1  | 4        | 0.51          |
| (1,2536) | 1:167:A:SER:HB3  | 1:225:A:TYR:HD2  | 4        | 0.51          |
| (1,1894) | 1:215:A:VAL:HG21 | 1:219:A:GLN:H    | 8        | 0.51          |
| (1,1894) | 1:215:A:VAL:HG22 | 1:219:A:GLN:H    | 8        | 0.51          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1894) | 1:215:A:VAL:HG23 | 1:219:A:GLN:H    | 8        | 0.51          |
| (1,1678) | 1:125:A:LEU:H    | 1:125:A:LEU:HB2  | 6        | 0.51          |
| (1,1584) | 1:122:A:VAL:H    | 1:122:A:VAL:HG11 | 2        | 0.51          |
| (1,1584) | 1:122:A:VAL:H    | 1:122:A:VAL:HG12 | 2        | 0.51          |
| (1,1584) | 1:122:A:VAL:H    | 1:122:A:VAL:HG13 | 2        | 0.51          |
| (1,1584) | 1:122:A:VAL:H    | 1:122:A:VAL:HG11 | 12       | 0.51          |
| (1,1584) | 1:122:A:VAL:H    | 1:122:A:VAL:HG12 | 12       | 0.51          |
| (1,1584) | 1:122:A:VAL:H    | 1:122:A:VAL:HG13 | 12       | 0.51          |
| (1,1523) | 1:162:A:TYR:HB3  | 1:182:A:ILE:HG12 | 14       | 0.51          |
| (1,1523) | 1:162:A:TYR:HB3  | 1:182:A:ILE:HG13 | 14       | 0.51          |
| (1,1303) | 1:137:A:PRO:HB2  | 1:213:A:MET:HG2  | 10       | 0.51          |
| (1,1256) | 1:184:A:ILE:HG13 | 1:206:A:MET:HG3  | 9        | 0.51          |
| (1,1212) | 1:184:A:ILE:HD11 | 1:206:A:MET:HB3  | 6        | 0.51          |
| (1,1212) | 1:184:A:ILE:HD12 | 1:206:A:MET:HB3  | 6        | 0.51          |
| (1,1212) | 1:184:A:ILE:HD13 | 1:206:A:MET:HB3  | 6        | 0.51          |
| (1,907)  | 1:226:A:TYR:HA   | 1:229:A:ARG:HB2  | 5        | 0.51          |
| (1,893)  | 1:162:A:TYR:HB3  | 1:182:A:ILE:HB   | 18       | 0.51          |
| (1,833)  | 1:207:A:GLU:HA   | 1:207:A:GLU:HG3  | 18       | 0.51          |
| (1,775)  | 1:203:A:VAL:HG11 | 1:206:A:MET:HE1  | 18       | 0.51          |
| (1,775)  | 1:203:A:VAL:HG11 | 1:206:A:MET:HE2  | 18       | 0.51          |
| (1,775)  | 1:203:A:VAL:HG11 | 1:206:A:MET:HE3  | 18       | 0.51          |
| (1,775)  | 1:203:A:VAL:HG12 | 1:206:A:MET:HE1  | 18       | 0.51          |
| (1,775)  | 1:203:A:VAL:HG12 | 1:206:A:MET:HE2  | 18       | 0.51          |
| (1,775)  | 1:203:A:VAL:HG12 | 1:206:A:MET:HE3  | 18       | 0.51          |
| (1,775)  | 1:203:A:VAL:HG13 | 1:206:A:MET:HE1  | 18       | 0.51          |
| (1,775)  | 1:203:A:VAL:HG13 | 1:206:A:MET:HE2  | 18       | 0.51          |
| (1,775)  | 1:203:A:VAL:HG13 | 1:206:A:MET:HE3  | 18       | 0.51          |
| (1,740)  | 1:197:A:ASN:HB2  | 1:198:A:PHE:H    | 9        | 0.51          |
| (1,663)  | 1:223:A:GLN:HG2  | 1:227:A:ASP:HB2  | 5        | 0.51          |
| (1,663)  | 1:223:A:GLN:HG2  | 1:227:A:ASP:HB3  | 5        | 0.51          |
| (1,663)  | 1:223:A:GLN:HG2  | 1:227:A:ASP:HB2  | 14       | 0.51          |
| (1,663)  | 1:223:A:GLN:HG2  | 1:227:A:ASP:HB3  | 14       | 0.51          |
| (1,567)  | 1:230:A:ARG:HB2  | 1:231:A:SER:HB3  | 5        | 0.51          |
| (1,389)  | 1:121:A:VAL:HA   | 1:122:A:VAL:HG11 | 18       | 0.51          |
| (1,389)  | 1:121:A:VAL:HA   | 1:122:A:VAL:HG12 | 18       | 0.51          |
| (1,389)  | 1:121:A:VAL:HA   | 1:122:A:VAL:HG13 | 18       | 0.51          |
| (1,359)  | 1:122:A:VAL:HG21 | 1:182:A:ILE:HG21 | 16       | 0.51          |
| (1,359)  | 1:122:A:VAL:HG21 | 1:182:A:ILE:HG22 | 16       | 0.51          |
| (1,359)  | 1:122:A:VAL:HG21 | 1:182:A:ILE:HG23 | 16       | 0.51          |
| (1,359)  | 1:122:A:VAL:HG22 | 1:182:A:ILE:HG21 | 16       | 0.51          |
| (1,359)  | 1:122:A:VAL:HG22 | 1:182:A:ILE:HG22 | 16       | 0.51          |
| (1,359)  | 1:122:A:VAL:HG22 | 1:182:A:ILE:HG23 | 16       | 0.51          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,359)  | 1:122:A:VAL:HG23 | 1:182:A:ILE:HG21 | 16       | 0.51          |
| (1,359)  | 1:122:A:VAL:HG23 | 1:182:A:ILE:HG22 | 16       | 0.51          |
| (1,359)  | 1:122:A:VAL:HG23 | 1:182:A:ILE:HG23 | 16       | 0.51          |
| (1,2774) | 1:128:A:TYR:HE1  | 1:162:A:TYR:HB3  | 3        | 0.5           |
| (1,2774) | 1:128:A:TYR:HE2  | 1:162:A:TYR:HB3  | 3        | 0.5           |
| (1,2774) | 1:128:A:TYR:HE1  | 1:162:A:TYR:HB3  | 19       | 0.5           |
| (1,2774) | 1:128:A:TYR:HE2  | 1:162:A:TYR:HB3  | 19       | 0.5           |
| (1,2759) | 1:139:A:ILE:HG12 | 1:150:A:TYR:HE1  | 11       | 0.5           |
| (1,2759) | 1:139:A:ILE:HG12 | 1:150:A:TYR:HE2  | 11       | 0.5           |
| (1,2548) | 1:162:A:TYR:HD1  | 1:186:A:GLN:HB3  | 14       | 0.5           |
| (1,2548) | 1:162:A:TYR:HD2  | 1:186:A:GLN:HB3  | 14       | 0.5           |
| (1,2482) | 1:163:A:TYR:HD1  | 1:221:A:GLU:HG2  | 15       | 0.5           |
| (1,2482) | 1:163:A:TYR:HD2  | 1:221:A:GLU:HG2  | 15       | 0.5           |
| (1,2445) | 1:122:A:VAL:HG21 | 1:124:A:GLY:H    | 18       | 0.5           |
| (1,2445) | 1:122:A:VAL:HG22 | 1:124:A:GLY:H    | 18       | 0.5           |
| (1,2445) | 1:122:A:VAL:HG23 | 1:124:A:GLY:H    | 18       | 0.5           |
| (1,2326) | 1:223:A:GLN:HE21 | 1:228:A:GLY:H    | 5        | 0.5           |
| (1,2326) | 1:223:A:GLN:HE21 | 1:228:A:GLY:H    | 10       | 0.5           |
| (1,2270) | 1:132:A:SER:H    | 1:132:A:SER:HB2  | 6        | 0.5           |
| (1,1937) | 1:220:A:LYS:H    | 1:221:A:GLU:HG3  | 5        | 0.5           |
| (1,1894) | 1:215:A:VAL:HG21 | 1:219:A:GLN:H    | 19       | 0.5           |
| (1,1894) | 1:215:A:VAL:HG22 | 1:219:A:GLN:H    | 19       | 0.5           |
| (1,1894) | 1:215:A:VAL:HG23 | 1:219:A:GLN:H    | 19       | 0.5           |
| (1,1893) | 1:208:A:ARG:HB3  | 1:209:A:VAL:H    | 10       | 0.5           |
| (1,1303) | 1:137:A:PRO:HB2  | 1:213:A:MET:HG2  | 14       | 0.5           |
| (1,1294) | 1:138:A:MET:HG3  | 1:139:A:ILE:H    | 12       | 0.5           |
| (1,1212) | 1:184:A:ILE:HD11 | 1:206:A:MET:HB3  | 8        | 0.5           |
| (1,1212) | 1:184:A:ILE:HD12 | 1:206:A:MET:HB3  | 8        | 0.5           |
| (1,1212) | 1:184:A:ILE:HD13 | 1:206:A:MET:HB3  | 8        | 0.5           |
| (1,957)  | 1:184:A:ILE:HD11 | 1:207:A:GLU:HG3  | 4        | 0.5           |
| (1,957)  | 1:184:A:ILE:HD12 | 1:207:A:GLU:HG3  | 4        | 0.5           |
| (1,957)  | 1:184:A:ILE:HD13 | 1:207:A:GLU:HG3  | 4        | 0.5           |
| (1,921)  | 1:167:A:SER:HA   | 1:168:A:GLN:HG3  | 4        | 0.5           |
| (1,901)  | 1:203:A:VAL:HG21 | 1:204:A:LYS:HA   | 7        | 0.5           |
| (1,901)  | 1:203:A:VAL:HG22 | 1:204:A:LYS:HA   | 7        | 0.5           |
| (1,901)  | 1:203:A:VAL:HG23 | 1:204:A:LYS:HA   | 7        | 0.5           |
| (1,873)  | 1:146:A:GLU:HA   | 1:150:A:TYR:HB3  | 10       | 0.5           |
| (1,862)  | 1:143:A:ASN:HD22 | 1:146:A:GLU:HG2  | 16       | 0.5           |
| (1,740)  | 1:197:A:ASN:HB2  | 1:198:A:PHE:H    | 5        | 0.5           |
| (1,663)  | 1:223:A:GLN:HG2  | 1:227:A:ASP:HB2  | 8        | 0.5           |
| (1,663)  | 1:223:A:GLN:HG2  | 1:227:A:ASP:HB3  | 8        | 0.5           |
| (1,663)  | 1:223:A:GLN:HG2  | 1:227:A:ASP:HB2  | 16       | 0.5           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,663)  | 1:223:A:GLN:HG2  | 1:227:A:ASP:HB3  | 16       | 0.5           |
| (1,634)  | 1:192:A:THR:HA   | 1:195:A:GLY:HA3  | 20       | 0.5           |
| (1,602)  | 1:230:A:ARG:H    | 1:231:A:SER:HB3  | 8        | 0.5           |
| (1,563)  | 1:132:A:SER:HB3  | 1:133:A:ALA:HB1  | 14       | 0.5           |
| (1,563)  | 1:132:A:SER:HB3  | 1:133:A:ALA:HB2  | 14       | 0.5           |
| (1,563)  | 1:132:A:SER:HB3  | 1:133:A:ALA:HB3  | 14       | 0.5           |
| (1,502)  | 1:162:A:TYR:HB3  | 1:183:A:THR:HA   | 3        | 0.5           |
| (1,445)  | 1:180:A:VAL:HA   | 1:184:A:ILE:HG12 | 16       | 0.5           |
| (1,389)  | 1:121:A:VAL:HA   | 1:122:A:VAL:HG11 | 15       | 0.5           |
| (1,389)  | 1:121:A:VAL:HA   | 1:122:A:VAL:HG12 | 15       | 0.5           |
| (1,389)  | 1:121:A:VAL:HA   | 1:122:A:VAL:HG13 | 15       | 0.5           |
| (1,179)  | 1:201:A:THR:HB   | 1:205:A:MET:HG3  | 4        | 0.5           |
| (1,166)  | 1:203:A:VAL:HG11 | 1:206:A:MET:HG2  | 18       | 0.5           |
| (1,166)  | 1:203:A:VAL:HG12 | 1:206:A:MET:HG2  | 18       | 0.5           |
| (1,166)  | 1:203:A:VAL:HG13 | 1:206:A:MET:HG2  | 18       | 0.5           |
| (1,2834) | 1:163:A:TYR:HE1  | 1:221:A:GLU:HG2  | 4        | 0.49          |
| (1,2834) | 1:163:A:TYR:HE2  | 1:221:A:GLU:HG2  | 4        | 0.49          |
| (1,2759) | 1:139:A:ILE:HG12 | 1:150:A:TYR:HE1  | 6        | 0.49          |
| (1,2759) | 1:139:A:ILE:HG12 | 1:150:A:TYR:HE2  | 6        | 0.49          |
| (1,2756) | 1:150:A:TYR:HE1  | 1:205:A:MET:HG2  | 1        | 0.49          |
| (1,2756) | 1:150:A:TYR:HE2  | 1:205:A:MET:HG2  | 1        | 0.49          |
| (1,2721) | 1:177:A:HIS:HD2  | 1:178:A:ASP:HB3  | 18       | 0.49          |
| (1,2699) | 1:141:A:PHE:HZ   | 1:150:A:TYR:HB3  | 17       | 0.49          |
| (1,2657) | 1:141:A:PHE:HE1  | 1:208:A:ARG:HB3  | 11       | 0.49          |
| (1,2657) | 1:141:A:PHE:HE2  | 1:208:A:ARG:HB3  | 11       | 0.49          |
| (1,2548) | 1:162:A:TYR:HD1  | 1:186:A:GLN:HB3  | 1        | 0.49          |
| (1,2548) | 1:162:A:TYR:HD2  | 1:186:A:GLN:HB3  | 1        | 0.49          |
| (1,2548) | 1:162:A:TYR:HD1  | 1:186:A:GLN:HB3  | 12       | 0.49          |
| (1,2548) | 1:162:A:TYR:HD2  | 1:186:A:GLN:HB3  | 12       | 0.49          |
| (1,2501) | 1:149:A:TYR:HD1  | 1:205:A:MET:HG2  | 13       | 0.49          |
| (1,2501) | 1:149:A:TYR:HD2  | 1:205:A:MET:HG2  | 13       | 0.49          |
| (1,2469) | 1:166:A:VAL:HG21 | 1:169:A:TYR:HD1  | 12       | 0.49          |
| (1,2469) | 1:166:A:VAL:HG21 | 1:169:A:TYR:HD2  | 12       | 0.49          |
| (1,2469) | 1:166:A:VAL:HG22 | 1:169:A:TYR:HD1  | 12       | 0.49          |
| (1,2469) | 1:166:A:VAL:HG22 | 1:169:A:TYR:HD2  | 12       | 0.49          |
| (1,2469) | 1:166:A:VAL:HG23 | 1:169:A:TYR:HD1  | 12       | 0.49          |
| (1,2469) | 1:166:A:VAL:HG23 | 1:169:A:TYR:HD2  | 12       | 0.49          |
| (1,2270) | 1:132:A:SER:H    | 1:132:A:SER:HB2  | 10       | 0.49          |
| (1,2129) | 1:186:A:GLN:H    | 1:186:A:GLN:HB3  | 5        | 0.49          |
| (1,2129) | 1:186:A:GLN:H    | 1:186:A:GLN:HB3  | 13       | 0.49          |
| (1,1861) | 1:147:A:ASP:HB2  | 1:148:A:ARG:H    | 4        | 0.49          |
| (1,1579) | 1:132:A:SER:HB3  | 1:133:A:ALA:H    | 7        | 0.49          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1523) | 1:162:A:TYR:HB3  | 1:182:A:ILE:HG12 | 20       | 0.49          |
| (1,1523) | 1:162:A:TYR:HB3  | 1:182:A:ILE:HG13 | 20       | 0.49          |
| (1,1303) | 1:137:A:PRO:HB2  | 1:213:A:MET:HG2  | 4        | 0.49          |
| (1,1256) | 1:184:A:ILE:HG13 | 1:206:A:MET:HG3  | 14       | 0.49          |
| (1,1227) | 1:210:A:VAL:HA   | 1:213:A:MET:HG2  | 12       | 0.49          |
| (1,1212) | 1:184:A:ILE:HD11 | 1:206:A:MET:HB3  | 2        | 0.49          |
| (1,1212) | 1:184:A:ILE:HD12 | 1:206:A:MET:HB3  | 2        | 0.49          |
| (1,1212) | 1:184:A:ILE:HD13 | 1:206:A:MET:HB3  | 2        | 0.49          |
| (1,1212) | 1:184:A:ILE:HD11 | 1:206:A:MET:HB3  | 3        | 0.49          |
| (1,1212) | 1:184:A:ILE:HD12 | 1:206:A:MET:HB3  | 3        | 0.49          |
| (1,1212) | 1:184:A:ILE:HD13 | 1:206:A:MET:HB3  | 3        | 0.49          |
| (1,1169) | 1:216:A:THR:HB   | 1:219:A:GLN:HG3  | 19       | 0.49          |
| (1,1168) | 1:223:A:GLN:H    | 1:223:A:GLN:HG2  | 8        | 0.49          |
| (1,901)  | 1:203:A:VAL:HG21 | 1:204:A:LYS:HA   | 8        | 0.49          |
| (1,901)  | 1:203:A:VAL:HG22 | 1:204:A:LYS:HA   | 8        | 0.49          |
| (1,901)  | 1:203:A:VAL:HG23 | 1:204:A:LYS:HA   | 8        | 0.49          |
| (1,893)  | 1:162:A:TYR:HB3  | 1:182:A:ILE:HB   | 7        | 0.49          |
| (1,881)  | 1:145:A:TRP:HE3  | 1:146:A:GLU:HG3  | 4        | 0.49          |
| (1,828)  | 1:222:A:SER:HA   | 1:226:A:TYR:HB3  | 1        | 0.49          |
| (1,740)  | 1:197:A:ASN:HB2  | 1:198:A:PHE:H    | 4        | 0.49          |
| (1,663)  | 1:223:A:GLN:HG2  | 1:227:A:ASP:HB2  | 3        | 0.49          |
| (1,663)  | 1:223:A:GLN:HG2  | 1:227:A:ASP:HB3  | 3        | 0.49          |
| (1,663)  | 1:223:A:GLN:HG2  | 1:227:A:ASP:HB2  | 9        | 0.49          |
| (1,663)  | 1:223:A:GLN:HG2  | 1:227:A:ASP:HB3  | 9        | 0.49          |
| (1,634)  | 1:192:A:THR:HA   | 1:195:A:GLY:HA3  | 18       | 0.49          |
| (1,598)  | 1:161:A:VAL:HG21 | 1:213:A:MET:HB3  | 10       | 0.49          |
| (1,598)  | 1:161:A:VAL:HG22 | 1:213:A:MET:HB3  | 10       | 0.49          |
| (1,598)  | 1:161:A:VAL:HG23 | 1:213:A:MET:HB3  | 10       | 0.49          |
| (1,569)  | 1:128:A:TYR:HE1  | 1:179:A:CYS:HB3  | 16       | 0.49          |
| (1,569)  | 1:128:A:TYR:HE2  | 1:179:A:CYS:HB3  | 16       | 0.49          |
| (1,445)  | 1:180:A:VAL:HA   | 1:184:A:ILE:HG12 | 1        | 0.49          |
| (1,336)  | 1:163:A:TYR:HD1  | 1:166:A:VAL:HG11 | 17       | 0.49          |
| (1,336)  | 1:163:A:TYR:HD1  | 1:166:A:VAL:HG12 | 17       | 0.49          |
| (1,336)  | 1:163:A:TYR:HD1  | 1:166:A:VAL:HG13 | 17       | 0.49          |
| (1,336)  | 1:163:A:TYR:HD2  | 1:166:A:VAL:HG11 | 17       | 0.49          |
| (1,336)  | 1:163:A:TYR:HD2  | 1:166:A:VAL:HG12 | 17       | 0.49          |
| (1,336)  | 1:163:A:TYR:HD2  | 1:166:A:VAL:HG13 | 17       | 0.49          |
| (1,216)  | 1:216:A:THR:HG21 | 1:220:A:LYS:HG3  | 19       | 0.49          |
| (1,216)  | 1:216:A:THR:HG22 | 1:220:A:LYS:HG3  | 19       | 0.49          |
| (1,216)  | 1:216:A:THR:HG23 | 1:220:A:LYS:HG3  | 19       | 0.49          |
| (1,177)  | 1:195:A:GLY:HA3  | 1:197:A:ASN:HD21 | 16       | 0.49          |
| (1,160)  | 1:223:A:GLN:HE21 | 1:228:A:GLY:HA2  | 4        | 0.49          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,160)  | 1:223:A:GLN:HE21 | 1:228:A:GLY:HA3  | 4        | 0.49          |
| (1,151)  | 1:126:A:GLY:HA3  | 1:164:A:ARG:HD3  | 18       | 0.49          |
| (1,89)   | 1:206:A:MET:HB3  | 1:210:A:VAL:HG21 | 17       | 0.49          |
| (1,89)   | 1:206:A:MET:HB3  | 1:210:A:VAL:HG22 | 17       | 0.49          |
| (1,89)   | 1:206:A:MET:HB3  | 1:210:A:VAL:HG23 | 17       | 0.49          |
| (1,79)   | 1:138:A:MET:H    | 1:209:A:VAL:HG11 | 17       | 0.49          |
| (1,79)   | 1:138:A:MET:H    | 1:209:A:VAL:HG12 | 17       | 0.49          |
| (1,79)   | 1:138:A:MET:H    | 1:209:A:VAL:HG13 | 17       | 0.49          |
| (1,2830) | 1:172:A:GLN:HG2  | 1:218:A:TYR:HE1  | 17       | 0.48          |
| (1,2830) | 1:172:A:GLN:HG2  | 1:218:A:TYR:HE2  | 17       | 0.48          |
| (1,2807) | 1:149:A:TYR:HE1  | 1:153:A:ASN:HB3  | 11       | 0.48          |
| (1,2807) | 1:149:A:TYR:HE2  | 1:153:A:ASN:HB3  | 11       | 0.48          |
| (1,2771) | 1:130:A:LEU:HB3  | 1:162:A:TYR:HE1  | 5        | 0.48          |
| (1,2771) | 1:130:A:LEU:HB3  | 1:162:A:TYR:HE2  | 5        | 0.48          |
| (1,2758) | 1:150:A:TYR:HE1  | 1:209:A:VAL:HG11 | 18       | 0.48          |
| (1,2758) | 1:150:A:TYR:HE1  | 1:209:A:VAL:HG12 | 18       | 0.48          |
| (1,2758) | 1:150:A:TYR:HE1  | 1:209:A:VAL:HG13 | 18       | 0.48          |
| (1,2758) | 1:150:A:TYR:HE2  | 1:209:A:VAL:HG11 | 18       | 0.48          |
| (1,2758) | 1:150:A:TYR:HE2  | 1:209:A:VAL:HG12 | 18       | 0.48          |
| (1,2758) | 1:150:A:TYR:HE2  | 1:209:A:VAL:HG13 | 18       | 0.48          |
| (1,2756) | 1:150:A:TYR:HE1  | 1:205:A:MET:HG2  | 16       | 0.48          |
| (1,2756) | 1:150:A:TYR:HE2  | 1:205:A:MET:HG2  | 16       | 0.48          |
| (1,2756) | 1:150:A:TYR:HE1  | 1:205:A:MET:HG2  | 18       | 0.48          |
| (1,2756) | 1:150:A:TYR:HE2  | 1:205:A:MET:HG2  | 18       | 0.48          |
| (1,2736) | 1:184:A:ILE:HG13 | 1:187:A:HIS:HD2  | 5        | 0.48          |
| (1,2736) | 1:184:A:ILE:HG13 | 1:187:A:HIS:HD2  | 9        | 0.48          |
| (1,2518) | 1:155:A:TYR:HD1  | 1:156:A:ARG:HD2  | 8        | 0.48          |
| (1,2518) | 1:155:A:TYR:HD2  | 1:156:A:ARG:HD2  | 8        | 0.48          |
| (1,2414) | 1:136:A:ARG:HB3  | 1:159:A:ASN:HD21 | 12       | 0.48          |
| (1,2129) | 1:186:A:GLN:H    | 1:186:A:GLN:HB3  | 3        | 0.48          |
| (1,2129) | 1:186:A:GLN:H    | 1:186:A:GLN:HB3  | 19       | 0.48          |
| (1,1679) | 1:122:A:VAL:HG21 | 1:125:A:LEU:H    | 6        | 0.48          |
| (1,1679) | 1:122:A:VAL:HG22 | 1:125:A:LEU:H    | 6        | 0.48          |
| (1,1679) | 1:122:A:VAL:HG23 | 1:125:A:LEU:H    | 6        | 0.48          |
| (1,1678) | 1:125:A:LEU:H    | 1:125:A:LEU:HB2  | 17       | 0.48          |
| (1,1523) | 1:162:A:TYR:HB3  | 1:182:A:ILE:HG12 | 5        | 0.48          |
| (1,1523) | 1:162:A:TYR:HB3  | 1:182:A:ILE:HG13 | 5        | 0.48          |
| (1,1523) | 1:162:A:TYR:HB3  | 1:182:A:ILE:HG12 | 13       | 0.48          |
| (1,1523) | 1:162:A:TYR:HB3  | 1:182:A:ILE:HG13 | 13       | 0.48          |
| (1,1285) | 1:205:A:MET:H    | 1:206:A:MET:HG2  | 6        | 0.48          |
| (1,1166) | 1:215:A:VAL:HG21 | 1:219:A:GLN:HG3  | 12       | 0.48          |
| (1,1166) | 1:215:A:VAL:HG22 | 1:219:A:GLN:HG3  | 12       | 0.48          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1166) | 1:215:A:VAL:HG23 | 1:219:A:GLN:HG3  | 12       | 0.48          |
| (1,1060) | 1:207:A:GLU:HG3  | 1:208:A:ARG:H    | 14       | 0.48          |
| (1,1015) | 1:152:A:GLU:HG2  | 1:153:A:ASN:HD22 | 20       | 0.48          |
| (1,862)  | 1:143:A:ASN:HD22 | 1:146:A:GLU:HG2  | 20       | 0.48          |
| (1,833)  | 1:207:A:GLU:HA   | 1:207:A:GLU:HG3  | 15       | 0.48          |
| (1,752)  | 1:138:A:MET:HE1  | 1:139:A:ILE:HG12 | 19       | 0.48          |
| (1,752)  | 1:138:A:MET:HE2  | 1:139:A:ILE:HG12 | 19       | 0.48          |
| (1,752)  | 1:138:A:MET:HE3  | 1:139:A:ILE:HG12 | 19       | 0.48          |
| (1,657)  | 1:213:A:MET:HB3  | 1:213:A:MET:HE1  | 11       | 0.48          |
| (1,657)  | 1:213:A:MET:HB3  | 1:213:A:MET:HE2  | 11       | 0.48          |
| (1,657)  | 1:213:A:MET:HB3  | 1:213:A:MET:HE3  | 11       | 0.48          |
| (1,634)  | 1:192:A:THR:HA   | 1:195:A:GLY:HA3  | 12       | 0.48          |
| (1,575)  | 1:134:A:MET:HE1  | 1:135:A:SER:HB2  | 3        | 0.48          |
| (1,575)  | 1:134:A:MET:HE2  | 1:135:A:SER:HB2  | 3        | 0.48          |
| (1,575)  | 1:134:A:MET:HE3  | 1:135:A:SER:HB2  | 3        | 0.48          |
| (1,563)  | 1:132:A:SER:HB3  | 1:133:A:ALA:HB1  | 10       | 0.48          |
| (1,563)  | 1:132:A:SER:HB3  | 1:133:A:ALA:HB2  | 10       | 0.48          |
| (1,563)  | 1:132:A:SER:HB3  | 1:133:A:ALA:HB3  | 10       | 0.48          |
| (1,507)  | 1:211:A:GLU:HG3  | 1:214:A:CYS:HB2  | 7        | 0.48          |
| (1,159)  | 1:228:A:GLY:HA2  | 1:230:A:ARG:HD2  | 1        | 0.48          |
| (1,159)  | 1:228:A:GLY:HA3  | 1:230:A:ARG:HD2  | 1        | 0.48          |
| (1,128)  | 1:161:A:VAL:HG11 | 1:213:A:MET:HB3  | 9        | 0.48          |
| (1,128)  | 1:161:A:VAL:HG12 | 1:213:A:MET:HB3  | 9        | 0.48          |
| (1,128)  | 1:161:A:VAL:HG13 | 1:213:A:MET:HB3  | 9        | 0.48          |
| (1,1)    | 1:138:A:MET:HG3  | 1:139:A:ILE:HG12 | 14       | 0.48          |
| (1,2830) | 1:172:A:GLN:HG2  | 1:218:A:TYR:HE1  | 13       | 0.47          |
| (1,2830) | 1:172:A:GLN:HG2  | 1:218:A:TYR:HE2  | 13       | 0.47          |
| (1,2759) | 1:139:A:ILE:HG12 | 1:150:A:TYR:HE1  | 10       | 0.47          |
| (1,2759) | 1:139:A:ILE:HG12 | 1:150:A:TYR:HE2  | 10       | 0.47          |
| (1,2756) | 1:150:A:TYR:HE1  | 1:205:A:MET:HG2  | 2        | 0.47          |
| (1,2756) | 1:150:A:TYR:HE2  | 1:205:A:MET:HG2  | 2        | 0.47          |
| (1,2681) | 1:141:A:PHE:HZ   | 1:208:A:ARG:HB3  | 13       | 0.47          |
| (1,2507) | 1:150:A:TYR:HD1  | 1:151:A:ARG:HG3  | 8        | 0.47          |
| (1,2507) | 1:150:A:TYR:HD2  | 1:151:A:ARG:HG3  | 8        | 0.47          |
| (1,2501) | 1:149:A:TYR:HD1  | 1:205:A:MET:HG2  | 15       | 0.47          |
| (1,2501) | 1:149:A:TYR:HD2  | 1:205:A:MET:HG2  | 15       | 0.47          |
| (1,2488) | 1:149:A:TYR:HD1  | 1:153:A:ASN:HB3  | 19       | 0.47          |
| (1,2488) | 1:149:A:TYR:HD2  | 1:153:A:ASN:HB3  | 19       | 0.47          |
| (1,2326) | 1:223:A:GLN:HE21 | 1:228:A:GLY:H    | 12       | 0.47          |
| (1,2320) | 1:160:A:GLN:HE22 | 1:213:A:MET:HB2  | 10       | 0.47          |
| (1,2313) | 1:159:A:ASN:HD22 | 1:160:A:GLN:HE21 | 9        | 0.47          |
| (1,1937) | 1:220:A:LYS:H    | 1:221:A:GLU:HG3  | 9        | 0.47          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1701) | 1:129:A:MET:H    | 1:129:A:MET:HG3  | 17       | 0.47          |
| (1,1579) | 1:132:A:SER:HB3  | 1:133:A:ALA:H    | 15       | 0.47          |
| (1,1538) | 1:164:A:ARG:HD2  | 1:165:A:PRO:HD3  | 8        | 0.47          |
| (1,1168) | 1:223:A:GLN:H    | 1:223:A:GLN:HG2  | 10       | 0.47          |
| (1,996)  | 1:176:A:VAL:HA   | 1:211:A:GLU:HG3  | 7        | 0.47          |
| (1,957)  | 1:184:A:ILE:HD11 | 1:207:A:GLU:HG3  | 10       | 0.47          |
| (1,957)  | 1:184:A:ILE:HD12 | 1:207:A:GLU:HG3  | 10       | 0.47          |
| (1,957)  | 1:184:A:ILE:HD13 | 1:207:A:GLU:HG3  | 10       | 0.47          |
| (1,944)  | 1:171:A:ASN:HB3  | 1:172:A:GLN:HA   | 2        | 0.47          |
| (1,873)  | 1:146:A:GLU:HA   | 1:150:A:TYR:HB3  | 14       | 0.47          |
| (1,775)  | 1:203:A:VAL:HG11 | 1:206:A:MET:HE1  | 7        | 0.47          |
| (1,775)  | 1:203:A:VAL:HG11 | 1:206:A:MET:HE2  | 7        | 0.47          |
| (1,775)  | 1:203:A:VAL:HG11 | 1:206:A:MET:HE3  | 7        | 0.47          |
| (1,775)  | 1:203:A:VAL:HG12 | 1:206:A:MET:HE1  | 7        | 0.47          |
| (1,775)  | 1:203:A:VAL:HG12 | 1:206:A:MET:HE2  | 7        | 0.47          |
| (1,775)  | 1:203:A:VAL:HG12 | 1:206:A:MET:HE3  | 7        | 0.47          |
| (1,775)  | 1:203:A:VAL:HG13 | 1:206:A:MET:HE1  | 7        | 0.47          |
| (1,775)  | 1:203:A:VAL:HG13 | 1:206:A:MET:HE2  | 7        | 0.47          |
| (1,775)  | 1:203:A:VAL:HG13 | 1:206:A:MET:HE3  | 7        | 0.47          |
| (1,740)  | 1:197:A:ASN:HB2  | 1:198:A:PHE:H    | 13       | 0.47          |
| (1,663)  | 1:223:A:GLN:HG2  | 1:227:A:ASP:HB2  | 11       | 0.47          |
| (1,663)  | 1:223:A:GLN:HG2  | 1:227:A:ASP:HB3  | 11       | 0.47          |
| (1,663)  | 1:223:A:GLN:HG2  | 1:227:A:ASP:HB2  | 18       | 0.47          |
| (1,663)  | 1:223:A:GLN:HG2  | 1:227:A:ASP:HB3  | 18       | 0.47          |
| (1,634)  | 1:192:A:THR:HA   | 1:195:A:GLY:HA3  | 11       | 0.47          |
| (1,634)  | 1:192:A:THR:HA   | 1:195:A:GLY:HA3  | 13       | 0.47          |
| (1,563)  | 1:132:A:SER:HB3  | 1:133:A:ALA:HB1  | 6        | 0.47          |
| (1,563)  | 1:132:A:SER:HB3  | 1:133:A:ALA:HB2  | 6        | 0.47          |
| (1,563)  | 1:132:A:SER:HB3  | 1:133:A:ALA:HB3  | 6        | 0.47          |
| (1,563)  | 1:132:A:SER:HB3  | 1:133:A:ALA:HB1  | 19       | 0.47          |
| (1,563)  | 1:132:A:SER:HB3  | 1:133:A:ALA:HB2  | 19       | 0.47          |
| (1,563)  | 1:132:A:SER:HB3  | 1:133:A:ALA:HB3  | 19       | 0.47          |
| (1,436)  | 1:229:A:ARG:HA   | 1:230:A:ARG:HD3  | 20       | 0.47          |
| (1,339)  | 1:209:A:VAL:HG21 | 1:210:A:VAL:HG21 | 18       | 0.47          |
| (1,339)  | 1:209:A:VAL:HG21 | 1:210:A:VAL:HG22 | 18       | 0.47          |
| (1,339)  | 1:209:A:VAL:HG21 | 1:210:A:VAL:HG23 | 18       | 0.47          |
| (1,339)  | 1:209:A:VAL:HG22 | 1:210:A:VAL:HG21 | 18       | 0.47          |
| (1,339)  | 1:209:A:VAL:HG22 | 1:210:A:VAL:HG22 | 18       | 0.47          |
| (1,339)  | 1:209:A:VAL:HG22 | 1:210:A:VAL:HG23 | 18       | 0.47          |
| (1,339)  | 1:209:A:VAL:HG23 | 1:210:A:VAL:HG21 | 18       | 0.47          |
| (1,339)  | 1:209:A:VAL:HG23 | 1:210:A:VAL:HG22 | 18       | 0.47          |
| (1,339)  | 1:209:A:VAL:HG23 | 1:210:A:VAL:HG23 | 18       | 0.47          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,323)  | 1:209:A:VAL:HG21 | 1:212:A:GLN:HB3  | 17       | 0.47          |
| (1,323)  | 1:209:A:VAL:HG22 | 1:212:A:GLN:HB3  | 17       | 0.47          |
| (1,323)  | 1:209:A:VAL:HG23 | 1:212:A:GLN:HB3  | 17       | 0.47          |
| (1,224)  | 1:127:A:GLY:HA3  | 1:128:A:TYR:HB2  | 1        | 0.47          |
| (1,224)  | 1:127:A:GLY:HA3  | 1:128:A:TYR:HB2  | 6        | 0.47          |
| (1,179)  | 1:201:A:THR:HB   | 1:205:A:MET:HG3  | 14       | 0.47          |
| (1,179)  | 1:201:A:THR:HB   | 1:205:A:MET:HG3  | 19       | 0.47          |
| (1,155)  | 1:125:A:LEU:HB3  | 1:126:A:GLY:HA3  | 16       | 0.47          |
| (1,79)   | 1:138:A:MET:H    | 1:209:A:VAL:HG11 | 19       | 0.47          |
| (1,79)   | 1:138:A:MET:H    | 1:209:A:VAL:HG12 | 19       | 0.47          |
| (1,79)   | 1:138:A:MET:H    | 1:209:A:VAL:HG13 | 19       | 0.47          |
| (1,2834) | 1:163:A:TYR:HE1  | 1:221:A:GLU:HG2  | 6        | 0.46          |
| (1,2834) | 1:163:A:TYR:HE2  | 1:221:A:GLU:HG2  | 6        | 0.46          |
| (1,2615) | 1:141:A:PHE:HD1  | 1:147:A:ASP:HB3  | 3        | 0.46          |
| (1,2615) | 1:141:A:PHE:HD2  | 1:147:A:ASP:HB3  | 3        | 0.46          |
| (1,2553) | 1:126:A:GLY:HA2  | 1:128:A:TYR:HD1  | 16       | 0.46          |
| (1,2553) | 1:126:A:GLY:HA2  | 1:128:A:TYR:HD2  | 16       | 0.46          |
| (1,2501) | 1:149:A:TYR:HD1  | 1:205:A:MET:HG2  | 6        | 0.46          |
| (1,2501) | 1:149:A:TYR:HD2  | 1:205:A:MET:HG2  | 6        | 0.46          |
| (1,2279) | 1:186:A:GLN:HB3  | 1:188:A:THR:H    | 15       | 0.46          |
| (1,2129) | 1:186:A:GLN:H    | 1:186:A:GLN:HB3  | 17       | 0.46          |
| (1,1861) | 1:147:A:ASP:HB2  | 1:148:A:ARG:H    | 8        | 0.46          |
| (1,1701) | 1:129:A:MET:H    | 1:129:A:MET:HG3  | 6        | 0.46          |
| (1,1701) | 1:129:A:MET:H    | 1:129:A:MET:HG3  | 12       | 0.46          |
| (1,1579) | 1:132:A:SER:HB3  | 1:133:A:ALA:H    | 14       | 0.46          |
| (1,1575) | 1:136:A:ARG:H    | 1:136:A:ARG:HD3  | 7        | 0.46          |
| (1,1212) | 1:184:A:ILE:HD11 | 1:206:A:MET:HB3  | 14       | 0.46          |
| (1,1212) | 1:184:A:ILE:HD12 | 1:206:A:MET:HB3  | 14       | 0.46          |
| (1,1212) | 1:184:A:ILE:HD13 | 1:206:A:MET:HB3  | 14       | 0.46          |
| (1,1197) | 1:160:A:GLN:HB2  | 1:183:A:THR:HG21 | 1        | 0.46          |
| (1,1197) | 1:160:A:GLN:HB2  | 1:183:A:THR:HG22 | 1        | 0.46          |
| (1,1197) | 1:160:A:GLN:HB2  | 1:183:A:THR:HG23 | 1        | 0.46          |
| (1,1197) | 1:160:A:GLN:HB2  | 1:183:A:THR:HG21 | 17       | 0.46          |
| (1,1197) | 1:160:A:GLN:HB2  | 1:183:A:THR:HG22 | 17       | 0.46          |
| (1,1197) | 1:160:A:GLN:HB2  | 1:183:A:THR:HG23 | 17       | 0.46          |
| (1,1104) | 1:213:A:MET:HB3  | 1:214:A:CYS:HA   | 12       | 0.46          |
| (1,1060) | 1:207:A:GLU:HG3  | 1:208:A:ARG:H    | 13       | 0.46          |
| (1,1023) | 1:206:A:MET:HG3  | 1:207:A:GLU:HG3  | 4        | 0.46          |
| (1,944)  | 1:171:A:ASN:HB3  | 1:172:A:GLN:HA   | 17       | 0.46          |
| (1,864)  | 1:134:A:MET:HB3  | 1:135:A:SER:HB2  | 6        | 0.46          |
| (1,862)  | 1:143:A:ASN:HD22 | 1:146:A:GLU:HG2  | 5        | 0.46          |
| (1,833)  | 1:207:A:GLU:HA   | 1:207:A:GLU:HG3  | 9        | 0.46          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,739)  | 1:166:A:VAL:HG11 | 1:222:A:SER:HB3  | 5        | 0.46          |
| (1,739)  | 1:166:A:VAL:HG12 | 1:222:A:SER:HB3  | 5        | 0.46          |
| (1,739)  | 1:166:A:VAL:HG13 | 1:222:A:SER:HB3  | 5        | 0.46          |
| (1,730)  | 1:166:A:VAL:HG11 | 1:167:A:SER:HB3  | 3        | 0.46          |
| (1,730)  | 1:166:A:VAL:HG12 | 1:167:A:SER:HB3  | 3        | 0.46          |
| (1,730)  | 1:166:A:VAL:HG13 | 1:167:A:SER:HB3  | 3        | 0.46          |
| (1,634)  | 1:192:A:THR:HA   | 1:195:A:GLY:HA3  | 1        | 0.46          |
| (1,506)  | 1:179:A:CYS:HB2  | 1:214:A:CYS:HB2  | 15       | 0.46          |
| (1,377)  | 1:209:A:VAL:HG21 | 1:213:A:MET:HG2  | 5        | 0.46          |
| (1,377)  | 1:209:A:VAL:HG22 | 1:213:A:MET:HG2  | 5        | 0.46          |
| (1,377)  | 1:209:A:VAL:HG23 | 1:213:A:MET:HG2  | 5        | 0.46          |
| (1,377)  | 1:209:A:VAL:HG21 | 1:213:A:MET:HG2  | 9        | 0.46          |
| (1,377)  | 1:209:A:VAL:HG22 | 1:213:A:MET:HG2  | 9        | 0.46          |
| (1,377)  | 1:209:A:VAL:HG23 | 1:213:A:MET:HG2  | 9        | 0.46          |
| (1,179)  | 1:201:A:THR:HB   | 1:205:A:MET:HG3  | 11       | 0.46          |
| (1,2807) | 1:149:A:TYR:HE1  | 1:153:A:ASN:HB3  | 16       | 0.45          |
| (1,2807) | 1:149:A:TYR:HE2  | 1:153:A:ASN:HB3  | 16       | 0.45          |
| (1,2759) | 1:139:A:ILE:HG12 | 1:150:A:TYR:HE1  | 1        | 0.45          |
| (1,2759) | 1:139:A:ILE:HG12 | 1:150:A:TYR:HE2  | 1        | 0.45          |
| (1,2756) | 1:150:A:TYR:HE1  | 1:205:A:MET:HG2  | 15       | 0.45          |
| (1,2756) | 1:150:A:TYR:HE2  | 1:205:A:MET:HG2  | 15       | 0.45          |
| (1,2699) | 1:141:A:PHE:HZ   | 1:150:A:TYR:HB3  | 19       | 0.45          |
| (1,2218) | 1:131:A:GLY:H    | 1:161:A:VAL:HG21 | 10       | 0.45          |
| (1,2218) | 1:131:A:GLY:H    | 1:161:A:VAL:HG22 | 10       | 0.45          |
| (1,2218) | 1:131:A:GLY:H    | 1:161:A:VAL:HG23 | 10       | 0.45          |
| (1,2129) | 1:186:A:GLN:H    | 1:186:A:GLN:HB3  | 1        | 0.45          |
| (1,2129) | 1:186:A:GLN:H    | 1:186:A:GLN:HB3  | 4        | 0.45          |
| (1,2129) | 1:186:A:GLN:H    | 1:186:A:GLN:HB3  | 9        | 0.45          |
| (1,1894) | 1:215:A:VAL:HG21 | 1:219:A:GLN:H    | 6        | 0.45          |
| (1,1894) | 1:215:A:VAL:HG22 | 1:219:A:GLN:H    | 6        | 0.45          |
| (1,1894) | 1:215:A:VAL:HG23 | 1:219:A:GLN:H    | 6        | 0.45          |
| (1,1893) | 1:208:A:ARG:HB3  | 1:209:A:VAL:H    | 19       | 0.45          |
| (1,1701) | 1:129:A:MET:H    | 1:129:A:MET:HG3  | 8        | 0.45          |
| (1,1678) | 1:125:A:LEU:H    | 1:125:A:LEU:HB2  | 10       | 0.45          |
| (1,1579) | 1:132:A:SER:HB3  | 1:133:A:ALA:H    | 13       | 0.45          |
| (1,1523) | 1:162:A:TYR:HB3  | 1:182:A:ILE:HG12 | 11       | 0.45          |
| (1,1523) | 1:162:A:TYR:HB3  | 1:182:A:ILE:HG13 | 11       | 0.45          |
| (1,1497) | 1:139:A:ILE:HD11 | 1:212:A:GLN:HB3  | 10       | 0.45          |
| (1,1497) | 1:139:A:ILE:HD12 | 1:212:A:GLN:HB3  | 10       | 0.45          |
| (1,1497) | 1:139:A:ILE:HD13 | 1:212:A:GLN:HB3  | 10       | 0.45          |
| (1,1466) | 1:210:A:VAL:H    | 1:211:A:GLU:HB3  | 7        | 0.45          |
| (1,1207) | 1:168:A:GLN:HA   | 1:168:A:GLN:HE22 | 1        | 0.45          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1060) | 1:207:A:GLU:HG3  | 1:208:A:ARG:H    | 15       | 0.45          |
| (1,931)  | 1:166:A:VAL:HG11 | 1:221:A:GLU:HG3  | 17       | 0.45          |
| (1,931)  | 1:166:A:VAL:HG12 | 1:221:A:GLU:HG3  | 17       | 0.45          |
| (1,931)  | 1:166:A:VAL:HG13 | 1:221:A:GLU:HG3  | 17       | 0.45          |
| (1,873)  | 1:146:A:GLU:HA   | 1:150:A:TYR:HB3  | 1        | 0.45          |
| (1,833)  | 1:207:A:GLU:HA   | 1:207:A:GLU:HG3  | 13       | 0.45          |
| (1,833)  | 1:207:A:GLU:HA   | 1:207:A:GLU:HG3  | 19       | 0.45          |
| (1,752)  | 1:138:A:MET:HE1  | 1:139:A:ILE:HG12 | 2        | 0.45          |
| (1,752)  | 1:138:A:MET:HE2  | 1:139:A:ILE:HG12 | 2        | 0.45          |
| (1,752)  | 1:138:A:MET:HE3  | 1:139:A:ILE:HG12 | 2        | 0.45          |
| (1,752)  | 1:138:A:MET:HE1  | 1:139:A:ILE:HG12 | 15       | 0.45          |
| (1,752)  | 1:138:A:MET:HE2  | 1:139:A:ILE:HG12 | 15       | 0.45          |
| (1,752)  | 1:138:A:MET:HE3  | 1:139:A:ILE:HG12 | 15       | 0.45          |
| (1,677)  | 1:135:A:SER:HB2  | 1:213:A:MET:HA   | 20       | 0.45          |
| (1,569)  | 1:128:A:TYR:HE1  | 1:179:A:CYS:HB3  | 7        | 0.45          |
| (1,569)  | 1:128:A:TYR:HE2  | 1:179:A:CYS:HB3  | 7        | 0.45          |
| (1,496)  | 1:130:A:LEU:HA   | 1:162:A:TYR:HB2  | 3        | 0.45          |
| (1,445)  | 1:180:A:VAL:HA   | 1:184:A:ILE:HG12 | 13       | 0.45          |
| (1,389)  | 1:121:A:VAL:HA   | 1:122:A:VAL:HG11 | 2        | 0.45          |
| (1,389)  | 1:121:A:VAL:HA   | 1:122:A:VAL:HG12 | 2        | 0.45          |
| (1,389)  | 1:121:A:VAL:HA   | 1:122:A:VAL:HG13 | 2        | 0.45          |
| (1,388)  | 1:122:A:VAL:HG11 | 1:186:A:GLN:HE21 | 2        | 0.45          |
| (1,388)  | 1:122:A:VAL:HG12 | 1:186:A:GLN:HE21 | 2        | 0.45          |
| (1,388)  | 1:122:A:VAL:HG13 | 1:186:A:GLN:HE21 | 2        | 0.45          |
| (1,336)  | 1:163:A:TYR:HD1  | 1:166:A:VAL:HG11 | 3        | 0.45          |
| (1,336)  | 1:163:A:TYR:HD1  | 1:166:A:VAL:HG12 | 3        | 0.45          |
| (1,336)  | 1:163:A:TYR:HD1  | 1:166:A:VAL:HG13 | 3        | 0.45          |
| (1,336)  | 1:163:A:TYR:HD2  | 1:166:A:VAL:HG11 | 3        | 0.45          |
| (1,336)  | 1:163:A:TYR:HD2  | 1:166:A:VAL:HG12 | 3        | 0.45          |
| (1,336)  | 1:163:A:TYR:HD2  | 1:166:A:VAL:HG13 | 3        | 0.45          |
| (1,224)  | 1:127:A:GLY:HA3  | 1:128:A:TYR:HB2  | 5        | 0.45          |
| (1,224)  | 1:127:A:GLY:HA3  | 1:128:A:TYR:HB2  | 12       | 0.45          |
| (1,224)  | 1:127:A:GLY:HA3  | 1:128:A:TYR:HB2  | 20       | 0.45          |
| (1,174)  | 1:202:A:ASP:HB3  | 1:203:A:VAL:HG11 | 18       | 0.45          |
| (1,174)  | 1:202:A:ASP:HB3  | 1:203:A:VAL:HG12 | 18       | 0.45          |
| (1,174)  | 1:202:A:ASP:HB3  | 1:203:A:VAL:HG13 | 18       | 0.45          |
| (1,151)  | 1:126:A:GLY:HA3  | 1:164:A:ARG:HD3  | 16       | 0.45          |
| (1,89)   | 1:206:A:MET:HB3  | 1:210:A:VAL:HG21 | 18       | 0.45          |
| (1,89)   | 1:206:A:MET:HB3  | 1:210:A:VAL:HG22 | 18       | 0.45          |
| (1,89)   | 1:206:A:MET:HB3  | 1:210:A:VAL:HG23 | 18       | 0.45          |
| (1,1)    | 1:138:A:MET:HG3  | 1:139:A:ILE:HG12 | 13       | 0.45          |
| (1,2834) | 1:163:A:TYR:HE1  | 1:221:A:GLU:HG2  | 14       | 0.44          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2834) | 1:163:A:TYR:HE2  | 1:221:A:GLU:HG2  | 14       | 0.44          |
| (1,2830) | 1:172:A:GLN:HG2  | 1:218:A:TYR:HE1  | 8        | 0.44          |
| (1,2830) | 1:172:A:GLN:HG2  | 1:218:A:TYR:HE2  | 8        | 0.44          |
| (1,2830) | 1:172:A:GLN:HG2  | 1:218:A:TYR:HE1  | 14       | 0.44          |
| (1,2830) | 1:172:A:GLN:HG2  | 1:218:A:TYR:HE2  | 14       | 0.44          |
| (1,2774) | 1:128:A:TYR:HE1  | 1:162:A:TYR:HB3  | 5        | 0.44          |
| (1,2774) | 1:128:A:TYR:HE2  | 1:162:A:TYR:HB3  | 5        | 0.44          |
| (1,2759) | 1:139:A:ILE:HG12 | 1:150:A:TYR:HE1  | 4        | 0.44          |
| (1,2759) | 1:139:A:ILE:HG12 | 1:150:A:TYR:HE2  | 4        | 0.44          |
| (1,2759) | 1:139:A:ILE:HG12 | 1:150:A:TYR:HE1  | 14       | 0.44          |
| (1,2759) | 1:139:A:ILE:HG12 | 1:150:A:TYR:HE2  | 14       | 0.44          |
| (1,2736) | 1:184:A:ILE:HG13 | 1:187:A:HIS:HD2  | 12       | 0.44          |
| (1,2711) | 1:145:A:TRP:HZ3  | 1:146:A:GLU:HG3  | 15       | 0.44          |
| (1,2699) | 1:141:A:PHE:HZ   | 1:150:A:TYR:HB3  | 12       | 0.44          |
| (1,2553) | 1:126:A:GLY:HA2  | 1:128:A:TYR:HD1  | 18       | 0.44          |
| (1,2553) | 1:126:A:GLY:HA2  | 1:128:A:TYR:HD2  | 18       | 0.44          |
| (1,2325) | 1:223:A:GLN:HE21 | 1:227:A:ASP:H    | 19       | 0.44          |
| (1,2129) | 1:186:A:GLN:H    | 1:186:A:GLN:HB3  | 2        | 0.44          |
| (1,2129) | 1:186:A:GLN:H    | 1:186:A:GLN:HB3  | 12       | 0.44          |
| (1,2129) | 1:186:A:GLN:H    | 1:186:A:GLN:HB3  | 14       | 0.44          |
| (1,2129) | 1:186:A:GLN:H    | 1:186:A:GLN:HB3  | 20       | 0.44          |
| (1,1907) | 1:178:A:ASP:HB2  | 1:179:A:CYS:H    | 3        | 0.44          |
| (1,1893) | 1:208:A:ARG:HB3  | 1:209:A:VAL:H    | 15       | 0.44          |
| (1,1584) | 1:122:A:VAL:H    | 1:122:A:VAL:HG11 | 6        | 0.44          |
| (1,1584) | 1:122:A:VAL:H    | 1:122:A:VAL:HG12 | 6        | 0.44          |
| (1,1584) | 1:122:A:VAL:H    | 1:122:A:VAL:HG13 | 6        | 0.44          |
| (1,1212) | 1:184:A:ILE:HD11 | 1:206:A:MET:HB3  | 1        | 0.44          |
| (1,1212) | 1:184:A:ILE:HD12 | 1:206:A:MET:HB3  | 1        | 0.44          |
| (1,1212) | 1:184:A:ILE:HD13 | 1:206:A:MET:HB3  | 1        | 0.44          |
| (1,1168) | 1:223:A:GLN:H    | 1:223:A:GLN:HG2  | 2        | 0.44          |
| (1,1168) | 1:223:A:GLN:H    | 1:223:A:GLN:HG2  | 4        | 0.44          |
| (1,1168) | 1:223:A:GLN:H    | 1:223:A:GLN:HG2  | 12       | 0.44          |
| (1,1168) | 1:223:A:GLN:H    | 1:223:A:GLN:HG2  | 13       | 0.44          |
| (1,1168) | 1:223:A:GLN:H    | 1:223:A:GLN:HG2  | 15       | 0.44          |
| (1,1168) | 1:223:A:GLN:H    | 1:223:A:GLN:HG2  | 20       | 0.44          |
| (1,1101) | 1:160:A:GLN:H    | 1:213:A:MET:HB3  | 4        | 0.44          |
| (1,1060) | 1:207:A:GLU:HG3  | 1:208:A:ARG:H    | 8        | 0.44          |
| (1,833)  | 1:207:A:GLU:HA   | 1:207:A:GLU:HG3  | 4        | 0.44          |
| (1,833)  | 1:207:A:GLU:HA   | 1:207:A:GLU:HG3  | 11       | 0.44          |
| (1,740)  | 1:197:A:ASN:HB2  | 1:198:A:PHE:H    | 16       | 0.44          |
| (1,634)  | 1:192:A:THR:HA   | 1:195:A:GLY:HA3  | 2        | 0.44          |
| (1,574)  | 1:153:A:ASN:HB2  | 1:155:A:TYR:HE1  | 5        | 0.44          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,574)  | 1:153:A:ASN:HB2  | 1:155:A:TYR:HE2  | 5        | 0.44          |
| (1,563)  | 1:132:A:SER:HB3  | 1:133:A:ALA:HB1  | 3        | 0.44          |
| (1,563)  | 1:132:A:SER:HB3  | 1:133:A:ALA:HB2  | 3        | 0.44          |
| (1,563)  | 1:132:A:SER:HB3  | 1:133:A:ALA:HB3  | 3        | 0.44          |
| (1,312)  | 1:166:A:VAL:HG21 | 1:170:A:SER:HB3  | 5        | 0.44          |
| (1,312)  | 1:166:A:VAL:HG22 | 1:170:A:SER:HB3  | 5        | 0.44          |
| (1,312)  | 1:166:A:VAL:HG23 | 1:170:A:SER:HB3  | 5        | 0.44          |
| (1,312)  | 1:166:A:VAL:HG21 | 1:170:A:SER:HB3  | 19       | 0.44          |
| (1,312)  | 1:166:A:VAL:HG22 | 1:170:A:SER:HB3  | 19       | 0.44          |
| (1,312)  | 1:166:A:VAL:HG23 | 1:170:A:SER:HB3  | 19       | 0.44          |
| (1,159)  | 1:228:A:GLY:HA2  | 1:230:A:ARG:HD2  | 5        | 0.44          |
| (1,159)  | 1:228:A:GLY:HA3  | 1:230:A:ARG:HD2  | 5        | 0.44          |
| (1,101)  | 1:138:A:MET:HA   | 1:209:A:VAL:HG11 | 12       | 0.44          |
| (1,101)  | 1:138:A:MET:HA   | 1:209:A:VAL:HG12 | 12       | 0.44          |
| (1,101)  | 1:138:A:MET:HA   | 1:209:A:VAL:HG13 | 12       | 0.44          |
| (1,89)   | 1:206:A:MET:HB3  | 1:210:A:VAL:HG21 | 13       | 0.44          |
| (1,89)   | 1:206:A:MET:HB3  | 1:210:A:VAL:HG22 | 13       | 0.44          |
| (1,89)   | 1:206:A:MET:HB3  | 1:210:A:VAL:HG23 | 13       | 0.44          |
| (1,2807) | 1:149:A:TYR:HE1  | 1:153:A:ASN:HB3  | 14       | 0.43          |
| (1,2807) | 1:149:A:TYR:HE2  | 1:153:A:ASN:HB3  | 14       | 0.43          |
| (1,2774) | 1:128:A:TYR:HE1  | 1:162:A:TYR:HB3  | 14       | 0.43          |
| (1,2774) | 1:128:A:TYR:HE2  | 1:162:A:TYR:HB3  | 14       | 0.43          |
| (1,2354) | 1:170:A:SER:HB2  | 1:174:A:ASN:HD21 | 15       | 0.43          |
| (1,1893) | 1:208:A:ARG:HB3  | 1:209:A:VAL:H    | 20       | 0.43          |
| (1,1861) | 1:147:A:ASP:HB2  | 1:148:A:ARG:H    | 9        | 0.43          |
| (1,1861) | 1:147:A:ASP:HB2  | 1:148:A:ARG:H    | 16       | 0.43          |
| (1,1678) | 1:125:A:LEU:H    | 1:125:A:LEU:HB2  | 19       | 0.43          |
| (1,1584) | 1:122:A:VAL:H    | 1:122:A:VAL:HG11 | 18       | 0.43          |
| (1,1584) | 1:122:A:VAL:H    | 1:122:A:VAL:HG12 | 18       | 0.43          |
| (1,1584) | 1:122:A:VAL:H    | 1:122:A:VAL:HG13 | 18       | 0.43          |
| (1,1060) | 1:207:A:GLU:HG3  | 1:208:A:ARG:H    | 11       | 0.43          |
| (1,996)  | 1:176:A:VAL:HA   | 1:211:A:GLU:HG3  | 18       | 0.43          |
| (1,862)  | 1:143:A:ASN:HD22 | 1:146:A:GLU:HG2  | 6        | 0.43          |
| (1,862)  | 1:143:A:ASN:HD22 | 1:146:A:GLU:HG2  | 15       | 0.43          |
| (1,833)  | 1:207:A:GLU:HA   | 1:207:A:GLU:HG3  | 8        | 0.43          |
| (1,833)  | 1:207:A:GLU:HA   | 1:207:A:GLU:HG3  | 10       | 0.43          |
| (1,833)  | 1:207:A:GLU:HA   | 1:207:A:GLU:HG3  | 14       | 0.43          |
| (1,574)  | 1:153:A:ASN:HB2  | 1:155:A:TYR:HE1  | 3        | 0.43          |
| (1,574)  | 1:153:A:ASN:HB2  | 1:155:A:TYR:HE2  | 3        | 0.43          |
| (1,569)  | 1:128:A:TYR:HE1  | 1:179:A:CYS:HB3  | 5        | 0.43          |
| (1,569)  | 1:128:A:TYR:HE2  | 1:179:A:CYS:HB3  | 5        | 0.43          |
| (1,563)  | 1:132:A:SER:HB3  | 1:133:A:ALA:HB1  | 13       | 0.43          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,563) | 1:132:A:SER:HB3  | 1:133:A:ALA:HB2  | 13       | 0.43          |
| (1,563) | 1:132:A:SER:HB3  | 1:133:A:ALA:HB3  | 13       | 0.43          |
| (1,525) | 1:132:A:SER:HB2  | 1:160:A:GLN:HE21 | 16       | 0.43          |
| (1,436) | 1:229:A:ARG:HA   | 1:230:A:ARG:HD3  | 5        | 0.43          |
| (1,348) | 1:122:A:VAL:HG21 | 1:124:A:GLY:HA2  | 15       | 0.43          |
| (1,348) | 1:122:A:VAL:HG21 | 1:124:A:GLY:HA3  | 15       | 0.43          |
| (1,348) | 1:122:A:VAL:HG22 | 1:124:A:GLY:HA2  | 15       | 0.43          |
| (1,348) | 1:122:A:VAL:HG22 | 1:124:A:GLY:HA3  | 15       | 0.43          |
| (1,348) | 1:122:A:VAL:HG23 | 1:124:A:GLY:HA2  | 15       | 0.43          |
| (1,348) | 1:122:A:VAL:HG23 | 1:124:A:GLY:HA3  | 15       | 0.43          |
| (1,339) | 1:209:A:VAL:HG21 | 1:210:A:VAL:HG21 | 17       | 0.43          |
| (1,339) | 1:209:A:VAL:HG21 | 1:210:A:VAL:HG22 | 17       | 0.43          |
| (1,339) | 1:209:A:VAL:HG21 | 1:210:A:VAL:HG23 | 17       | 0.43          |
| (1,339) | 1:209:A:VAL:HG22 | 1:210:A:VAL:HG21 | 17       | 0.43          |
| (1,339) | 1:209:A:VAL:HG22 | 1:210:A:VAL:HG22 | 17       | 0.43          |
| (1,339) | 1:209:A:VAL:HG22 | 1:210:A:VAL:HG23 | 17       | 0.43          |
| (1,339) | 1:209:A:VAL:HG23 | 1:210:A:VAL:HG21 | 17       | 0.43          |
| (1,339) | 1:209:A:VAL:HG23 | 1:210:A:VAL:HG22 | 17       | 0.43          |
| (1,339) | 1:209:A:VAL:HG23 | 1:210:A:VAL:HG23 | 17       | 0.43          |
| (1,312) | 1:166:A:VAL:HG21 | 1:170:A:SER:HB3  | 14       | 0.43          |
| (1,312) | 1:166:A:VAL:HG22 | 1:170:A:SER:HB3  | 14       | 0.43          |
| (1,312) | 1:166:A:VAL:HG23 | 1:170:A:SER:HB3  | 14       | 0.43          |
| (1,312) | 1:166:A:VAL:HG21 | 1:170:A:SER:HB3  | 18       | 0.43          |
| (1,312) | 1:166:A:VAL:HG22 | 1:170:A:SER:HB3  | 18       | 0.43          |
| (1,312) | 1:166:A:VAL:HG23 | 1:170:A:SER:HB3  | 18       | 0.43          |
| (1,272) | 1:166:A:VAL:HG11 | 1:221:A:GLU:HB3  | 17       | 0.43          |
| (1,272) | 1:166:A:VAL:HG12 | 1:221:A:GLU:HB3  | 17       | 0.43          |
| (1,272) | 1:166:A:VAL:HG13 | 1:221:A:GLU:HB3  | 17       | 0.43          |
| (1,224) | 1:127:A:GLY:HA3  | 1:128:A:TYR:HB2  | 14       | 0.43          |
| (1,179) | 1:201:A:THR:HB   | 1:205:A:MET:HG3  | 1        | 0.43          |
| (1,179) | 1:201:A:THR:HB   | 1:205:A:MET:HG3  | 2        | 0.43          |
| (1,174) | 1:202:A:ASP:HB3  | 1:203:A:VAL:HG11 | 2        | 0.43          |
| (1,174) | 1:202:A:ASP:HB3  | 1:203:A:VAL:HG12 | 2        | 0.43          |
| (1,174) | 1:202:A:ASP:HB3  | 1:203:A:VAL:HG13 | 2        | 0.43          |
| (1,79)  | 1:138:A:MET:H    | 1:209:A:VAL:HG11 | 2        | 0.43          |
| (1,79)  | 1:138:A:MET:H    | 1:209:A:VAL:HG12 | 2        | 0.43          |
| (1,79)  | 1:138:A:MET:H    | 1:209:A:VAL:HG13 | 2        | 0.43          |
| (1,77)  | 1:208:A:ARG:H    | 1:209:A:VAL:HG11 | 12       | 0.43          |
| (1,77)  | 1:208:A:ARG:H    | 1:209:A:VAL:HG12 | 12       | 0.43          |
| (1,77)  | 1:208:A:ARG:H    | 1:209:A:VAL:HG13 | 12       | 0.43          |
| (1,71)  | 1:122:A:VAL:HA   | 1:125:A:LEU:HD11 | 6        | 0.43          |
| (1,71)  | 1:122:A:VAL:HA   | 1:125:A:LEU:HD12 | 6        | 0.43          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,71)   | 1:122:A:VAL:HA   | 1:125:A:LEU:HD13 | 6        | 0.43          |
| (1,2807) | 1:149:A:TYR:HE1  | 1:153:A:ASN:HB3  | 19       | 0.42          |
| (1,2807) | 1:149:A:TYR:HE2  | 1:153:A:ASN:HB3  | 19       | 0.42          |
| (1,2792) | 1:128:A:TYR:HE1  | 1:164:A:ARG:HD3  | 12       | 0.42          |
| (1,2792) | 1:128:A:TYR:HE2  | 1:164:A:ARG:HD3  | 12       | 0.42          |
| (1,2759) | 1:139:A:ILE:HG12 | 1:150:A:TYR:HE1  | 15       | 0.42          |
| (1,2759) | 1:139:A:ILE:HG12 | 1:150:A:TYR:HE2  | 15       | 0.42          |
| (1,2736) | 1:184:A:ILE:HG13 | 1:187:A:HIS:HD2  | 2        | 0.42          |
| (1,2537) | 1:166:A:VAL:HG11 | 1:225:A:TYR:HD1  | 17       | 0.42          |
| (1,2537) | 1:166:A:VAL:HG11 | 1:225:A:TYR:HD2  | 17       | 0.42          |
| (1,2537) | 1:166:A:VAL:HG12 | 1:225:A:TYR:HD1  | 17       | 0.42          |
| (1,2537) | 1:166:A:VAL:HG12 | 1:225:A:TYR:HD2  | 17       | 0.42          |
| (1,2537) | 1:166:A:VAL:HG13 | 1:225:A:TYR:HD1  | 17       | 0.42          |
| (1,2537) | 1:166:A:VAL:HG13 | 1:225:A:TYR:HD2  | 17       | 0.42          |
| (1,2414) | 1:136:A:ARG:HB3  | 1:159:A:ASN:HD21 | 7        | 0.42          |
| (1,2129) | 1:186:A:GLN:H    | 1:186:A:GLN:HB3  | 10       | 0.42          |
| (1,1937) | 1:220:A:LYS:H    | 1:221:A:GLU:HG3  | 3        | 0.42          |
| (1,1538) | 1:164:A:ARG:HD2  | 1:165:A:PRO:HD3  | 10       | 0.42          |
| (1,1207) | 1:168:A:GLN:HA   | 1:168:A:GLN:HE22 | 3        | 0.42          |
| (1,1104) | 1:213:A:MET:HB3  | 1:214:A:CYS:HA   | 1        | 0.42          |
| (1,1101) | 1:160:A:GLN:H    | 1:213:A:MET:HB3  | 2        | 0.42          |
| (1,1101) | 1:160:A:GLN:H    | 1:213:A:MET:HB3  | 11       | 0.42          |
| (1,1101) | 1:160:A:GLN:H    | 1:213:A:MET:HB3  | 20       | 0.42          |
| (1,873)  | 1:146:A:GLU:HA   | 1:150:A:TYR:HB3  | 16       | 0.42          |
| (1,752)  | 1:138:A:MET:HE1  | 1:139:A:ILE:HG12 | 3        | 0.42          |
| (1,752)  | 1:138:A:MET:HE2  | 1:139:A:ILE:HG12 | 3        | 0.42          |
| (1,752)  | 1:138:A:MET:HE3  | 1:139:A:ILE:HG12 | 3        | 0.42          |
| (1,740)  | 1:197:A:ASN:HB2  | 1:198:A:PHE:H    | 1        | 0.42          |
| (1,740)  | 1:197:A:ASN:HB2  | 1:198:A:PHE:H    | 15       | 0.42          |
| (1,377)  | 1:209:A:VAL:HG21 | 1:213:A:MET:HG2  | 6        | 0.42          |
| (1,377)  | 1:209:A:VAL:HG22 | 1:213:A:MET:HG2  | 6        | 0.42          |
| (1,377)  | 1:209:A:VAL:HG23 | 1:213:A:MET:HG2  | 6        | 0.42          |
| (1,179)  | 1:201:A:THR:HB   | 1:205:A:MET:HG3  | 9        | 0.42          |
| (1,79)   | 1:138:A:MET:H    | 1:209:A:VAL:HG11 | 4        | 0.42          |
| (1,79)   | 1:138:A:MET:H    | 1:209:A:VAL:HG12 | 4        | 0.42          |
| (1,79)   | 1:138:A:MET:H    | 1:209:A:VAL:HG13 | 4        | 0.42          |
| (1,77)   | 1:208:A:ARG:H    | 1:209:A:VAL:HG11 | 2        | 0.42          |
| (1,77)   | 1:208:A:ARG:H    | 1:209:A:VAL:HG12 | 2        | 0.42          |
| (1,77)   | 1:208:A:ARG:H    | 1:209:A:VAL:HG13 | 2        | 0.42          |
| (1,58)   | 1:122:A:VAL:HG21 | 1:125:A:LEU:HD11 | 19       | 0.42          |
| (1,58)   | 1:122:A:VAL:HG21 | 1:125:A:LEU:HD12 | 19       | 0.42          |
| (1,58)   | 1:122:A:VAL:HG21 | 1:125:A:LEU:HD13 | 19       | 0.42          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,58)   | 1:122:A:VAL:HG22 | 1:125:A:LEU:HD11 | 19       | 0.42          |
| (1,58)   | 1:122:A:VAL:HG22 | 1:125:A:LEU:HD12 | 19       | 0.42          |
| (1,58)   | 1:122:A:VAL:HG22 | 1:125:A:LEU:HD13 | 19       | 0.42          |
| (1,58)   | 1:122:A:VAL:HG23 | 1:125:A:LEU:HD11 | 19       | 0.42          |
| (1,58)   | 1:122:A:VAL:HG23 | 1:125:A:LEU:HD12 | 19       | 0.42          |
| (1,58)   | 1:122:A:VAL:HG23 | 1:125:A:LEU:HD13 | 19       | 0.42          |
| (1,2834) | 1:163:A:TYR:HE1  | 1:221:A:GLU:HG2  | 7        | 0.41          |
| (1,2834) | 1:163:A:TYR:HE2  | 1:221:A:GLU:HG2  | 7        | 0.41          |
| (1,2830) | 1:172:A:GLN:HG2  | 1:218:A:TYR:HE1  | 5        | 0.41          |
| (1,2830) | 1:172:A:GLN:HG2  | 1:218:A:TYR:HE2  | 5        | 0.41          |
| (1,2774) | 1:128:A:TYR:HE1  | 1:162:A:TYR:HB3  | 4        | 0.41          |
| (1,2774) | 1:128:A:TYR:HE2  | 1:162:A:TYR:HB3  | 4        | 0.41          |
| (1,2763) | 1:155:A:TYR:HE1  | 1:156:A:ARG:HD2  | 12       | 0.41          |
| (1,2763) | 1:155:A:TYR:HE2  | 1:156:A:ARG:HD2  | 12       | 0.41          |
| (1,2681) | 1:141:A:PHE:HZ   | 1:208:A:ARG:HB3  | 9        | 0.41          |
| (1,2474) | 1:168:A:GLN:HG2  | 1:169:A:TYR:HD1  | 20       | 0.41          |
| (1,2474) | 1:168:A:GLN:HG2  | 1:169:A:TYR:HD2  | 20       | 0.41          |
| (1,2469) | 1:166:A:VAL:HG21 | 1:169:A:TYR:HD1  | 3        | 0.41          |
| (1,2469) | 1:166:A:VAL:HG21 | 1:169:A:TYR:HD2  | 3        | 0.41          |
| (1,2469) | 1:166:A:VAL:HG22 | 1:169:A:TYR:HD1  | 3        | 0.41          |
| (1,2469) | 1:166:A:VAL:HG22 | 1:169:A:TYR:HD2  | 3        | 0.41          |
| (1,2469) | 1:166:A:VAL:HG23 | 1:169:A:TYR:HD1  | 3        | 0.41          |
| (1,2469) | 1:166:A:VAL:HG23 | 1:169:A:TYR:HD2  | 3        | 0.41          |
| (1,2439) | 1:229:A:ARG:HE   | 1:230:A:ARG:HB3  | 11       | 0.41          |
| (1,2305) | 1:171:A:ASN:HD21 | 1:173:A:LYS:HB2  | 7        | 0.41          |
| (1,2129) | 1:186:A:GLN:H    | 1:186:A:GLN:HB3  | 11       | 0.41          |
| (1,2076) | 1:208:A:ARG:H    | 1:208:A:ARG:HG3  | 8        | 0.41          |
| (1,1466) | 1:210:A:VAL:H    | 1:211:A:GLU:HB3  | 6        | 0.41          |
| (1,1213) | 1:230:A:ARG:HA   | 1:230:A:ARG:HG3  | 7        | 0.41          |
| (1,1212) | 1:184:A:ILE:HD11 | 1:206:A:MET:HB3  | 4        | 0.41          |
| (1,1212) | 1:184:A:ILE:HD12 | 1:206:A:MET:HB3  | 4        | 0.41          |
| (1,1212) | 1:184:A:ILE:HD13 | 1:206:A:MET:HB3  | 4        | 0.41          |
| (1,1168) | 1:223:A:GLN:H    | 1:223:A:GLN:HG2  | 11       | 0.41          |
| (1,1104) | 1:213:A:MET:HB3  | 1:214:A:CYS:HA   | 18       | 0.41          |
| (1,1101) | 1:160:A:GLN:H    | 1:213:A:MET:HB3  | 13       | 0.41          |
| (1,1101) | 1:160:A:GLN:H    | 1:213:A:MET:HB3  | 19       | 0.41          |
| (1,893)  | 1:162:A:TYR:HB3  | 1:182:A:ILE:HB   | 14       | 0.41          |
| (1,833)  | 1:207:A:GLU:HA   | 1:207:A:GLU:HG3  | 16       | 0.41          |
| (1,833)  | 1:207:A:GLU:HA   | 1:207:A:GLU:HG3  | 17       | 0.41          |
| (1,656)  | 1:138:A:MET:HG3  | 1:154:A:MET:HE1  | 8        | 0.41          |
| (1,656)  | 1:138:A:MET:HG3  | 1:154:A:MET:HE2  | 8        | 0.41          |
| (1,656)  | 1:138:A:MET:HG3  | 1:154:A:MET:HE3  | 8        | 0.41          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,496)  | 1:130:A:LEU:HA   | 1:162:A:TYR:HB2  | 5        | 0.41          |
| (1,467)  | 1:122:A:VAL:HG21 | 1:125:A:LEU:HB3  | 4        | 0.41          |
| (1,467)  | 1:122:A:VAL:HG22 | 1:125:A:LEU:HB3  | 4        | 0.41          |
| (1,467)  | 1:122:A:VAL:HG23 | 1:125:A:LEU:HB3  | 4        | 0.41          |
| (1,445)  | 1:180:A:VAL:HA   | 1:184:A:ILE:HG12 | 5        | 0.41          |
| (1,357)  | 1:122:A:VAL:HG21 | 1:125:A:LEU:HG   | 16       | 0.41          |
| (1,357)  | 1:122:A:VAL:HG22 | 1:125:A:LEU:HG   | 16       | 0.41          |
| (1,357)  | 1:122:A:VAL:HG23 | 1:125:A:LEU:HG   | 16       | 0.41          |
| (1,339)  | 1:209:A:VAL:HG21 | 1:210:A:VAL:HG21 | 1        | 0.41          |
| (1,339)  | 1:209:A:VAL:HG21 | 1:210:A:VAL:HG22 | 1        | 0.41          |
| (1,339)  | 1:209:A:VAL:HG21 | 1:210:A:VAL:HG23 | 1        | 0.41          |
| (1,339)  | 1:209:A:VAL:HG22 | 1:210:A:VAL:HG21 | 1        | 0.41          |
| (1,339)  | 1:209:A:VAL:HG22 | 1:210:A:VAL:HG22 | 1        | 0.41          |
| (1,339)  | 1:209:A:VAL:HG22 | 1:210:A:VAL:HG23 | 1        | 0.41          |
| (1,339)  | 1:209:A:VAL:HG23 | 1:210:A:VAL:HG21 | 1        | 0.41          |
| (1,339)  | 1:209:A:VAL:HG23 | 1:210:A:VAL:HG22 | 1        | 0.41          |
| (1,339)  | 1:209:A:VAL:HG23 | 1:210:A:VAL:HG23 | 1        | 0.41          |
| (1,339)  | 1:209:A:VAL:HG21 | 1:210:A:VAL:HG21 | 8        | 0.41          |
| (1,339)  | 1:209:A:VAL:HG21 | 1:210:A:VAL:HG22 | 8        | 0.41          |
| (1,339)  | 1:209:A:VAL:HG21 | 1:210:A:VAL:HG23 | 8        | 0.41          |
| (1,339)  | 1:209:A:VAL:HG22 | 1:210:A:VAL:HG21 | 8        | 0.41          |
| (1,339)  | 1:209:A:VAL:HG22 | 1:210:A:VAL:HG22 | 8        | 0.41          |
| (1,339)  | 1:209:A:VAL:HG22 | 1:210:A:VAL:HG23 | 8        | 0.41          |
| (1,339)  | 1:209:A:VAL:HG23 | 1:210:A:VAL:HG21 | 8        | 0.41          |
| (1,339)  | 1:209:A:VAL:HG23 | 1:210:A:VAL:HG22 | 8        | 0.41          |
| (1,339)  | 1:209:A:VAL:HG23 | 1:210:A:VAL:HG23 | 8        | 0.41          |
| (1,260)  | 1:186:A:GLN:HB2  | 1:190:A:THR:HG21 | 7        | 0.41          |
| (1,260)  | 1:186:A:GLN:HB2  | 1:190:A:THR:HG22 | 7        | 0.41          |
| (1,260)  | 1:186:A:GLN:HB2  | 1:190:A:THR:HG23 | 7        | 0.41          |
| (1,224)  | 1:127:A:GLY:HA3  | 1:128:A:TYR:HB2  | 15       | 0.41          |
| (1,101)  | 1:138:A:MET:HA   | 1:209:A:VAL:HG11 | 17       | 0.41          |
| (1,101)  | 1:138:A:MET:HA   | 1:209:A:VAL:HG12 | 17       | 0.41          |
| (1,101)  | 1:138:A:MET:HA   | 1:209:A:VAL:HG13 | 17       | 0.41          |
| (1,89)   | 1:206:A:MET:HB3  | 1:210:A:VAL:HG21 | 1        | 0.41          |
| (1,89)   | 1:206:A:MET:HB3  | 1:210:A:VAL:HG22 | 1        | 0.41          |
| (1,89)   | 1:206:A:MET:HB3  | 1:210:A:VAL:HG23 | 1        | 0.41          |
| (1,2830) | 1:172:A:GLN:HG2  | 1:218:A:TYR:HE1  | 16       | 0.4           |
| (1,2830) | 1:172:A:GLN:HG2  | 1:218:A:TYR:HE2  | 16       | 0.4           |
| (1,2792) | 1:128:A:TYR:HE1  | 1:164:A:ARG:HD3  | 10       | 0.4           |
| (1,2792) | 1:128:A:TYR:HE2  | 1:164:A:ARG:HD3  | 10       | 0.4           |
| (1,2759) | 1:139:A:ILE:HG12 | 1:150:A:TYR:HE1  | 13       | 0.4           |
| (1,2759) | 1:139:A:ILE:HG12 | 1:150:A:TYR:HE2  | 13       | 0.4           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2756) | 1:150:A:TYR:HE1  | 1:205:A:MET:HG2  | 10       | 0.4           |
| (1,2756) | 1:150:A:TYR:HE2  | 1:205:A:MET:HG2  | 10       | 0.4           |
| (1,2593) | 1:175:A:PHE:HE1  | 1:221:A:GLU:HG2  | 14       | 0.4           |
| (1,2593) | 1:175:A:PHE:HE2  | 1:221:A:GLU:HG2  | 14       | 0.4           |
| (1,2270) | 1:132:A:SER:H    | 1:132:A:SER:HB2  | 2        | 0.4           |
| (1,2270) | 1:132:A:SER:H    | 1:132:A:SER:HB2  | 5        | 0.4           |
| (1,2129) | 1:186:A:GLN:H    | 1:186:A:GLN:HB3  | 15       | 0.4           |
| (1,1861) | 1:147:A:ASP:HB2  | 1:148:A:ARG:H    | 1        | 0.4           |
| (1,1861) | 1:147:A:ASP:HB2  | 1:148:A:ARG:H    | 13       | 0.4           |
| (1,1861) | 1:147:A:ASP:HB2  | 1:148:A:ARG:H    | 19       | 0.4           |
| (1,1655) | 1:230:A:ARG:H    | 1:230:A:ARG:HG3  | 13       | 0.4           |
| (1,1575) | 1:136:A:ARG:H    | 1:136:A:ARG:HD3  | 16       | 0.4           |
| (1,1213) | 1:230:A:ARG:HA   | 1:230:A:ARG:HG3  | 8        | 0.4           |
| (1,1213) | 1:230:A:ARG:HA   | 1:230:A:ARG:HG3  | 16       | 0.4           |
| (1,1212) | 1:184:A:ILE:HD11 | 1:206:A:MET:HB3  | 13       | 0.4           |
| (1,1212) | 1:184:A:ILE:HD12 | 1:206:A:MET:HB3  | 13       | 0.4           |
| (1,1212) | 1:184:A:ILE:HD13 | 1:206:A:MET:HB3  | 13       | 0.4           |
| (1,1197) | 1:160:A:GLN:HB2  | 1:183:A:THR:HG21 | 15       | 0.4           |
| (1,1197) | 1:160:A:GLN:HB2  | 1:183:A:THR:HG22 | 15       | 0.4           |
| (1,1197) | 1:160:A:GLN:HB2  | 1:183:A:THR:HG23 | 15       | 0.4           |
| (1,1168) | 1:223:A:GLN:H    | 1:223:A:GLN:HG2  | 6        | 0.4           |
| (1,1168) | 1:223:A:GLN:H    | 1:223:A:GLN:HG2  | 17       | 0.4           |
| (1,1060) | 1:207:A:GLU:HG3  | 1:208:A:ARG:H    | 18       | 0.4           |
| (1,1050) | 1:128:A:TYR:HA   | 1:129:A:MET:HG3  | 9        | 0.4           |
| (1,1050) | 1:128:A:TYR:HA   | 1:129:A:MET:HG3  | 11       | 0.4           |
| (1,881)  | 1:145:A:TRP:HE3  | 1:146:A:GLU:HG3  | 5        | 0.4           |
| (1,828)  | 1:222:A:SER:HA   | 1:226:A:TYR:HB3  | 7        | 0.4           |
| (1,775)  | 1:203:A:VAL:HG11 | 1:206:A:MET:HE1  | 8        | 0.4           |
| (1,775)  | 1:203:A:VAL:HG11 | 1:206:A:MET:HE2  | 8        | 0.4           |
| (1,775)  | 1:203:A:VAL:HG11 | 1:206:A:MET:HE3  | 8        | 0.4           |
| (1,775)  | 1:203:A:VAL:HG12 | 1:206:A:MET:HE1  | 8        | 0.4           |
| (1,775)  | 1:203:A:VAL:HG12 | 1:206:A:MET:HE2  | 8        | 0.4           |
| (1,775)  | 1:203:A:VAL:HG12 | 1:206:A:MET:HE3  | 8        | 0.4           |
| (1,775)  | 1:203:A:VAL:HG13 | 1:206:A:MET:HE1  | 8        | 0.4           |
| (1,775)  | 1:203:A:VAL:HG13 | 1:206:A:MET:HE2  | 8        | 0.4           |
| (1,775)  | 1:203:A:VAL:HG13 | 1:206:A:MET:HE3  | 8        | 0.4           |
| (1,740)  | 1:197:A:ASN:HB2  | 1:198:A:PHE:H    | 20       | 0.4           |
| (1,563)  | 1:132:A:SER:HB3  | 1:133:A:ALA:HB1  | 2        | 0.4           |
| (1,563)  | 1:132:A:SER:HB3  | 1:133:A:ALA:HB2  | 2        | 0.4           |
| (1,563)  | 1:132:A:SER:HB3  | 1:133:A:ALA:HB3  | 2        | 0.4           |
| (1,563)  | 1:132:A:SER:HB3  | 1:133:A:ALA:HB1  | 7        | 0.4           |
| (1,563)  | 1:132:A:SER:HB3  | 1:133:A:ALA:HB2  | 7        | 0.4           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,563)  | 1:132:A:SER:HB3  | 1:133:A:ALA:HB3  | 7        | 0.4           |
| (1,521)  | 1:223:A:GLN:HG3  | 1:224:A:ALA:HB1  | 6        | 0.4           |
| (1,521)  | 1:223:A:GLN:HG3  | 1:224:A:ALA:HB2  | 6        | 0.4           |
| (1,521)  | 1:223:A:GLN:HG3  | 1:224:A:ALA:HB3  | 6        | 0.4           |
| (1,445)  | 1:180:A:VAL:HA   | 1:184:A:ILE:HG12 | 3        | 0.4           |
| (1,435)  | 1:230:A:ARG:HA   | 1:230:A:ARG:HD2  | 6        | 0.4           |
| (1,388)  | 1:122:A:VAL:HG11 | 1:186:A:GLN:HE21 | 19       | 0.4           |
| (1,388)  | 1:122:A:VAL:HG12 | 1:186:A:GLN:HE21 | 19       | 0.4           |
| (1,388)  | 1:122:A:VAL:HG13 | 1:186:A:GLN:HE21 | 19       | 0.4           |
| (1,359)  | 1:122:A:VAL:HG21 | 1:182:A:ILE:HG21 | 2        | 0.4           |
| (1,359)  | 1:122:A:VAL:HG21 | 1:182:A:ILE:HG22 | 2        | 0.4           |
| (1,359)  | 1:122:A:VAL:HG21 | 1:182:A:ILE:HG23 | 2        | 0.4           |
| (1,359)  | 1:122:A:VAL:HG22 | 1:182:A:ILE:HG21 | 2        | 0.4           |
| (1,359)  | 1:122:A:VAL:HG22 | 1:182:A:ILE:HG22 | 2        | 0.4           |
| (1,359)  | 1:122:A:VAL:HG22 | 1:182:A:ILE:HG23 | 2        | 0.4           |
| (1,359)  | 1:122:A:VAL:HG23 | 1:182:A:ILE:HG21 | 2        | 0.4           |
| (1,359)  | 1:122:A:VAL:HG23 | 1:182:A:ILE:HG22 | 2        | 0.4           |
| (1,359)  | 1:122:A:VAL:HG23 | 1:182:A:ILE:HG23 | 2        | 0.4           |
| (1,349)  | 1:122:A:VAL:HG21 | 1:186:A:GLN:HE21 | 3        | 0.4           |
| (1,349)  | 1:122:A:VAL:HG22 | 1:186:A:GLN:HE21 | 3        | 0.4           |
| (1,349)  | 1:122:A:VAL:HG23 | 1:186:A:GLN:HE21 | 3        | 0.4           |
| (1,322)  | 1:158:A:PRO:HD3  | 1:209:A:VAL:HG21 | 16       | 0.4           |
| (1,322)  | 1:158:A:PRO:HD3  | 1:209:A:VAL:HG22 | 16       | 0.4           |
| (1,322)  | 1:158:A:PRO:HD3  | 1:209:A:VAL:HG23 | 16       | 0.4           |
| (1,312)  | 1:166:A:VAL:HG21 | 1:170:A:SER:HB3  | 6        | 0.4           |
| (1,312)  | 1:166:A:VAL:HG22 | 1:170:A:SER:HB3  | 6        | 0.4           |
| (1,312)  | 1:166:A:VAL:HG23 | 1:170:A:SER:HB3  | 6        | 0.4           |
| (1,312)  | 1:166:A:VAL:HG21 | 1:170:A:SER:HB3  | 7        | 0.4           |
| (1,312)  | 1:166:A:VAL:HG22 | 1:170:A:SER:HB3  | 7        | 0.4           |
| (1,312)  | 1:166:A:VAL:HG23 | 1:170:A:SER:HB3  | 7        | 0.4           |
| (1,224)  | 1:127:A:GLY:HA3  | 1:128:A:TYR:HB2  | 9        | 0.4           |
| (1,179)  | 1:201:A:THR:HB   | 1:205:A:MET:HG3  | 15       | 0.4           |
| (1,179)  | 1:201:A:THR:HB   | 1:205:A:MET:HG3  | 17       | 0.4           |
| (1,160)  | 1:223:A:GLN:HE21 | 1:228:A:GLY:HA2  | 13       | 0.4           |
| (1,160)  | 1:223:A:GLN:HE21 | 1:228:A:GLY:HA3  | 13       | 0.4           |
| (1,77)   | 1:208:A:ARG:H    | 1:209:A:VAL:HG11 | 4        | 0.4           |
| (1,77)   | 1:208:A:ARG:H    | 1:209:A:VAL:HG12 | 4        | 0.4           |
| (1,77)   | 1:208:A:ARG:H    | 1:209:A:VAL:HG13 | 4        | 0.4           |
| (1,2824) | 1:218:A:TYR:HE1  | 1:222:A:SER:HB3  | 5        | 0.39          |
| (1,2824) | 1:218:A:TYR:HE2  | 1:222:A:SER:HB3  | 5        | 0.39          |
| (1,2756) | 1:150:A:TYR:HE1  | 1:205:A:MET:HG2  | 13       | 0.39          |
| (1,2756) | 1:150:A:TYR:HE2  | 1:205:A:MET:HG2  | 13       | 0.39          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2699) | 1:141:A:PHE:HZ   | 1:150:A:TYR:HB3  | 18       | 0.39          |
| (1,2501) | 1:149:A:TYR:HD1  | 1:205:A:MET:HG2  | 20       | 0.39          |
| (1,2501) | 1:149:A:TYR:HD2  | 1:205:A:MET:HG2  | 20       | 0.39          |
| (1,2270) | 1:132:A:SER:H    | 1:132:A:SER:HB2  | 7        | 0.39          |
| (1,2045) | 1:230:A:ARG:HG3  | 1:231:A:SER:H    | 5        | 0.39          |
| (1,1893) | 1:208:A:ARG:HB3  | 1:209:A:VAL:H    | 14       | 0.39          |
| (1,1861) | 1:147:A:ASP:HB2  | 1:148:A:ARG:H    | 20       | 0.39          |
| (1,1847) | 1:197:A:ASN:H    | 1:197:A:ASN:HB3  | 12       | 0.39          |
| (1,1303) | 1:137:A:PRO:HB2  | 1:213:A:MET:HG2  | 8        | 0.39          |
| (1,1294) | 1:138:A:MET:HG3  | 1:139:A:ILE:H    | 5        | 0.39          |
| (1,1212) | 1:184:A:ILE:HD11 | 1:206:A:MET:HB3  | 17       | 0.39          |
| (1,1212) | 1:184:A:ILE:HD12 | 1:206:A:MET:HB3  | 17       | 0.39          |
| (1,1212) | 1:184:A:ILE:HD13 | 1:206:A:MET:HB3  | 17       | 0.39          |
| (1,1104) | 1:213:A:MET:HB3  | 1:214:A:CYS:HA   | 2        | 0.39          |
| (1,1101) | 1:160:A:GLN:H    | 1:213:A:MET:HB3  | 14       | 0.39          |
| (1,1095) | 1:165:A:PRO:HA   | 1:168:A:GLN:HG2  | 20       | 0.39          |
| (1,740)  | 1:197:A:ASN:HB2  | 1:198:A:PHE:H    | 7        | 0.39          |
| (1,663)  | 1:223:A:GLN:HG2  | 1:227:A:ASP:HB2  | 1        | 0.39          |
| (1,663)  | 1:223:A:GLN:HG2  | 1:227:A:ASP:HB3  | 1        | 0.39          |
| (1,637)  | 1:147:A:ASP:HB2  | 1:148:A:ARG:HG2  | 9        | 0.39          |
| (1,579)  | 1:152:A:GLU:HB2  | 1:153:A:ASN:HB3  | 8        | 0.39          |
| (1,579)  | 1:152:A:GLU:HB3  | 1:153:A:ASN:HB3  | 8        | 0.39          |
| (1,563)  | 1:132:A:SER:HB3  | 1:133:A:ALA:HB1  | 5        | 0.39          |
| (1,563)  | 1:132:A:SER:HB3  | 1:133:A:ALA:HB2  | 5        | 0.39          |
| (1,563)  | 1:132:A:SER:HB3  | 1:133:A:ALA:HB3  | 5        | 0.39          |
| (1,389)  | 1:121:A:VAL:HA   | 1:122:A:VAL:HG11 | 19       | 0.39          |
| (1,389)  | 1:121:A:VAL:HA   | 1:122:A:VAL:HG12 | 19       | 0.39          |
| (1,389)  | 1:121:A:VAL:HA   | 1:122:A:VAL:HG13 | 19       | 0.39          |
| (1,359)  | 1:122:A:VAL:HG21 | 1:182:A:ILE:HG21 | 1        | 0.39          |
| (1,359)  | 1:122:A:VAL:HG21 | 1:182:A:ILE:HG22 | 1        | 0.39          |
| (1,359)  | 1:122:A:VAL:HG21 | 1:182:A:ILE:HG23 | 1        | 0.39          |
| (1,359)  | 1:122:A:VAL:HG22 | 1:182:A:ILE:HG21 | 1        | 0.39          |
| (1,359)  | 1:122:A:VAL:HG22 | 1:182:A:ILE:HG22 | 1        | 0.39          |
| (1,359)  | 1:122:A:VAL:HG22 | 1:182:A:ILE:HG23 | 1        | 0.39          |
| (1,359)  | 1:122:A:VAL:HG23 | 1:182:A:ILE:HG21 | 1        | 0.39          |
| (1,359)  | 1:122:A:VAL:HG23 | 1:182:A:ILE:HG22 | 1        | 0.39          |
| (1,359)  | 1:122:A:VAL:HG23 | 1:182:A:ILE:HG23 | 1        | 0.39          |
| (1,339)  | 1:209:A:VAL:HG21 | 1:210:A:VAL:HG21 | 2        | 0.39          |
| (1,339)  | 1:209:A:VAL:HG21 | 1:210:A:VAL:HG22 | 2        | 0.39          |
| (1,339)  | 1:209:A:VAL:HG21 | 1:210:A:VAL:HG23 | 2        | 0.39          |
| (1,339)  | 1:209:A:VAL:HG22 | 1:210:A:VAL:HG21 | 2        | 0.39          |
| (1,339)  | 1:209:A:VAL:HG22 | 1:210:A:VAL:HG22 | 2        | 0.39          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,339)  | 1:209:A:VAL:HG22 | 1:210:A:VAL:HG23 | 2        | 0.39          |
| (1,339)  | 1:209:A:VAL:HG23 | 1:210:A:VAL:HG21 | 2        | 0.39          |
| (1,339)  | 1:209:A:VAL:HG23 | 1:210:A:VAL:HG22 | 2        | 0.39          |
| (1,339)  | 1:209:A:VAL:HG23 | 1:210:A:VAL:HG23 | 2        | 0.39          |
| (1,216)  | 1:216:A:THR:HG21 | 1:220:A:LYS:HG3  | 18       | 0.39          |
| (1,216)  | 1:216:A:THR:HG22 | 1:220:A:LYS:HG3  | 18       | 0.39          |
| (1,216)  | 1:216:A:THR:HG23 | 1:220:A:LYS:HG3  | 18       | 0.39          |
| (1,2830) | 1:172:A:GLN:HG2  | 1:218:A:TYR:HE1  | 2        | 0.38          |
| (1,2830) | 1:172:A:GLN:HG2  | 1:218:A:TYR:HE2  | 2        | 0.38          |
| (1,2824) | 1:218:A:TYR:HE1  | 1:222:A:SER:HB3  | 12       | 0.38          |
| (1,2824) | 1:218:A:TYR:HE2  | 1:222:A:SER:HB3  | 12       | 0.38          |
| (1,2759) | 1:139:A:ILE:HG12 | 1:150:A:TYR:HE1  | 7        | 0.38          |
| (1,2759) | 1:139:A:ILE:HG12 | 1:150:A:TYR:HE2  | 7        | 0.38          |
| (1,2553) | 1:126:A:GLY:HA2  | 1:128:A:TYR:HD1  | 19       | 0.38          |
| (1,2553) | 1:126:A:GLY:HA2  | 1:128:A:TYR:HD2  | 19       | 0.38          |
| (1,2364) | 1:171:A:ASN:HD22 | 1:174:A:ASN:HD22 | 4        | 0.38          |
| (1,2326) | 1:223:A:GLN:HE21 | 1:228:A:GLY:H    | 7        | 0.38          |
| (1,2129) | 1:186:A:GLN:H    | 1:186:A:GLN:HB3  | 6        | 0.38          |
| (1,2129) | 1:186:A:GLN:H    | 1:186:A:GLN:HB3  | 7        | 0.38          |
| (1,2045) | 1:230:A:ARG:HG3  | 1:231:A:SER:H    | 14       | 0.38          |
| (1,1746) | 1:184:A:ILE:H    | 1:184:A:ILE:HG12 | 4        | 0.38          |
| (1,1701) | 1:129:A:MET:H    | 1:129:A:MET:HG3  | 4        | 0.38          |
| (1,1584) | 1:122:A:VAL:H    | 1:122:A:VAL:HG11 | 19       | 0.38          |
| (1,1584) | 1:122:A:VAL:H    | 1:122:A:VAL:HG12 | 19       | 0.38          |
| (1,1584) | 1:122:A:VAL:H    | 1:122:A:VAL:HG13 | 19       | 0.38          |
| (1,1256) | 1:184:A:ILE:HG13 | 1:206:A:MET:HG3  | 16       | 0.38          |
| (1,1231) | 1:209:A:VAL:HG21 | 1:213:A:MET:HG3  | 1        | 0.38          |
| (1,1231) | 1:209:A:VAL:HG22 | 1:213:A:MET:HG3  | 1        | 0.38          |
| (1,1231) | 1:209:A:VAL:HG23 | 1:213:A:MET:HG3  | 1        | 0.38          |
| (1,1213) | 1:230:A:ARG:HA   | 1:230:A:ARG:HG3  | 10       | 0.38          |
| (1,1212) | 1:184:A:ILE:HD11 | 1:206:A:MET:HB3  | 9        | 0.38          |
| (1,1212) | 1:184:A:ILE:HD12 | 1:206:A:MET:HB3  | 9        | 0.38          |
| (1,1212) | 1:184:A:ILE:HD13 | 1:206:A:MET:HB3  | 9        | 0.38          |
| (1,1101) | 1:160:A:GLN:H    | 1:213:A:MET:HB3  | 15       | 0.38          |
| (1,1101) | 1:160:A:GLN:H    | 1:213:A:MET:HB3  | 17       | 0.38          |
| (1,1097) | 1:165:A:PRO:HB3  | 1:168:A:GLN:HG2  | 3        | 0.38          |
| (1,881)  | 1:145:A:TRP:HE3  | 1:146:A:GLU:HG3  | 18       | 0.38          |
| (1,873)  | 1:146:A:GLU:HA   | 1:150:A:TYR:HB3  | 4        | 0.38          |
| (1,873)  | 1:146:A:GLU:HA   | 1:150:A:TYR:HB3  | 15       | 0.38          |
| (1,828)  | 1:222:A:SER:HA   | 1:226:A:TYR:HB3  | 12       | 0.38          |
| (1,752)  | 1:138:A:MET:HE1  | 1:139:A:ILE:HG12 | 8        | 0.38          |
| (1,752)  | 1:138:A:MET:HE2  | 1:139:A:ILE:HG12 | 8        | 0.38          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,752)  | 1:138:A:MET:HE3  | 1:139:A:ILE:HG12 | 8        | 0.38          |
| (1,752)  | 1:138:A:MET:HE1  | 1:139:A:ILE:HG12 | 14       | 0.38          |
| (1,752)  | 1:138:A:MET:HE2  | 1:139:A:ILE:HG12 | 14       | 0.38          |
| (1,752)  | 1:138:A:MET:HE3  | 1:139:A:ILE:HG12 | 14       | 0.38          |
| (1,730)  | 1:166:A:VAL:HG11 | 1:167:A:SER:HB3  | 1        | 0.38          |
| (1,730)  | 1:166:A:VAL:HG12 | 1:167:A:SER:HB3  | 1        | 0.38          |
| (1,730)  | 1:166:A:VAL:HG13 | 1:167:A:SER:HB3  | 1        | 0.38          |
| (1,705)  | 1:161:A:VAL:HG11 | 1:213:A:MET:HE1  | 10       | 0.38          |
| (1,705)  | 1:161:A:VAL:HG11 | 1:213:A:MET:HE2  | 10       | 0.38          |
| (1,705)  | 1:161:A:VAL:HG11 | 1:213:A:MET:HE3  | 10       | 0.38          |
| (1,705)  | 1:161:A:VAL:HG12 | 1:213:A:MET:HE1  | 10       | 0.38          |
| (1,705)  | 1:161:A:VAL:HG12 | 1:213:A:MET:HE2  | 10       | 0.38          |
| (1,705)  | 1:161:A:VAL:HG12 | 1:213:A:MET:HE3  | 10       | 0.38          |
| (1,705)  | 1:161:A:VAL:HG13 | 1:213:A:MET:HE1  | 10       | 0.38          |
| (1,705)  | 1:161:A:VAL:HG13 | 1:213:A:MET:HE2  | 10       | 0.38          |
| (1,705)  | 1:161:A:VAL:HG13 | 1:213:A:MET:HE3  | 10       | 0.38          |
| (1,657)  | 1:213:A:MET:HB3  | 1:213:A:MET:HE1  | 14       | 0.38          |
| (1,657)  | 1:213:A:MET:HB3  | 1:213:A:MET:HE2  | 14       | 0.38          |
| (1,657)  | 1:213:A:MET:HB3  | 1:213:A:MET:HE3  | 14       | 0.38          |
| (1,502)  | 1:162:A:TYR:HB3  | 1:183:A:THR:HA   | 7        | 0.38          |
| (1,389)  | 1:121:A:VAL:HA   | 1:122:A:VAL:HG11 | 4        | 0.38          |
| (1,389)  | 1:121:A:VAL:HA   | 1:122:A:VAL:HG12 | 4        | 0.38          |
| (1,389)  | 1:121:A:VAL:HA   | 1:122:A:VAL:HG13 | 4        | 0.38          |
| (1,272)  | 1:166:A:VAL:HG11 | 1:221:A:GLU:HB3  | 3        | 0.38          |
| (1,272)  | 1:166:A:VAL:HG12 | 1:221:A:GLU:HB3  | 3        | 0.38          |
| (1,272)  | 1:166:A:VAL:HG13 | 1:221:A:GLU:HB3  | 3        | 0.38          |
| (1,220)  | 1:127:A:GLY:HA2  | 1:164:A:ARG:HE   | 9        | 0.38          |
| (1,216)  | 1:216:A:THR:HG21 | 1:220:A:LYS:HG3  | 6        | 0.38          |
| (1,216)  | 1:216:A:THR:HG22 | 1:220:A:LYS:HG3  | 6        | 0.38          |
| (1,216)  | 1:216:A:THR:HG23 | 1:220:A:LYS:HG3  | 6        | 0.38          |
| (1,202)  | 1:183:A:THR:HG21 | 1:184:A:ILE:HG12 | 11       | 0.38          |
| (1,202)  | 1:183:A:THR:HG22 | 1:184:A:ILE:HG12 | 11       | 0.38          |
| (1,202)  | 1:183:A:THR:HG23 | 1:184:A:ILE:HG12 | 11       | 0.38          |
| (1,188)  | 1:124:A:GLY:HA2  | 1:125:A:LEU:HD21 | 6        | 0.38          |
| (1,188)  | 1:124:A:GLY:HA2  | 1:125:A:LEU:HD22 | 6        | 0.38          |
| (1,188)  | 1:124:A:GLY:HA2  | 1:125:A:LEU:HD23 | 6        | 0.38          |
| (1,188)  | 1:124:A:GLY:HA3  | 1:125:A:LEU:HD21 | 6        | 0.38          |
| (1,188)  | 1:124:A:GLY:HA3  | 1:125:A:LEU:HD22 | 6        | 0.38          |
| (1,188)  | 1:124:A:GLY:HA3  | 1:125:A:LEU:HD23 | 6        | 0.38          |
| (1,179)  | 1:201:A:THR:HB   | 1:205:A:MET:HG3  | 5        | 0.38          |
| (1,2851) | 1:184:A:ILE:HG13 | 1:187:A:HIS:HE1  | 12       | 0.37          |
| (1,2830) | 1:172:A:GLN:HG2  | 1:218:A:TYR:HE1  | 9        | 0.37          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2830) | 1:172:A:GLN:HG2  | 1:218:A:TYR:HE2 | 9        | 0.37          |
| (1,2792) | 1:128:A:TYR:HE1  | 1:164:A:ARG:HD3 | 11       | 0.37          |
| (1,2792) | 1:128:A:TYR:HE2  | 1:164:A:ARG:HD3 | 11       | 0.37          |
| (1,2771) | 1:130:A:LEU:HB3  | 1:162:A:TYR:HE1 | 13       | 0.37          |
| (1,2771) | 1:130:A:LEU:HB3  | 1:162:A:TYR:HE2 | 13       | 0.37          |
| (1,2553) | 1:126:A:GLY:HA2  | 1:128:A:TYR:HD1 | 2        | 0.37          |
| (1,2553) | 1:126:A:GLY:HA2  | 1:128:A:TYR:HD2 | 2        | 0.37          |
| (1,2501) | 1:149:A:TYR:HD1  | 1:205:A:MET:HG2 | 17       | 0.37          |
| (1,2501) | 1:149:A:TYR:HD2  | 1:205:A:MET:HG2 | 17       | 0.37          |
| (1,2474) | 1:168:A:GLN:HG2  | 1:169:A:TYR:HD1 | 9        | 0.37          |
| (1,2474) | 1:168:A:GLN:HG2  | 1:169:A:TYR:HD2 | 9        | 0.37          |
| (1,2270) | 1:132:A:SER:H    | 1:132:A:SER:HB2 | 16       | 0.37          |
| (1,2237) | 1:166:A:VAL:HG11 | 1:222:A:SER:H   | 12       | 0.37          |
| (1,2237) | 1:166:A:VAL:HG12 | 1:222:A:SER:H   | 12       | 0.37          |
| (1,2237) | 1:166:A:VAL:HG13 | 1:222:A:SER:H   | 12       | 0.37          |
| (1,2129) | 1:186:A:GLN:H    | 1:186:A:GLN:HB3 | 18       | 0.37          |
| (1,1893) | 1:208:A:ARG:HB3  | 1:209:A:VAL:H   | 11       | 0.37          |
| (1,1579) | 1:132:A:SER:HB3  | 1:133:A:ALA:H   | 5        | 0.37          |
| (1,1212) | 1:184:A:ILE:HD11 | 1:206:A:MET:HB3 | 12       | 0.37          |
| (1,1212) | 1:184:A:ILE:HD12 | 1:206:A:MET:HB3 | 12       | 0.37          |
| (1,1212) | 1:184:A:ILE:HD13 | 1:206:A:MET:HB3 | 12       | 0.37          |
| (1,1131) | 1:223:A:GLN:HG2  | 1:226:A:TYR:H   | 3        | 0.37          |
| (1,983)  | 1:149:A:TYR:H    | 1:152:A:GLU:HG2 | 14       | 0.37          |
| (1,833)  | 1:207:A:GLU:HA   | 1:207:A:GLU:HG3 | 2        | 0.37          |
| (1,740)  | 1:197:A:ASN:HB2  | 1:198:A:PHE:H   | 6        | 0.37          |
| (1,739)  | 1:166:A:VAL:HG11 | 1:222:A:SER:HB3 | 1        | 0.37          |
| (1,739)  | 1:166:A:VAL:HG12 | 1:222:A:SER:HB3 | 1        | 0.37          |
| (1,739)  | 1:166:A:VAL:HG13 | 1:222:A:SER:HB3 | 1        | 0.37          |
| (1,657)  | 1:213:A:MET:HB3  | 1:213:A:MET:HE1 | 19       | 0.37          |
| (1,657)  | 1:213:A:MET:HB3  | 1:213:A:MET:HE2 | 19       | 0.37          |
| (1,657)  | 1:213:A:MET:HB3  | 1:213:A:MET:HE3 | 19       | 0.37          |
| (1,657)  | 1:213:A:MET:HB3  | 1:213:A:MET:HE1 | 20       | 0.37          |
| (1,657)  | 1:213:A:MET:HB3  | 1:213:A:MET:HE2 | 20       | 0.37          |
| (1,657)  | 1:213:A:MET:HB3  | 1:213:A:MET:HE3 | 20       | 0.37          |
| (1,569)  | 1:128:A:TYR:HE1  | 1:179:A:CYS:HB3 | 19       | 0.37          |
| (1,569)  | 1:128:A:TYR:HE2  | 1:179:A:CYS:HB3 | 19       | 0.37          |
| (1,224)  | 1:127:A:GLY:HA3  | 1:128:A:TYR:HB2 | 10       | 0.37          |
| (1,216)  | 1:216:A:THR:HG21 | 1:220:A:LYS:HG3 | 11       | 0.37          |
| (1,216)  | 1:216:A:THR:HG22 | 1:220:A:LYS:HG3 | 11       | 0.37          |
| (1,216)  | 1:216:A:THR:HG23 | 1:220:A:LYS:HG3 | 11       | 0.37          |
| (1,179)  | 1:201:A:THR:HB   | 1:205:A:MET:HG3 | 3        | 0.37          |
| (1,179)  | 1:201:A:THR:HB   | 1:205:A:MET:HG3 | 12       | 0.37          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,174)  | 1:202:A:ASP:HB3  | 1:203:A:VAL:HG11 | 5        | 0.37          |
| (1,174)  | 1:202:A:ASP:HB3  | 1:203:A:VAL:HG12 | 5        | 0.37          |
| (1,174)  | 1:202:A:ASP:HB3  | 1:203:A:VAL:HG13 | 5        | 0.37          |
| (1,167)  | 1:203:A:VAL:H    | 1:203:A:VAL:HG11 | 2        | 0.37          |
| (1,167)  | 1:203:A:VAL:H    | 1:203:A:VAL:HG12 | 2        | 0.37          |
| (1,167)  | 1:203:A:VAL:H    | 1:203:A:VAL:HG13 | 2        | 0.37          |
| (1,167)  | 1:203:A:VAL:H    | 1:203:A:VAL:HG11 | 7        | 0.37          |
| (1,167)  | 1:203:A:VAL:H    | 1:203:A:VAL:HG12 | 7        | 0.37          |
| (1,167)  | 1:203:A:VAL:H    | 1:203:A:VAL:HG13 | 7        | 0.37          |
| (1,128)  | 1:161:A:VAL:HG11 | 1:213:A:MET:HB3  | 5        | 0.37          |
| (1,128)  | 1:161:A:VAL:HG12 | 1:213:A:MET:HB3  | 5        | 0.37          |
| (1,128)  | 1:161:A:VAL:HG13 | 1:213:A:MET:HB3  | 5        | 0.37          |
| (1,2763) | 1:155:A:TYR:HE1  | 1:156:A:ARG:HD2  | 4        | 0.36          |
| (1,2763) | 1:155:A:TYR:HE2  | 1:156:A:ARG:HD2  | 4        | 0.36          |
| (1,2615) | 1:141:A:PHE:HD1  | 1:147:A:ASP:HB3  | 5        | 0.36          |
| (1,2615) | 1:141:A:PHE:HD2  | 1:147:A:ASP:HB3  | 5        | 0.36          |
| (1,2548) | 1:162:A:TYR:HD1  | 1:186:A:GLN:HB3  | 3        | 0.36          |
| (1,2548) | 1:162:A:TYR:HD2  | 1:186:A:GLN:HB3  | 3        | 0.36          |
| (1,2279) | 1:186:A:GLN:HB3  | 1:188:A:THR:H    | 18       | 0.36          |
| (1,1937) | 1:220:A:LYS:H    | 1:221:A:GLU:HG3  | 14       | 0.36          |
| (1,1861) | 1:147:A:ASP:HB2  | 1:148:A:ARG:H    | 11       | 0.36          |
| (1,1861) | 1:147:A:ASP:HB2  | 1:148:A:ARG:H    | 14       | 0.36          |
| (1,1861) | 1:147:A:ASP:HB2  | 1:148:A:ARG:H    | 18       | 0.36          |
| (1,1746) | 1:184:A:ILE:H    | 1:184:A:ILE:HG12 | 18       | 0.36          |
| (1,1495) | 1:212:A:GLN:HB2  | 1:216:A:THR:H    | 2        | 0.36          |
| (1,1227) | 1:210:A:VAL:HA   | 1:213:A:MET:HG2  | 19       | 0.36          |
| (1,1213) | 1:230:A:ARG:HA   | 1:230:A:ARG:HG3  | 2        | 0.36          |
| (1,1213) | 1:230:A:ARG:HA   | 1:230:A:ARG:HG3  | 18       | 0.36          |
| (1,1168) | 1:223:A:GLN:H    | 1:223:A:GLN:HG2  | 9        | 0.36          |
| (1,1168) | 1:223:A:GLN:H    | 1:223:A:GLN:HG2  | 19       | 0.36          |
| (1,1101) | 1:160:A:GLN:H    | 1:213:A:MET:HB3  | 8        | 0.36          |
| (1,1101) | 1:160:A:GLN:H    | 1:213:A:MET:HB3  | 9        | 0.36          |
| (1,1101) | 1:160:A:GLN:H    | 1:213:A:MET:HB3  | 18       | 0.36          |
| (1,1015) | 1:152:A:GLU:HG2  | 1:153:A:ASN:HD22 | 15       | 0.36          |
| (1,957)  | 1:184:A:ILE:HD11 | 1:207:A:GLU:HG3  | 18       | 0.36          |
| (1,957)  | 1:184:A:ILE:HD12 | 1:207:A:GLU:HG3  | 18       | 0.36          |
| (1,957)  | 1:184:A:ILE:HD13 | 1:207:A:GLU:HG3  | 18       | 0.36          |
| (1,862)  | 1:143:A:ASN:HD22 | 1:146:A:GLU:HG2  | 18       | 0.36          |
| (1,634)  | 1:192:A:THR:HA   | 1:195:A:GLY:HA3  | 4        | 0.36          |
| (1,357)  | 1:122:A:VAL:HG21 | 1:125:A:LEU:HG   | 4        | 0.36          |
| (1,357)  | 1:122:A:VAL:HG22 | 1:125:A:LEU:HG   | 4        | 0.36          |
| (1,357)  | 1:122:A:VAL:HG23 | 1:125:A:LEU:HG   | 4        | 0.36          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,323)  | 1:209:A:VAL:HG21 | 1:212:A:GLN:HB3  | 10       | 0.36          |
| (1,323)  | 1:209:A:VAL:HG22 | 1:212:A:GLN:HB3  | 10       | 0.36          |
| (1,323)  | 1:209:A:VAL:HG23 | 1:212:A:GLN:HB3  | 10       | 0.36          |
| (1,318)  | 1:153:A:ASN:HB2  | 1:156:A:ARG:HD3  | 13       | 0.36          |
| (1,268)  | 1:166:A:VAL:HG11 | 1:225:A:TYR:HB3  | 17       | 0.36          |
| (1,268)  | 1:166:A:VAL:HG12 | 1:225:A:TYR:HB3  | 17       | 0.36          |
| (1,268)  | 1:166:A:VAL:HG13 | 1:225:A:TYR:HB3  | 17       | 0.36          |
| (1,224)  | 1:127:A:GLY:HA3  | 1:128:A:TYR:HB2  | 16       | 0.36          |
| (1,179)  | 1:201:A:THR:HB   | 1:205:A:MET:HG3  | 20       | 0.36          |
| (1,79)   | 1:138:A:MET:H    | 1:209:A:VAL:HG11 | 1        | 0.36          |
| (1,79)   | 1:138:A:MET:H    | 1:209:A:VAL:HG12 | 1        | 0.36          |
| (1,79)   | 1:138:A:MET:H    | 1:209:A:VAL:HG13 | 1        | 0.36          |
| (1,79)   | 1:138:A:MET:H    | 1:209:A:VAL:HG11 | 12       | 0.36          |
| (1,79)   | 1:138:A:MET:H    | 1:209:A:VAL:HG12 | 12       | 0.36          |
| (1,79)   | 1:138:A:MET:H    | 1:209:A:VAL:HG13 | 12       | 0.36          |
| (1,77)   | 1:208:A:ARG:H    | 1:209:A:VAL:HG11 | 1        | 0.36          |
| (1,77)   | 1:208:A:ARG:H    | 1:209:A:VAL:HG12 | 1        | 0.36          |
| (1,77)   | 1:208:A:ARG:H    | 1:209:A:VAL:HG13 | 1        | 0.36          |
| (1,2830) | 1:172:A:GLN:HG2  | 1:218:A:TYR:HE1  | 19       | 0.35          |
| (1,2830) | 1:172:A:GLN:HG2  | 1:218:A:TYR:HE2  | 19       | 0.35          |
| (1,2830) | 1:172:A:GLN:HG2  | 1:218:A:TYR:HE1  | 20       | 0.35          |
| (1,2830) | 1:172:A:GLN:HG2  | 1:218:A:TYR:HE2  | 20       | 0.35          |
| (1,2824) | 1:218:A:TYR:HE1  | 1:222:A:SER:HB3  | 7        | 0.35          |
| (1,2824) | 1:218:A:TYR:HE2  | 1:222:A:SER:HB3  | 7        | 0.35          |
| (1,2807) | 1:149:A:TYR:HE1  | 1:153:A:ASN:HB3  | 17       | 0.35          |
| (1,2807) | 1:149:A:TYR:HE2  | 1:153:A:ASN:HB3  | 17       | 0.35          |
| (1,2756) | 1:150:A:TYR:HE1  | 1:205:A:MET:HG2  | 3        | 0.35          |
| (1,2756) | 1:150:A:TYR:HE2  | 1:205:A:MET:HG2  | 3        | 0.35          |
| (1,2699) | 1:141:A:PHE:HZ   | 1:150:A:TYR:HB3  | 20       | 0.35          |
| (1,2553) | 1:126:A:GLY:HA2  | 1:128:A:TYR:HD1  | 5        | 0.35          |
| (1,2553) | 1:126:A:GLY:HA2  | 1:128:A:TYR:HD2  | 5        | 0.35          |
| (1,2474) | 1:168:A:GLN:HG2  | 1:169:A:TYR:HD1  | 10       | 0.35          |
| (1,2474) | 1:168:A:GLN:HG2  | 1:169:A:TYR:HD2  | 10       | 0.35          |
| (1,2234) | 1:221:A:GLU:HG3  | 1:222:A:SER:H    | 12       | 0.35          |
| (1,2129) | 1:186:A:GLN:H    | 1:186:A:GLN:HB3  | 8        | 0.35          |
| (1,1861) | 1:147:A:ASP:HB2  | 1:148:A:ARG:H    | 12       | 0.35          |
| (1,1847) | 1:197:A:ASN:H    | 1:197:A:ASN:HB3  | 10       | 0.35          |
| (1,1256) | 1:184:A:ILE:HG13 | 1:206:A:MET:HG3  | 5        | 0.35          |
| (1,1213) | 1:230:A:ARG:HA   | 1:230:A:ARG:HG3  | 17       | 0.35          |
| (1,1212) | 1:184:A:ILE:HD11 | 1:206:A:MET:HB3  | 15       | 0.35          |
| (1,1212) | 1:184:A:ILE:HD12 | 1:206:A:MET:HB3  | 15       | 0.35          |
| (1,1212) | 1:184:A:ILE:HD13 | 1:206:A:MET:HB3  | 15       | 0.35          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1168) | 1:223:A:GLN:H    | 1:223:A:GLN:HG2  | 7        | 0.35          |
| (1,1168) | 1:223:A:GLN:H    | 1:223:A:GLN:HG2  | 18       | 0.35          |
| (1,1166) | 1:215:A:VAL:HG21 | 1:219:A:GLN:HG3  | 13       | 0.35          |
| (1,1166) | 1:215:A:VAL:HG22 | 1:219:A:GLN:HG3  | 13       | 0.35          |
| (1,1166) | 1:215:A:VAL:HG23 | 1:219:A:GLN:HG3  | 13       | 0.35          |
| (1,1131) | 1:223:A:GLN:HG2  | 1:226:A:TYR:H    | 15       | 0.35          |
| (1,1101) | 1:160:A:GLN:H    | 1:213:A:MET:HB3  | 5        | 0.35          |
| (1,1097) | 1:165:A:PRO:HB3  | 1:168:A:GLN:HG2  | 2        | 0.35          |
| (1,1095) | 1:165:A:PRO:HA   | 1:168:A:GLN:HG2  | 9        | 0.35          |
| (1,1070) | 1:152:A:GLU:HA   | 1:152:A:GLU:HG3  | 12       | 0.35          |
| (1,1060) | 1:207:A:GLU:HG3  | 1:208:A:ARG:H    | 19       | 0.35          |
| (1,1050) | 1:128:A:TYR:HA   | 1:129:A:MET:HG3  | 14       | 0.35          |
| (1,944)  | 1:171:A:ASN:HB3  | 1:172:A:GLN:HA   | 16       | 0.35          |
| (1,881)  | 1:145:A:TRP:HE3  | 1:146:A:GLU:HG3  | 16       | 0.35          |
| (1,873)  | 1:146:A:GLU:HA   | 1:150:A:TYR:HB3  | 6        | 0.35          |
| (1,752)  | 1:138:A:MET:HE1  | 1:139:A:ILE:HG12 | 4        | 0.35          |
| (1,752)  | 1:138:A:MET:HE2  | 1:139:A:ILE:HG12 | 4        | 0.35          |
| (1,752)  | 1:138:A:MET:HE3  | 1:139:A:ILE:HG12 | 4        | 0.35          |
| (1,740)  | 1:197:A:ASN:HB2  | 1:198:A:PHE:H    | 17       | 0.35          |
| (1,637)  | 1:147:A:ASP:HB2  | 1:148:A:ARG:HG2  | 7        | 0.35          |
| (1,569)  | 1:128:A:TYR:HE1  | 1:179:A:CYS:HB3  | 13       | 0.35          |
| (1,569)  | 1:128:A:TYR:HE2  | 1:179:A:CYS:HB3  | 13       | 0.35          |
| (1,429)  | 1:122:A:VAL:HG11 | 1:186:A:GLN:HA   | 12       | 0.35          |
| (1,429)  | 1:122:A:VAL:HG12 | 1:186:A:GLN:HA   | 12       | 0.35          |
| (1,429)  | 1:122:A:VAL:HG13 | 1:186:A:GLN:HA   | 12       | 0.35          |
| (1,318)  | 1:153:A:ASN:HB2  | 1:156:A:ARG:HD3  | 2        | 0.35          |
| (1,318)  | 1:153:A:ASN:HB2  | 1:156:A:ARG:HD3  | 5        | 0.35          |
| (1,174)  | 1:202:A:ASP:HB3  | 1:203:A:VAL:HG11 | 12       | 0.35          |
| (1,174)  | 1:202:A:ASP:HB3  | 1:203:A:VAL:HG12 | 12       | 0.35          |
| (1,174)  | 1:202:A:ASP:HB3  | 1:203:A:VAL:HG13 | 12       | 0.35          |
| (1,77)   | 1:208:A:ARG:H    | 1:209:A:VAL:HG11 | 19       | 0.35          |
| (1,77)   | 1:208:A:ARG:H    | 1:209:A:VAL:HG12 | 19       | 0.35          |
| (1,77)   | 1:208:A:ARG:H    | 1:209:A:VAL:HG13 | 19       | 0.35          |
| (1,2851) | 1:184:A:ILE:HG13 | 1:187:A:HIS:HE1  | 11       | 0.34          |
| (1,2699) | 1:141:A:PHE:HZ   | 1:150:A:TYR:HB3  | 4        | 0.34          |
| (1,2593) | 1:175:A:PHE:HE1  | 1:221:A:GLU:HG2  | 1        | 0.34          |
| (1,2593) | 1:175:A:PHE:HE2  | 1:221:A:GLU:HG2  | 1        | 0.34          |
| (1,2366) | 1:164:A:ARG:HE   | 1:168:A:GLN:HE22 | 13       | 0.34          |
| (1,2356) | 1:169:A:TYR:HB2  | 1:174:A:ASN:HD21 | 12       | 0.34          |
| (1,2309) | 1:171:A:ASN:HD22 | 1:174:A:ASN:HD21 | 4        | 0.34          |
| (1,2270) | 1:132:A:SER:H    | 1:132:A:SER:HB2  | 13       | 0.34          |
| (1,2129) | 1:186:A:GLN:H    | 1:186:A:GLN:HB3  | 16       | 0.34          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1893) | 1:208:A:ARG:HB3  | 1:209:A:VAL:H    | 13       | 0.34          |
| (1,1861) | 1:147:A:ASP:HB2  | 1:148:A:ARG:H    | 5        | 0.34          |
| (1,1861) | 1:147:A:ASP:HB2  | 1:148:A:ARG:H    | 7        | 0.34          |
| (1,1861) | 1:147:A:ASP:HB2  | 1:148:A:ARG:H    | 10       | 0.34          |
| (1,1213) | 1:230:A:ARG:HA   | 1:230:A:ARG:HG3  | 14       | 0.34          |
| (1,1212) | 1:184:A:ILE:HD11 | 1:206:A:MET:HB3  | 19       | 0.34          |
| (1,1212) | 1:184:A:ILE:HD12 | 1:206:A:MET:HB3  | 19       | 0.34          |
| (1,1212) | 1:184:A:ILE:HD13 | 1:206:A:MET:HB3  | 19       | 0.34          |
| (1,1168) | 1:223:A:GLN:H    | 1:223:A:GLN:HG2  | 3        | 0.34          |
| (1,893)  | 1:162:A:TYR:HB3  | 1:182:A:ILE:HB   | 5        | 0.34          |
| (1,740)  | 1:197:A:ASN:HB2  | 1:198:A:PHE:H    | 2        | 0.34          |
| (1,739)  | 1:166:A:VAL:HG11 | 1:222:A:SER:HB3  | 6        | 0.34          |
| (1,739)  | 1:166:A:VAL:HG12 | 1:222:A:SER:HB3  | 6        | 0.34          |
| (1,739)  | 1:166:A:VAL:HG13 | 1:222:A:SER:HB3  | 6        | 0.34          |
| (1,657)  | 1:213:A:MET:HB3  | 1:213:A:MET:HE1  | 9        | 0.34          |
| (1,657)  | 1:213:A:MET:HB3  | 1:213:A:MET:HE2  | 9        | 0.34          |
| (1,657)  | 1:213:A:MET:HB3  | 1:213:A:MET:HE3  | 9        | 0.34          |
| (1,528)  | 1:143:A:ASN:HB2  | 1:147:A:ASP:HB3  | 8        | 0.34          |
| (1,528)  | 1:143:A:ASN:HB3  | 1:147:A:ASP:HB3  | 8        | 0.34          |
| (1,445)  | 1:180:A:VAL:HA   | 1:184:A:ILE:HG12 | 20       | 0.34          |
| (1,224)  | 1:127:A:GLY:HA3  | 1:128:A:TYR:HB2  | 13       | 0.34          |
| (1,224)  | 1:127:A:GLY:HA3  | 1:128:A:TYR:HB2  | 18       | 0.34          |
| (1,179)  | 1:201:A:THR:HB   | 1:205:A:MET:HG3  | 18       | 0.34          |
| (1,79)   | 1:138:A:MET:H    | 1:209:A:VAL:HG11 | 13       | 0.34          |
| (1,79)   | 1:138:A:MET:H    | 1:209:A:VAL:HG12 | 13       | 0.34          |
| (1,79)   | 1:138:A:MET:H    | 1:209:A:VAL:HG13 | 13       | 0.34          |
| (1,77)   | 1:208:A:ARG:H    | 1:209:A:VAL:HG11 | 7        | 0.34          |
| (1,77)   | 1:208:A:ARG:H    | 1:209:A:VAL:HG12 | 7        | 0.34          |
| (1,77)   | 1:208:A:ARG:H    | 1:209:A:VAL:HG13 | 7        | 0.34          |
| (1,2834) | 1:163:A:TYR:HE1  | 1:221:A:GLU:HG2  | 19       | 0.33          |
| (1,2834) | 1:163:A:TYR:HE2  | 1:221:A:GLU:HG2  | 19       | 0.33          |
| (1,2771) | 1:130:A:LEU:HB3  | 1:162:A:TYR:HE1  | 11       | 0.33          |
| (1,2771) | 1:130:A:LEU:HB3  | 1:162:A:TYR:HE2  | 11       | 0.33          |
| (1,2759) | 1:139:A:ILE:HG12 | 1:150:A:TYR:HE1  | 8        | 0.33          |
| (1,2759) | 1:139:A:ILE:HG12 | 1:150:A:TYR:HE2  | 8        | 0.33          |
| (1,2553) | 1:126:A:GLY:HA2  | 1:128:A:TYR:HD1  | 7        | 0.33          |
| (1,2553) | 1:126:A:GLY:HA2  | 1:128:A:TYR:HD2  | 7        | 0.33          |
| (1,2553) | 1:126:A:GLY:HA2  | 1:128:A:TYR:HD1  | 9        | 0.33          |
| (1,2553) | 1:126:A:GLY:HA2  | 1:128:A:TYR:HD2  | 9        | 0.33          |
| (1,2553) | 1:126:A:GLY:HA2  | 1:128:A:TYR:HD1  | 20       | 0.33          |
| (1,2553) | 1:126:A:GLY:HA2  | 1:128:A:TYR:HD2  | 20       | 0.33          |
| (1,2548) | 1:162:A:TYR:HD1  | 1:186:A:GLN:HB3  | 20       | 0.33          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2548) | 1:162:A:TYR:HD2  | 1:186:A:GLN:HB3  | 20       | 0.33          |
| (1,2529) | 1:125:A:LEU:HD11 | 1:162:A:TYR:HD1  | 15       | 0.33          |
| (1,2529) | 1:125:A:LEU:HD11 | 1:162:A:TYR:HD2  | 15       | 0.33          |
| (1,2529) | 1:125:A:LEU:HD12 | 1:162:A:TYR:HD1  | 15       | 0.33          |
| (1,2529) | 1:125:A:LEU:HD12 | 1:162:A:TYR:HD2  | 15       | 0.33          |
| (1,2529) | 1:125:A:LEU:HD13 | 1:162:A:TYR:HD1  | 15       | 0.33          |
| (1,2529) | 1:125:A:LEU:HD13 | 1:162:A:TYR:HD2  | 15       | 0.33          |
| (1,2488) | 1:149:A:TYR:HD1  | 1:153:A:ASN:HB3  | 7        | 0.33          |
| (1,2488) | 1:149:A:TYR:HD2  | 1:153:A:ASN:HB3  | 7        | 0.33          |
| (1,2474) | 1:168:A:GLN:HG2  | 1:169:A:TYR:HD1  | 7        | 0.33          |
| (1,2474) | 1:168:A:GLN:HG2  | 1:169:A:TYR:HD2  | 7        | 0.33          |
| (1,2309) | 1:171:A:ASN:HD22 | 1:174:A:ASN:HD21 | 8        | 0.33          |
| (1,2279) | 1:186:A:GLN:HB3  | 1:188:A:THR:H    | 8        | 0.33          |
| (1,1558) | 1:208:A:ARG:HG3  | 1:209:A:VAL:H    | 14       | 0.33          |
| (1,1538) | 1:164:A:ARG:HD2  | 1:165:A:PRO:HD3  | 20       | 0.33          |
| (1,1396) | 1:148:A:ARG:HA   | 1:151:A:ARG:HB2  | 13       | 0.33          |
| (1,1250) | 1:205:A:MET:HB2  | 1:206:A:MET:HG2  | 12       | 0.33          |
| (1,1058) | 1:203:A:VAL:HG21 | 1:207:A:GLU:HG3  | 12       | 0.33          |
| (1,1058) | 1:203:A:VAL:HG22 | 1:207:A:GLU:HG3  | 12       | 0.33          |
| (1,1058) | 1:203:A:VAL:HG23 | 1:207:A:GLU:HG3  | 12       | 0.33          |
| (1,1033) | 1:205:A:MET:H    | 1:207:A:GLU:HG3  | 4        | 0.33          |
| (1,957)  | 1:184:A:ILE:HD11 | 1:207:A:GLU:HG3  | 12       | 0.33          |
| (1,957)  | 1:184:A:ILE:HD12 | 1:207:A:GLU:HG3  | 12       | 0.33          |
| (1,957)  | 1:184:A:ILE:HD13 | 1:207:A:GLU:HG3  | 12       | 0.33          |
| (1,893)  | 1:162:A:TYR:HB3  | 1:182:A:ILE:HB   | 1        | 0.33          |
| (1,864)  | 1:134:A:MET:HB3  | 1:135:A:SER:HB2  | 10       | 0.33          |
| (1,839)  | 1:176:A:VAL:HG21 | 1:214:A:CYS:HA   | 12       | 0.33          |
| (1,839)  | 1:176:A:VAL:HG22 | 1:214:A:CYS:HA   | 12       | 0.33          |
| (1,839)  | 1:176:A:VAL:HG23 | 1:214:A:CYS:HA   | 12       | 0.33          |
| (1,833)  | 1:207:A:GLU:HA   | 1:207:A:GLU:HG3  | 12       | 0.33          |
| (1,567)  | 1:230:A:ARG:HB2  | 1:231:A:SER:HB3  | 9        | 0.33          |
| (1,563)  | 1:132:A:SER:HB3  | 1:133:A:ALA:HB1  | 11       | 0.33          |
| (1,563)  | 1:132:A:SER:HB3  | 1:133:A:ALA:HB2  | 11       | 0.33          |
| (1,563)  | 1:132:A:SER:HB3  | 1:133:A:ALA:HB3  | 11       | 0.33          |
| (1,510)  | 1:211:A:GLU:HG3  | 1:214:A:CYS:HB3  | 8        | 0.33          |
| (1,389)  | 1:121:A:VAL:HA   | 1:122:A:VAL:HG11 | 12       | 0.33          |
| (1,389)  | 1:121:A:VAL:HA   | 1:122:A:VAL:HG12 | 12       | 0.33          |
| (1,389)  | 1:121:A:VAL:HA   | 1:122:A:VAL:HG13 | 12       | 0.33          |
| (1,318)  | 1:153:A:ASN:HB2  | 1:156:A:ARG:HD3  | 15       | 0.33          |
| (1,224)  | 1:127:A:GLY:HA3  | 1:128:A:TYR:HB2  | 3        | 0.33          |
| (1,2782) | 1:150:A:TYR:HE1  | 1:154:A:MET:HG3  | 3        | 0.32          |
| (1,2782) | 1:150:A:TYR:HE2  | 1:154:A:MET:HG3  | 3        | 0.32          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2771) | 1:130:A:LEU:HB3  | 1:162:A:TYR:HE1  | 6        | 0.32          |
| (1,2771) | 1:130:A:LEU:HB3  | 1:162:A:TYR:HE2  | 6        | 0.32          |
| (1,2674) | 1:175:A:PHE:HZ   | 1:221:A:GLU:HG2  | 18       | 0.32          |
| (1,2328) | 1:223:A:GLN:HE21 | 1:227:A:ASP:HB2  | 5        | 0.32          |
| (1,2328) | 1:223:A:GLN:HE21 | 1:227:A:ASP:HB3  | 5        | 0.32          |
| (1,2309) | 1:171:A:ASN:HD22 | 1:174:A:ASN:HD21 | 3        | 0.32          |
| (1,2270) | 1:132:A:SER:H    | 1:132:A:SER:HB2  | 14       | 0.32          |
| (1,2270) | 1:132:A:SER:H    | 1:132:A:SER:HB2  | 19       | 0.32          |
| (1,2045) | 1:230:A:ARG:HG3  | 1:231:A:SER:H    | 17       | 0.32          |
| (1,1584) | 1:122:A:VAL:H    | 1:122:A:VAL:HG11 | 8        | 0.32          |
| (1,1584) | 1:122:A:VAL:H    | 1:122:A:VAL:HG12 | 8        | 0.32          |
| (1,1584) | 1:122:A:VAL:H    | 1:122:A:VAL:HG13 | 8        | 0.32          |
| (1,1558) | 1:208:A:ARG:HG3  | 1:209:A:VAL:H    | 15       | 0.32          |
| (1,1501) | 1:137:A:PRO:HD3  | 1:209:A:VAL:HG21 | 1        | 0.32          |
| (1,1501) | 1:137:A:PRO:HD3  | 1:209:A:VAL:HG22 | 1        | 0.32          |
| (1,1501) | 1:137:A:PRO:HD3  | 1:209:A:VAL:HG23 | 1        | 0.32          |
| (1,1495) | 1:212:A:GLN:HB2  | 1:216:A:THR:H    | 9        | 0.32          |
| (1,1407) | 1:134:A:MET:HB3  | 1:220:A:LYS:HD2  | 11       | 0.32          |
| (1,1407) | 1:134:A:MET:HB3  | 1:220:A:LYS:HD3  | 11       | 0.32          |
| (1,1294) | 1:138:A:MET:HG3  | 1:139:A:ILE:H    | 6        | 0.32          |
| (1,1212) | 1:184:A:ILE:HD11 | 1:206:A:MET:HB3  | 20       | 0.32          |
| (1,1212) | 1:184:A:ILE:HD12 | 1:206:A:MET:HB3  | 20       | 0.32          |
| (1,1212) | 1:184:A:ILE:HD13 | 1:206:A:MET:HB3  | 20       | 0.32          |
| (1,1097) | 1:165:A:PRO:HB3  | 1:168:A:GLN:HG2  | 7        | 0.32          |
| (1,1023) | 1:206:A:MET:HG3  | 1:207:A:GLU:HG3  | 11       | 0.32          |
| (1,987)  | 1:149:A:TYR:HA   | 1:152:A:GLU:HG2  | 8        | 0.32          |
| (1,873)  | 1:146:A:GLU:HA   | 1:150:A:TYR:HB3  | 17       | 0.32          |
| (1,739)  | 1:166:A:VAL:HG11 | 1:222:A:SER:HB3  | 7        | 0.32          |
| (1,739)  | 1:166:A:VAL:HG12 | 1:222:A:SER:HB3  | 7        | 0.32          |
| (1,739)  | 1:166:A:VAL:HG13 | 1:222:A:SER:HB3  | 7        | 0.32          |
| (1,657)  | 1:213:A:MET:HB3  | 1:213:A:MET:HE1  | 5        | 0.32          |
| (1,657)  | 1:213:A:MET:HB3  | 1:213:A:MET:HE2  | 5        | 0.32          |
| (1,657)  | 1:213:A:MET:HB3  | 1:213:A:MET:HE3  | 5        | 0.32          |
| (1,634)  | 1:192:A:THR:HA   | 1:195:A:GLY:HA3  | 15       | 0.32          |
| (1,574)  | 1:153:A:ASN:HB2  | 1:155:A:TYR:HE1  | 14       | 0.32          |
| (1,574)  | 1:153:A:ASN:HB2  | 1:155:A:TYR:HE2  | 14       | 0.32          |
| (1,521)  | 1:223:A:GLN:HG3  | 1:224:A:ALA:HB1  | 18       | 0.32          |
| (1,521)  | 1:223:A:GLN:HG3  | 1:224:A:ALA:HB2  | 18       | 0.32          |
| (1,521)  | 1:223:A:GLN:HG3  | 1:224:A:ALA:HB3  | 18       | 0.32          |
| (1,497)  | 1:128:A:TYR:HB2  | 1:162:A:TYR:HB2  | 3        | 0.32          |
| (1,445)  | 1:180:A:VAL:HA   | 1:184:A:ILE:HG12 | 12       | 0.32          |
| (1,389)  | 1:121:A:VAL:HA   | 1:122:A:VAL:HG11 | 1        | 0.32          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,389)  | 1:121:A:VAL:HA   | 1:122:A:VAL:HG12 | 1        | 0.32          |
| (1,389)  | 1:121:A:VAL:HA   | 1:122:A:VAL:HG13 | 1        | 0.32          |
| (1,323)  | 1:209:A:VAL:HG21 | 1:212:A:GLN:HB3  | 12       | 0.32          |
| (1,323)  | 1:209:A:VAL:HG22 | 1:212:A:GLN:HB3  | 12       | 0.32          |
| (1,323)  | 1:209:A:VAL:HG23 | 1:212:A:GLN:HB3  | 12       | 0.32          |
| (1,202)  | 1:183:A:THR:HG21 | 1:184:A:ILE:HG12 | 10       | 0.32          |
| (1,202)  | 1:183:A:THR:HG22 | 1:184:A:ILE:HG12 | 10       | 0.32          |
| (1,202)  | 1:183:A:THR:HG23 | 1:184:A:ILE:HG12 | 10       | 0.32          |
| (1,179)  | 1:201:A:THR:HB   | 1:205:A:MET:HG3  | 13       | 0.32          |
| (1,166)  | 1:203:A:VAL:HG11 | 1:206:A:MET:HG2  | 5        | 0.32          |
| (1,166)  | 1:203:A:VAL:HG12 | 1:206:A:MET:HG2  | 5        | 0.32          |
| (1,166)  | 1:203:A:VAL:HG13 | 1:206:A:MET:HG2  | 5        | 0.32          |
| (1,151)  | 1:126:A:GLY:HA3  | 1:164:A:ARG:HD3  | 8        | 0.32          |
| (1,151)  | 1:126:A:GLY:HA3  | 1:164:A:ARG:HD3  | 12       | 0.32          |
| (1,129)  | 1:161:A:VAL:HG11 | 1:210:A:VAL:HG11 | 10       | 0.32          |
| (1,129)  | 1:161:A:VAL:HG11 | 1:210:A:VAL:HG12 | 10       | 0.32          |
| (1,129)  | 1:161:A:VAL:HG11 | 1:210:A:VAL:HG13 | 10       | 0.32          |
| (1,129)  | 1:161:A:VAL:HG12 | 1:210:A:VAL:HG11 | 10       | 0.32          |
| (1,129)  | 1:161:A:VAL:HG12 | 1:210:A:VAL:HG12 | 10       | 0.32          |
| (1,129)  | 1:161:A:VAL:HG12 | 1:210:A:VAL:HG13 | 10       | 0.32          |
| (1,129)  | 1:161:A:VAL:HG13 | 1:210:A:VAL:HG11 | 10       | 0.32          |
| (1,129)  | 1:161:A:VAL:HG13 | 1:210:A:VAL:HG12 | 10       | 0.32          |
| (1,129)  | 1:161:A:VAL:HG13 | 1:210:A:VAL:HG13 | 10       | 0.32          |
| (1,2834) | 1:163:A:TYR:HE1  | 1:221:A:GLU:HG2  | 2        | 0.31          |
| (1,2834) | 1:163:A:TYR:HE2  | 1:221:A:GLU:HG2  | 2        | 0.31          |
| (1,2824) | 1:218:A:TYR:HE1  | 1:222:A:SER:HB3  | 15       | 0.31          |
| (1,2824) | 1:218:A:TYR:HE2  | 1:222:A:SER:HB3  | 15       | 0.31          |
| (1,2721) | 1:177:A:HIS:HD2  | 1:178:A:ASP:HB3  | 4        | 0.31          |
| (1,2593) | 1:175:A:PHE:HE1  | 1:221:A:GLU:HG2  | 4        | 0.31          |
| (1,2593) | 1:175:A:PHE:HE2  | 1:221:A:GLU:HG2  | 4        | 0.31          |
| (1,2553) | 1:126:A:GLY:HA2  | 1:128:A:TYR:HD1  | 4        | 0.31          |
| (1,2553) | 1:126:A:GLY:HA2  | 1:128:A:TYR:HD2  | 4        | 0.31          |
| (1,1893) | 1:208:A:ARG:HB3  | 1:209:A:VAL:H    | 12       | 0.31          |
| (1,1746) | 1:184:A:ILE:H    | 1:184:A:ILE:HG12 | 7        | 0.31          |
| (1,1701) | 1:129:A:MET:H    | 1:129:A:MET:HG3  | 5        | 0.31          |
| (1,1655) | 1:230:A:ARG:H    | 1:230:A:ARG:HG3  | 14       | 0.31          |
| (1,1655) | 1:230:A:ARG:H    | 1:230:A:ARG:HG3  | 17       | 0.31          |
| (1,1495) | 1:212:A:GLN:HB2  | 1:216:A:THR:H    | 18       | 0.31          |
| (1,1480) | 1:203:A:VAL:HG21 | 1:207:A:GLU:HB2  | 18       | 0.31          |
| (1,1480) | 1:203:A:VAL:HG22 | 1:207:A:GLU:HB2  | 18       | 0.31          |
| (1,1480) | 1:203:A:VAL:HG23 | 1:207:A:GLU:HB2  | 18       | 0.31          |
| (1,1392) | 1:133:A:ALA:HA   | 1:159:A:ASN:HB2  | 10       | 0.31          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1285) | 1:205:A:MET:H    | 1:206:A:MET:HG2  | 3        | 0.31          |
| (1,1213) | 1:230:A:ARG:HA   | 1:230:A:ARG:HG3  | 13       | 0.31          |
| (1,1015) | 1:152:A:GLU:HG2  | 1:153:A:ASN:HD22 | 19       | 0.31          |
| (1,983)  | 1:149:A:TYR:H    | 1:152:A:GLU:HG2  | 16       | 0.31          |
| (1,957)  | 1:184:A:ILE:HD11 | 1:207:A:GLU:HG3  | 19       | 0.31          |
| (1,957)  | 1:184:A:ILE:HD12 | 1:207:A:GLU:HG3  | 19       | 0.31          |
| (1,957)  | 1:184:A:ILE:HD13 | 1:207:A:GLU:HG3  | 19       | 0.31          |
| (1,893)  | 1:162:A:TYR:HB3  | 1:182:A:ILE:HB   | 16       | 0.31          |
| (1,881)  | 1:145:A:TRP:HE3  | 1:146:A:GLU:HG3  | 13       | 0.31          |
| (1,881)  | 1:145:A:TRP:HE3  | 1:146:A:GLU:HG3  | 20       | 0.31          |
| (1,656)  | 1:138:A:MET:HG3  | 1:154:A:MET:HE1  | 4        | 0.31          |
| (1,656)  | 1:138:A:MET:HG3  | 1:154:A:MET:HE2  | 4        | 0.31          |
| (1,656)  | 1:138:A:MET:HG3  | 1:154:A:MET:HE3  | 4        | 0.31          |
| (1,563)  | 1:132:A:SER:HB3  | 1:133:A:ALA:HB1  | 17       | 0.31          |
| (1,563)  | 1:132:A:SER:HB3  | 1:133:A:ALA:HB2  | 17       | 0.31          |
| (1,563)  | 1:132:A:SER:HB3  | 1:133:A:ALA:HB3  | 17       | 0.31          |
| (1,496)  | 1:130:A:LEU:HA   | 1:162:A:TYR:HB2  | 8        | 0.31          |
| (1,350)  | 1:122:A:VAL:HG21 | 1:123:A:GLY:H    | 1        | 0.31          |
| (1,350)  | 1:122:A:VAL:HG22 | 1:123:A:GLY:H    | 1        | 0.31          |
| (1,350)  | 1:122:A:VAL:HG23 | 1:123:A:GLY:H    | 1        | 0.31          |
| (1,350)  | 1:122:A:VAL:HG21 | 1:123:A:GLY:H    | 9        | 0.31          |
| (1,350)  | 1:122:A:VAL:HG22 | 1:123:A:GLY:H    | 9        | 0.31          |
| (1,350)  | 1:122:A:VAL:HG23 | 1:123:A:GLY:H    | 9        | 0.31          |
| (1,323)  | 1:209:A:VAL:HG21 | 1:212:A:GLN:HB3  | 16       | 0.31          |
| (1,323)  | 1:209:A:VAL:HG22 | 1:212:A:GLN:HB3  | 16       | 0.31          |
| (1,323)  | 1:209:A:VAL:HG23 | 1:212:A:GLN:HB3  | 16       | 0.31          |
| (1,249)  | 1:203:A:VAL:HA   | 1:206:A:MET:HB2  | 5        | 0.31          |
| (1,177)  | 1:195:A:GLY:HA3  | 1:197:A:ASN:HD21 | 5        | 0.31          |
| (1,89)   | 1:206:A:MET:HB3  | 1:210:A:VAL:HG21 | 19       | 0.31          |
| (1,89)   | 1:206:A:MET:HB3  | 1:210:A:VAL:HG22 | 19       | 0.31          |
| (1,89)   | 1:206:A:MET:HB3  | 1:210:A:VAL:HG23 | 19       | 0.31          |
| (1,2774) | 1:128:A:TYR:HE1  | 1:162:A:TYR:HB3  | 1        | 0.3           |
| (1,2774) | 1:128:A:TYR:HE2  | 1:162:A:TYR:HB3  | 1        | 0.3           |
| (1,2771) | 1:130:A:LEU:HB3  | 1:162:A:TYR:HE1  | 15       | 0.3           |
| (1,2771) | 1:130:A:LEU:HB3  | 1:162:A:TYR:HE2  | 15       | 0.3           |
| (1,2736) | 1:184:A:ILE:HG13 | 1:187:A:HIS:HD2  | 6        | 0.3           |
| (1,2674) | 1:175:A:PHE:HZ   | 1:221:A:GLU:HG2  | 11       | 0.3           |
| (1,2593) | 1:175:A:PHE:HE1  | 1:221:A:GLU:HG2  | 3        | 0.3           |
| (1,2593) | 1:175:A:PHE:HE2  | 1:221:A:GLU:HG2  | 3        | 0.3           |
| (1,2270) | 1:132:A:SER:H    | 1:132:A:SER:HB2  | 11       | 0.3           |
| (1,1893) | 1:208:A:ARG:HB3  | 1:209:A:VAL:H    | 4        | 0.3           |
| (1,1655) | 1:230:A:ARG:H    | 1:230:A:ARG:HG3  | 7        | 0.3           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1579) | 1:132:A:SER:HB3  | 1:133:A:ALA:H    | 11       | 0.3           |
| (1,1501) | 1:137:A:PRO:HD3  | 1:209:A:VAL:HG21 | 7        | 0.3           |
| (1,1501) | 1:137:A:PRO:HD3  | 1:209:A:VAL:HG22 | 7        | 0.3           |
| (1,1501) | 1:137:A:PRO:HD3  | 1:209:A:VAL:HG23 | 7        | 0.3           |
| (1,1497) | 1:139:A:ILE:HD11 | 1:212:A:GLN:HB3  | 19       | 0.3           |
| (1,1497) | 1:139:A:ILE:HD12 | 1:212:A:GLN:HB3  | 19       | 0.3           |
| (1,1497) | 1:139:A:ILE:HD13 | 1:212:A:GLN:HB3  | 19       | 0.3           |
| (1,1479) | 1:145:A:TRP:HB2  | 1:146:A:GLU:HG2  | 15       | 0.3           |
| (1,1479) | 1:145:A:TRP:HB3  | 1:146:A:GLU:HG2  | 15       | 0.3           |
| (1,1466) | 1:210:A:VAL:H    | 1:211:A:GLU:HB3  | 8        | 0.3           |
| (1,1294) | 1:138:A:MET:HG3  | 1:139:A:ILE:H    | 18       | 0.3           |
| (1,1168) | 1:223:A:GLN:H    | 1:223:A:GLN:HG2  | 16       | 0.3           |
| (1,1060) | 1:207:A:GLU:HG3  | 1:208:A:ARG:H    | 10       | 0.3           |
| (1,1050) | 1:128:A:TYR:HA   | 1:129:A:MET:HG3  | 20       | 0.3           |
| (1,988)  | 1:148:A:ARG:HA   | 1:152:A:GLU:HG3  | 5        | 0.3           |
| (1,983)  | 1:149:A:TYR:H    | 1:152:A:GLU:HG2  | 4        | 0.3           |
| (1,893)  | 1:162:A:TYR:HB3  | 1:182:A:ILE:HB   | 3        | 0.3           |
| (1,634)  | 1:192:A:THR:HA   | 1:195:A:GLY:HA3  | 5        | 0.3           |
| (1,525)  | 1:132:A:SER:HB2  | 1:160:A:GLN:HE21 | 6        | 0.3           |
| (1,448)  | 1:226:A:TYR:HE1  | 1:230:A:ARG:HD2  | 13       | 0.3           |
| (1,448)  | 1:226:A:TYR:HE2  | 1:230:A:ARG:HD2  | 13       | 0.3           |
| (1,339)  | 1:209:A:VAL:HG21 | 1:210:A:VAL:HG21 | 12       | 0.3           |
| (1,339)  | 1:209:A:VAL:HG21 | 1:210:A:VAL:HG22 | 12       | 0.3           |
| (1,339)  | 1:209:A:VAL:HG21 | 1:210:A:VAL:HG23 | 12       | 0.3           |
| (1,339)  | 1:209:A:VAL:HG22 | 1:210:A:VAL:HG21 | 12       | 0.3           |
| (1,339)  | 1:209:A:VAL:HG22 | 1:210:A:VAL:HG22 | 12       | 0.3           |
| (1,339)  | 1:209:A:VAL:HG22 | 1:210:A:VAL:HG23 | 12       | 0.3           |
| (1,339)  | 1:209:A:VAL:HG23 | 1:210:A:VAL:HG21 | 12       | 0.3           |
| (1,339)  | 1:209:A:VAL:HG23 | 1:210:A:VAL:HG22 | 12       | 0.3           |
| (1,339)  | 1:209:A:VAL:HG23 | 1:210:A:VAL:HG23 | 12       | 0.3           |
| (1,318)  | 1:153:A:ASN:HB2  | 1:156:A:ARG:HD3  | 14       | 0.3           |
| (1,268)  | 1:166:A:VAL:HG11 | 1:225:A:TYR:HB3  | 12       | 0.3           |
| (1,268)  | 1:166:A:VAL:HG12 | 1:225:A:TYR:HB3  | 12       | 0.3           |
| (1,268)  | 1:166:A:VAL:HG13 | 1:225:A:TYR:HB3  | 12       | 0.3           |
| (1,249)  | 1:203:A:VAL:HA   | 1:206:A:MET:HB2  | 2        | 0.3           |
| (1,249)  | 1:203:A:VAL:HA   | 1:206:A:MET:HB2  | 15       | 0.3           |
| (1,249)  | 1:203:A:VAL:HA   | 1:206:A:MET:HB2  | 16       | 0.3           |
| (1,167)  | 1:203:A:VAL:H    | 1:203:A:VAL:HG11 | 8        | 0.3           |
| (1,167)  | 1:203:A:VAL:H    | 1:203:A:VAL:HG12 | 8        | 0.3           |
| (1,167)  | 1:203:A:VAL:H    | 1:203:A:VAL:HG13 | 8        | 0.3           |
| (1,138)  | 1:125:A:LEU:HA   | 1:125:A:LEU:HD21 | 11       | 0.3           |
| (1,138)  | 1:125:A:LEU:HA   | 1:125:A:LEU:HD22 | 11       | 0.3           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,138)  | 1:125:A:LEU:HA   | 1:125:A:LEU:HD23 | 11       | 0.3           |
| (1,77)   | 1:208:A:ARG:H    | 1:209:A:VAL:HG11 | 20       | 0.3           |
| (1,77)   | 1:208:A:ARG:H    | 1:209:A:VAL:HG12 | 20       | 0.3           |
| (1,77)   | 1:208:A:ARG:H    | 1:209:A:VAL:HG13 | 20       | 0.3           |
| (1,73)   | 1:176:A:VAL:HG21 | 1:214:A:CYS:H    | 12       | 0.3           |
| (1,73)   | 1:176:A:VAL:HG22 | 1:214:A:CYS:H    | 12       | 0.3           |
| (1,73)   | 1:176:A:VAL:HG23 | 1:214:A:CYS:H    | 12       | 0.3           |
| (1,1)    | 1:138:A:MET:HG3  | 1:139:A:ILE:HG12 | 10       | 0.3           |
| (1,2807) | 1:149:A:TYR:HE1  | 1:153:A:ASN:HB3  | 1        | 0.29          |
| (1,2807) | 1:149:A:TYR:HE2  | 1:153:A:ASN:HB3  | 1        | 0.29          |
| (1,2699) | 1:141:A:PHE:HZ   | 1:150:A:TYR:HB3  | 13       | 0.29          |
| (1,2657) | 1:141:A:PHE:HE1  | 1:208:A:ARG:HB3  | 3        | 0.29          |
| (1,2657) | 1:141:A:PHE:HE2  | 1:208:A:ARG:HB3  | 3        | 0.29          |
| (1,2593) | 1:175:A:PHE:HE1  | 1:221:A:GLU:HG2  | 11       | 0.29          |
| (1,2593) | 1:175:A:PHE:HE2  | 1:221:A:GLU:HG2  | 11       | 0.29          |
| (1,2488) | 1:149:A:TYR:HD1  | 1:153:A:ASN:HB3  | 15       | 0.29          |
| (1,2488) | 1:149:A:TYR:HD2  | 1:153:A:ASN:HB3  | 15       | 0.29          |
| (1,2438) | 1:229:A:ARG:HE   | 1:230:A:ARG:HD2  | 10       | 0.29          |
| (1,2076) | 1:208:A:ARG:H    | 1:208:A:ARG:HG3  | 15       | 0.29          |
| (1,2040) | 1:128:A:TYR:H    | 1:164:A:ARG:HG3  | 14       | 0.29          |
| (1,1407) | 1:134:A:MET:HB3  | 1:220:A:LYS:HD2  | 3        | 0.29          |
| (1,1407) | 1:134:A:MET:HB3  | 1:220:A:LYS:HD3  | 3        | 0.29          |
| (1,1207) | 1:168:A:GLN:HA   | 1:168:A:GLN:HE22 | 10       | 0.29          |
| (1,1207) | 1:168:A:GLN:HA   | 1:168:A:GLN:HE22 | 20       | 0.29          |
| (1,1197) | 1:160:A:GLN:HB2  | 1:183:A:THR:HG21 | 6        | 0.29          |
| (1,1197) | 1:160:A:GLN:HB2  | 1:183:A:THR:HG22 | 6        | 0.29          |
| (1,1197) | 1:160:A:GLN:HB2  | 1:183:A:THR:HG23 | 6        | 0.29          |
| (1,1058) | 1:203:A:VAL:HG21 | 1:207:A:GLU:HG3  | 8        | 0.29          |
| (1,1058) | 1:203:A:VAL:HG22 | 1:207:A:GLU:HG3  | 8        | 0.29          |
| (1,1058) | 1:203:A:VAL:HG23 | 1:207:A:GLU:HG3  | 8        | 0.29          |
| (1,1015) | 1:152:A:GLU:HG2  | 1:153:A:ASN:HD22 | 3        | 0.29          |
| (1,1015) | 1:152:A:GLU:HG2  | 1:153:A:ASN:HD22 | 17       | 0.29          |
| (1,957)  | 1:184:A:ILE:HD11 | 1:207:A:GLU:HG3  | 9        | 0.29          |
| (1,957)  | 1:184:A:ILE:HD12 | 1:207:A:GLU:HG3  | 9        | 0.29          |
| (1,957)  | 1:184:A:ILE:HD13 | 1:207:A:GLU:HG3  | 9        | 0.29          |
| (1,873)  | 1:146:A:GLU:HA   | 1:150:A:TYR:HB3  | 18       | 0.29          |
| (1,814)  | 1:226:A:TYR:HB2  | 1:227:A:ASP:HA   | 3        | 0.29          |
| (1,448)  | 1:226:A:TYR:HE1  | 1:230:A:ARG:HD2  | 10       | 0.29          |
| (1,448)  | 1:226:A:TYR:HE2  | 1:230:A:ARG:HD2  | 10       | 0.29          |
| (1,445)  | 1:180:A:VAL:HA   | 1:184:A:ILE:HG12 | 9        | 0.29          |
| (1,436)  | 1:229:A:ARG:HA   | 1:230:A:ARG:HD3  | 1        | 0.29          |
| (1,388)  | 1:122:A:VAL:HG11 | 1:186:A:GLN:HE21 | 3        | 0.29          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,388)  | 1:122:A:VAL:HG12 | 1:186:A:GLN:HE21 | 3        | 0.29          |
| (1,388)  | 1:122:A:VAL:HG13 | 1:186:A:GLN:HE21 | 3        | 0.29          |
| (1,249)  | 1:203:A:VAL:HA   | 1:206:A:MET:HB2  | 1        | 0.29          |
| (1,249)  | 1:203:A:VAL:HA   | 1:206:A:MET:HB2  | 7        | 0.29          |
| (1,249)  | 1:203:A:VAL:HA   | 1:206:A:MET:HB2  | 9        | 0.29          |
| (1,249)  | 1:203:A:VAL:HA   | 1:206:A:MET:HB2  | 10       | 0.29          |
| (1,249)  | 1:203:A:VAL:HA   | 1:206:A:MET:HB2  | 12       | 0.29          |
| (1,249)  | 1:203:A:VAL:HA   | 1:206:A:MET:HB2  | 13       | 0.29          |
| (1,249)  | 1:203:A:VAL:HA   | 1:206:A:MET:HB2  | 17       | 0.29          |
| (1,249)  | 1:203:A:VAL:HA   | 1:206:A:MET:HB2  | 18       | 0.29          |
| (1,162)  | 1:226:A:TYR:HB2  | 1:228:A:GLY:HA2  | 3        | 0.29          |
| (1,162)  | 1:226:A:TYR:HB2  | 1:228:A:GLY:HA3  | 3        | 0.29          |
| (1,162)  | 1:226:A:TYR:HB2  | 1:228:A:GLY:HA2  | 17       | 0.29          |
| (1,162)  | 1:226:A:TYR:HB2  | 1:228:A:GLY:HA3  | 17       | 0.29          |
| (1,31)   | 1:219:A:GLN:HA   | 1:220:A:LYS:HG3  | 9        | 0.29          |
| (1,2830) | 1:172:A:GLN:HG2  | 1:218:A:TYR:HE1  | 4        | 0.28          |
| (1,2830) | 1:172:A:GLN:HG2  | 1:218:A:TYR:HE2  | 4        | 0.28          |
| (1,2830) | 1:172:A:GLN:HG2  | 1:218:A:TYR:HE1  | 18       | 0.28          |
| (1,2830) | 1:172:A:GLN:HG2  | 1:218:A:TYR:HE2  | 18       | 0.28          |
| (1,2759) | 1:139:A:ILE:HG12 | 1:150:A:TYR:HE1  | 3        | 0.28          |
| (1,2759) | 1:139:A:ILE:HG12 | 1:150:A:TYR:HE2  | 3        | 0.28          |
| (1,2759) | 1:139:A:ILE:HG12 | 1:150:A:TYR:HE1  | 9        | 0.28          |
| (1,2759) | 1:139:A:ILE:HG12 | 1:150:A:TYR:HE2  | 9        | 0.28          |
| (1,2699) | 1:141:A:PHE:HZ   | 1:150:A:TYR:HB3  | 16       | 0.28          |
| (1,2593) | 1:175:A:PHE:HE1  | 1:221:A:GLU:HG2  | 2        | 0.28          |
| (1,2593) | 1:175:A:PHE:HE2  | 1:221:A:GLU:HG2  | 2        | 0.28          |
| (1,2488) | 1:149:A:TYR:HD1  | 1:153:A:ASN:HB3  | 6        | 0.28          |
| (1,2488) | 1:149:A:TYR:HD2  | 1:153:A:ASN:HB3  | 6        | 0.28          |
| (1,2313) | 1:159:A:ASN:HD22 | 1:160:A:GLN:HE21 | 13       | 0.28          |
| (1,2076) | 1:208:A:ARG:H    | 1:208:A:ARG:HG3  | 14       | 0.28          |
| (1,2043) | 1:231:A:SER:H    | 1:231:A:SER:HB3  | 5        | 0.28          |
| (1,2043) | 1:231:A:SER:H    | 1:231:A:SER:HB3  | 12       | 0.28          |
| (1,1937) | 1:220:A:LYS:H    | 1:221:A:GLU:HG3  | 2        | 0.28          |
| (1,1861) | 1:147:A:ASP:HB2  | 1:148:A:ARG:H    | 2        | 0.28          |
| (1,1540) | 1:164:A:ARG:HG3  | 1:165:A:PRO:HD3  | 5        | 0.28          |
| (1,1501) | 1:137:A:PRO:HD3  | 1:209:A:VAL:HG21 | 20       | 0.28          |
| (1,1501) | 1:137:A:PRO:HD3  | 1:209:A:VAL:HG22 | 20       | 0.28          |
| (1,1501) | 1:137:A:PRO:HD3  | 1:209:A:VAL:HG23 | 20       | 0.28          |
| (1,1375) | 1:136:A:ARG:HD2  | 1:154:A:MET:HG3  | 16       | 0.28          |
| (1,1294) | 1:138:A:MET:HG3  | 1:139:A:ILE:H    | 20       | 0.28          |
| (1,1250) | 1:205:A:MET:HB2  | 1:206:A:MET:HG2  | 10       | 0.28          |
| (1,1168) | 1:223:A:GLN:H    | 1:223:A:GLN:HG2  | 1        | 0.28          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1166) | 1:215:A:VAL:HG21 | 1:219:A:GLN:HG3  | 6        | 0.28          |
| (1,1166) | 1:215:A:VAL:HG22 | 1:219:A:GLN:HG3  | 6        | 0.28          |
| (1,1166) | 1:215:A:VAL:HG23 | 1:219:A:GLN:HG3  | 6        | 0.28          |
| (1,1097) | 1:165:A:PRO:HB3  | 1:168:A:GLN:HG2  | 10       | 0.28          |
| (1,1070) | 1:152:A:GLU:HA   | 1:152:A:GLU:HG3  | 10       | 0.28          |
| (1,1070) | 1:152:A:GLU:HA   | 1:152:A:GLU:HG3  | 15       | 0.28          |
| (1,1050) | 1:128:A:TYR:HA   | 1:129:A:MET:HG3  | 12       | 0.28          |
| (1,974)  | 1:148:A:ARG:HE   | 1:152:A:GLU:HG2  | 15       | 0.28          |
| (1,921)  | 1:167:A:SER:HA   | 1:168:A:GLN:HG3  | 18       | 0.28          |
| (1,873)  | 1:146:A:GLU:HA   | 1:150:A:TYR:HB3  | 5        | 0.28          |
| (1,873)  | 1:146:A:GLU:HA   | 1:150:A:TYR:HB3  | 11       | 0.28          |
| (1,862)  | 1:143:A:ASN:HD22 | 1:146:A:GLU:HG2  | 4        | 0.28          |
| (1,730)  | 1:166:A:VAL:HG11 | 1:167:A:SER:HB3  | 12       | 0.28          |
| (1,730)  | 1:166:A:VAL:HG12 | 1:167:A:SER:HB3  | 12       | 0.28          |
| (1,730)  | 1:166:A:VAL:HG13 | 1:167:A:SER:HB3  | 12       | 0.28          |
| (1,574)  | 1:153:A:ASN:HB2  | 1:155:A:TYR:HE1  | 6        | 0.28          |
| (1,574)  | 1:153:A:ASN:HB2  | 1:155:A:TYR:HE2  | 6        | 0.28          |
| (1,521)  | 1:223:A:GLN:HG3  | 1:224:A:ALA:HB1  | 20       | 0.28          |
| (1,521)  | 1:223:A:GLN:HG3  | 1:224:A:ALA:HB2  | 20       | 0.28          |
| (1,521)  | 1:223:A:GLN:HG3  | 1:224:A:ALA:HB3  | 20       | 0.28          |
| (1,502)  | 1:162:A:TYR:HB3  | 1:183:A:THR:HA   | 4        | 0.28          |
| (1,435)  | 1:230:A:ARG:HA   | 1:230:A:ARG:HD2  | 9        | 0.28          |
| (1,435)  | 1:230:A:ARG:HA   | 1:230:A:ARG:HD2  | 12       | 0.28          |
| (1,339)  | 1:209:A:VAL:HG21 | 1:210:A:VAL:HG21 | 13       | 0.28          |
| (1,339)  | 1:209:A:VAL:HG21 | 1:210:A:VAL:HG22 | 13       | 0.28          |
| (1,339)  | 1:209:A:VAL:HG21 | 1:210:A:VAL:HG23 | 13       | 0.28          |
| (1,339)  | 1:209:A:VAL:HG22 | 1:210:A:VAL:HG21 | 13       | 0.28          |
| (1,339)  | 1:209:A:VAL:HG22 | 1:210:A:VAL:HG22 | 13       | 0.28          |
| (1,339)  | 1:209:A:VAL:HG22 | 1:210:A:VAL:HG23 | 13       | 0.28          |
| (1,339)  | 1:209:A:VAL:HG23 | 1:210:A:VAL:HG21 | 13       | 0.28          |
| (1,339)  | 1:209:A:VAL:HG23 | 1:210:A:VAL:HG22 | 13       | 0.28          |
| (1,339)  | 1:209:A:VAL:HG23 | 1:210:A:VAL:HG23 | 13       | 0.28          |
| (1,333)  | 1:172:A:GLN:HE22 | 1:215:A:VAL:HG21 | 2        | 0.28          |
| (1,333)  | 1:172:A:GLN:HE22 | 1:215:A:VAL:HG22 | 2        | 0.28          |
| (1,333)  | 1:172:A:GLN:HE22 | 1:215:A:VAL:HG23 | 2        | 0.28          |
| (1,333)  | 1:172:A:GLN:HE22 | 1:215:A:VAL:HG21 | 17       | 0.28          |
| (1,333)  | 1:172:A:GLN:HE22 | 1:215:A:VAL:HG22 | 17       | 0.28          |
| (1,333)  | 1:172:A:GLN:HE22 | 1:215:A:VAL:HG23 | 17       | 0.28          |
| (1,327)  | 1:189:A:VAL:HA   | 1:189:A:VAL:HG21 | 11       | 0.28          |
| (1,327)  | 1:189:A:VAL:HA   | 1:189:A:VAL:HG22 | 11       | 0.28          |
| (1,327)  | 1:189:A:VAL:HA   | 1:189:A:VAL:HG23 | 11       | 0.28          |
| (1,249)  | 1:203:A:VAL:HA   | 1:206:A:MET:HB2  | 3        | 0.28          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,249)  | 1:203:A:VAL:HA   | 1:206:A:MET:HB2  | 4        | 0.28          |
| (1,249)  | 1:203:A:VAL:HA   | 1:206:A:MET:HB2  | 6        | 0.28          |
| (1,249)  | 1:203:A:VAL:HA   | 1:206:A:MET:HB2  | 8        | 0.28          |
| (1,249)  | 1:203:A:VAL:HA   | 1:206:A:MET:HB2  | 11       | 0.28          |
| (1,249)  | 1:203:A:VAL:HA   | 1:206:A:MET:HB2  | 14       | 0.28          |
| (1,234)  | 1:176:A:VAL:HG11 | 1:214:A:CYS:HB2  | 12       | 0.28          |
| (1,234)  | 1:176:A:VAL:HG12 | 1:214:A:CYS:HB2  | 12       | 0.28          |
| (1,234)  | 1:176:A:VAL:HG13 | 1:214:A:CYS:HB2  | 12       | 0.28          |
| (1,167)  | 1:203:A:VAL:H    | 1:203:A:VAL:HG11 | 5        | 0.28          |
| (1,167)  | 1:203:A:VAL:H    | 1:203:A:VAL:HG12 | 5        | 0.28          |
| (1,167)  | 1:203:A:VAL:H    | 1:203:A:VAL:HG13 | 5        | 0.28          |
| (1,162)  | 1:226:A:TYR:HB2  | 1:228:A:GLY:HA2  | 5        | 0.28          |
| (1,162)  | 1:226:A:TYR:HB2  | 1:228:A:GLY:HA3  | 5        | 0.28          |
| (1,162)  | 1:226:A:TYR:HB2  | 1:228:A:GLY:HA2  | 12       | 0.28          |
| (1,162)  | 1:226:A:TYR:HB2  | 1:228:A:GLY:HA3  | 12       | 0.28          |
| (1,162)  | 1:226:A:TYR:HB2  | 1:228:A:GLY:HA2  | 15       | 0.28          |
| (1,162)  | 1:226:A:TYR:HB2  | 1:228:A:GLY:HA3  | 15       | 0.28          |
| (1,162)  | 1:226:A:TYR:HB2  | 1:228:A:GLY:HA2  | 20       | 0.28          |
| (1,162)  | 1:226:A:TYR:HB2  | 1:228:A:GLY:HA3  | 20       | 0.28          |
| (1,151)  | 1:126:A:GLY:HA3  | 1:164:A:ARG:HD3  | 6        | 0.28          |
| (1,105)  | 1:212:A:GLN:HA   | 1:215:A:VAL:HG11 | 4        | 0.28          |
| (1,105)  | 1:212:A:GLN:HA   | 1:215:A:VAL:HG12 | 4        | 0.28          |
| (1,105)  | 1:212:A:GLN:HA   | 1:215:A:VAL:HG13 | 4        | 0.28          |
| (1,101)  | 1:138:A:MET:HA   | 1:209:A:VAL:HG11 | 20       | 0.28          |
| (1,101)  | 1:138:A:MET:HA   | 1:209:A:VAL:HG12 | 20       | 0.28          |
| (1,101)  | 1:138:A:MET:HA   | 1:209:A:VAL:HG13 | 20       | 0.28          |
| (1,2792) | 1:128:A:TYR:HE1  | 1:164:A:ARG:HD3  | 16       | 0.27          |
| (1,2792) | 1:128:A:TYR:HE2  | 1:164:A:ARG:HD3  | 16       | 0.27          |
| (1,2791) | 1:126:A:GLY:HA2  | 1:128:A:TYR:HE1  | 17       | 0.27          |
| (1,2791) | 1:126:A:GLY:HA2  | 1:128:A:TYR:HE2  | 17       | 0.27          |
| (1,2759) | 1:139:A:ILE:HG12 | 1:150:A:TYR:HE1  | 5        | 0.27          |
| (1,2759) | 1:139:A:ILE:HG12 | 1:150:A:TYR:HE2  | 5        | 0.27          |
| (1,2553) | 1:126:A:GLY:HA2  | 1:128:A:TYR:HD1  | 11       | 0.27          |
| (1,2553) | 1:126:A:GLY:HA2  | 1:128:A:TYR:HD2  | 11       | 0.27          |
| (1,2279) | 1:186:A:GLN:HB3  | 1:188:A:THR:H    | 16       | 0.27          |
| (1,2234) | 1:221:A:GLU:HG3  | 1:222:A:SER:H    | 6        | 0.27          |
| (1,2043) | 1:231:A:SER:H    | 1:231:A:SER:HB3  | 2        | 0.27          |
| (1,1974) | 1:166:A:VAL:HG11 | 1:225:A:TYR:H    | 17       | 0.27          |
| (1,1974) | 1:166:A:VAL:HG12 | 1:225:A:TYR:H    | 17       | 0.27          |
| (1,1974) | 1:166:A:VAL:HG13 | 1:225:A:TYR:H    | 17       | 0.27          |
| (1,1679) | 1:122:A:VAL:HG21 | 1:125:A:LEU:H    | 18       | 0.27          |
| (1,1679) | 1:122:A:VAL:HG22 | 1:125:A:LEU:H    | 18       | 0.27          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1679) | 1:122:A:VAL:HG23 | 1:125:A:LEU:H    | 18       | 0.27          |
| (1,1655) | 1:230:A:ARG:H    | 1:230:A:ARG:HG3  | 10       | 0.27          |
| (1,1396) | 1:148:A:ARG:HA   | 1:151:A:ARG:HB2  | 8        | 0.27          |
| (1,1207) | 1:168:A:GLN:HA   | 1:168:A:GLN:HE22 | 8        | 0.27          |
| (1,1155) | 1:130:A:LEU:HB3  | 1:162:A:TYR:HA   | 11       | 0.27          |
| (1,1135) | 1:137:A:PRO:HB3  | 1:212:A:GLN:HG2  | 1        | 0.27          |
| (1,1015) | 1:152:A:GLU:HG2  | 1:153:A:ASN:HD22 | 13       | 0.27          |
| (1,1011) | 1:208:A:ARG:HA   | 1:208:A:ARG:HG3  | 2        | 0.27          |
| (1,907)  | 1:226:A:TYR:HA   | 1:229:A:ARG:HB2  | 3        | 0.27          |
| (1,828)  | 1:222:A:SER:HA   | 1:226:A:TYR:HB3  | 5        | 0.27          |
| (1,552)  | 1:153:A:ASN:HB2  | 1:156:A:ARG:HD2  | 2        | 0.27          |
| (1,528)  | 1:143:A:ASN:HB2  | 1:147:A:ASP:HB3  | 16       | 0.27          |
| (1,528)  | 1:143:A:ASN:HB3  | 1:147:A:ASP:HB3  | 16       | 0.27          |
| (1,525)  | 1:132:A:SER:HB2  | 1:160:A:GLN:HE21 | 13       | 0.27          |
| (1,521)  | 1:223:A:GLN:HG3  | 1:224:A:ALA:HB1  | 11       | 0.27          |
| (1,521)  | 1:223:A:GLN:HG3  | 1:224:A:ALA:HB2  | 11       | 0.27          |
| (1,521)  | 1:223:A:GLN:HG3  | 1:224:A:ALA:HB3  | 11       | 0.27          |
| (1,501)  | 1:161:A:VAL:HA   | 1:162:A:TYR:HB3  | 12       | 0.27          |
| (1,496)  | 1:130:A:LEU:HA   | 1:162:A:TYR:HB2  | 10       | 0.27          |
| (1,445)  | 1:180:A:VAL:HA   | 1:184:A:ILE:HG12 | 6        | 0.27          |
| (1,350)  | 1:122:A:VAL:HG21 | 1:123:A:GLY:H    | 19       | 0.27          |
| (1,350)  | 1:122:A:VAL:HG22 | 1:123:A:GLY:H    | 19       | 0.27          |
| (1,350)  | 1:122:A:VAL:HG23 | 1:123:A:GLY:H    | 19       | 0.27          |
| (1,349)  | 1:122:A:VAL:HG21 | 1:186:A:GLN:HE21 | 14       | 0.27          |
| (1,349)  | 1:122:A:VAL:HG22 | 1:186:A:GLN:HE21 | 14       | 0.27          |
| (1,349)  | 1:122:A:VAL:HG23 | 1:186:A:GLN:HE21 | 14       | 0.27          |
| (1,339)  | 1:209:A:VAL:HG21 | 1:210:A:VAL:HG21 | 19       | 0.27          |
| (1,339)  | 1:209:A:VAL:HG21 | 1:210:A:VAL:HG22 | 19       | 0.27          |
| (1,339)  | 1:209:A:VAL:HG21 | 1:210:A:VAL:HG23 | 19       | 0.27          |
| (1,339)  | 1:209:A:VAL:HG22 | 1:210:A:VAL:HG21 | 19       | 0.27          |
| (1,339)  | 1:209:A:VAL:HG22 | 1:210:A:VAL:HG22 | 19       | 0.27          |
| (1,339)  | 1:209:A:VAL:HG22 | 1:210:A:VAL:HG23 | 19       | 0.27          |
| (1,339)  | 1:209:A:VAL:HG23 | 1:210:A:VAL:HG21 | 19       | 0.27          |
| (1,339)  | 1:209:A:VAL:HG23 | 1:210:A:VAL:HG22 | 19       | 0.27          |
| (1,339)  | 1:209:A:VAL:HG23 | 1:210:A:VAL:HG23 | 19       | 0.27          |
| (1,323)  | 1:209:A:VAL:HG21 | 1:212:A:GLN:HB3  | 18       | 0.27          |
| (1,323)  | 1:209:A:VAL:HG22 | 1:212:A:GLN:HB3  | 18       | 0.27          |
| (1,323)  | 1:209:A:VAL:HG23 | 1:212:A:GLN:HB3  | 18       | 0.27          |
| (1,220)  | 1:127:A:GLY:HA2  | 1:164:A:ARG:HE   | 11       | 0.27          |
| (1,216)  | 1:216:A:THR:HG21 | 1:220:A:LYS:HG3  | 7        | 0.27          |
| (1,216)  | 1:216:A:THR:HG22 | 1:220:A:LYS:HG3  | 7        | 0.27          |
| (1,216)  | 1:216:A:THR:HG23 | 1:220:A:LYS:HG3  | 7        | 0.27          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,202)  | 1:183:A:THR:HG21 | 1:184:A:ILE:HG12 | 4        | 0.27          |
| (1,202)  | 1:183:A:THR:HG22 | 1:184:A:ILE:HG12 | 4        | 0.27          |
| (1,202)  | 1:183:A:THR:HG23 | 1:184:A:ILE:HG12 | 4        | 0.27          |
| (1,162)  | 1:226:A:TYR:HB2  | 1:228:A:GLY:HA2  | 6        | 0.27          |
| (1,162)  | 1:226:A:TYR:HB2  | 1:228:A:GLY:HA3  | 6        | 0.27          |
| (1,105)  | 1:212:A:GLN:HA   | 1:215:A:VAL:HG11 | 2        | 0.27          |
| (1,105)  | 1:212:A:GLN:HA   | 1:215:A:VAL:HG12 | 2        | 0.27          |
| (1,105)  | 1:212:A:GLN:HA   | 1:215:A:VAL:HG13 | 2        | 0.27          |
| (1,2681) | 1:141:A:PHE:HZ   | 1:208:A:ARG:HB3  | 17       | 0.26          |
| (1,2375) | 1:164:A:ARG:HD2  | 1:168:A:GLN:HE22 | 18       | 0.26          |
| (1,2261) | 1:160:A:GLN:H    | 1:161:A:VAL:HG11 | 10       | 0.26          |
| (1,2261) | 1:160:A:GLN:H    | 1:161:A:VAL:HG12 | 10       | 0.26          |
| (1,2261) | 1:160:A:GLN:H    | 1:161:A:VAL:HG13 | 10       | 0.26          |
| (1,1937) | 1:220:A:LYS:H    | 1:221:A:GLU:HG3  | 19       | 0.26          |
| (1,1847) | 1:197:A:ASN:H    | 1:197:A:ASN:HB3  | 7        | 0.26          |
| (1,1558) | 1:208:A:ARG:HG3  | 1:209:A:VAL:H    | 8        | 0.26          |
| (1,1407) | 1:134:A:MET:HB3  | 1:220:A:LYS:HD2  | 10       | 0.26          |
| (1,1407) | 1:134:A:MET:HB3  | 1:220:A:LYS:HD3  | 10       | 0.26          |
| (1,1392) | 1:133:A:ALA:HA   | 1:159:A:ASN:HB2  | 1        | 0.26          |
| (1,1340) | 1:160:A:GLN:HA   | 1:213:A:MET:HB2  | 11       | 0.26          |
| (1,1304) | 1:153:A:ASN:HA   | 1:156:A:ARG:HD3  | 20       | 0.26          |
| (1,1285) | 1:205:A:MET:H    | 1:206:A:MET:HG2  | 12       | 0.26          |
| (1,1168) | 1:223:A:GLN:H    | 1:223:A:GLN:HG2  | 14       | 0.26          |
| (1,1155) | 1:130:A:LEU:HB3  | 1:162:A:TYR:HA   | 1        | 0.26          |
| (1,1155) | 1:130:A:LEU:HB3  | 1:162:A:TYR:HA   | 4        | 0.26          |
| (1,1155) | 1:130:A:LEU:HB3  | 1:162:A:TYR:HA   | 10       | 0.26          |
| (1,1155) | 1:130:A:LEU:HB3  | 1:162:A:TYR:HA   | 14       | 0.26          |
| (1,1095) | 1:165:A:PRO:HA   | 1:168:A:GLN:HG2  | 7        | 0.26          |
| (1,1095) | 1:165:A:PRO:HA   | 1:168:A:GLN:HG2  | 10       | 0.26          |
| (1,1089) | 1:182:A:ILE:HD11 | 1:186:A:GLN:HE21 | 7        | 0.26          |
| (1,1089) | 1:182:A:ILE:HD12 | 1:186:A:GLN:HE21 | 7        | 0.26          |
| (1,1089) | 1:182:A:ILE:HD13 | 1:186:A:GLN:HE21 | 7        | 0.26          |
| (1,1070) | 1:152:A:GLU:HA   | 1:152:A:GLU:HG3  | 17       | 0.26          |
| (1,983)  | 1:149:A:TYR:H    | 1:152:A:GLU:HG2  | 18       | 0.26          |
| (1,814)  | 1:226:A:TYR:HB2  | 1:227:A:ASP:HA   | 10       | 0.26          |
| (1,637)  | 1:147:A:ASP:HB2  | 1:148:A:ARG:HG2  | 12       | 0.26          |
| (1,496)  | 1:130:A:LEU:HA   | 1:162:A:TYR:HB2  | 19       | 0.26          |
| (1,333)  | 1:172:A:GLN:HE22 | 1:215:A:VAL:HG21 | 12       | 0.26          |
| (1,333)  | 1:172:A:GLN:HE22 | 1:215:A:VAL:HG22 | 12       | 0.26          |
| (1,333)  | 1:172:A:GLN:HE22 | 1:215:A:VAL:HG23 | 12       | 0.26          |
| (1,333)  | 1:172:A:GLN:HE22 | 1:215:A:VAL:HG21 | 13       | 0.26          |
| (1,333)  | 1:172:A:GLN:HE22 | 1:215:A:VAL:HG22 | 13       | 0.26          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,333)  | 1:172:A:GLN:HE22 | 1:215:A:VAL:HG23 | 13       | 0.26          |
| (1,312)  | 1:166:A:VAL:HG21 | 1:170:A:SER:HB3  | 13       | 0.26          |
| (1,312)  | 1:166:A:VAL:HG22 | 1:170:A:SER:HB3  | 13       | 0.26          |
| (1,312)  | 1:166:A:VAL:HG23 | 1:170:A:SER:HB3  | 13       | 0.26          |
| (1,260)  | 1:186:A:GLN:HB2  | 1:190:A:THR:HG21 | 11       | 0.26          |
| (1,260)  | 1:186:A:GLN:HB2  | 1:190:A:THR:HG22 | 11       | 0.26          |
| (1,260)  | 1:186:A:GLN:HB2  | 1:190:A:THR:HG23 | 11       | 0.26          |
| (1,249)  | 1:203:A:VAL:HA   | 1:206:A:MET:HB2  | 19       | 0.26          |
| (1,249)  | 1:203:A:VAL:HA   | 1:206:A:MET:HB2  | 20       | 0.26          |
| (1,179)  | 1:201:A:THR:HB   | 1:205:A:MET:HG3  | 8        | 0.26          |
| (1,177)  | 1:195:A:GLY:HA3  | 1:197:A:ASN:HD21 | 4        | 0.26          |
| (1,162)  | 1:226:A:TYR:HB2  | 1:228:A:GLY:HA2  | 10       | 0.26          |
| (1,162)  | 1:226:A:TYR:HB2  | 1:228:A:GLY:HA3  | 10       | 0.26          |
| (1,89)   | 1:206:A:MET:HB3  | 1:210:A:VAL:HG21 | 16       | 0.26          |
| (1,89)   | 1:206:A:MET:HB3  | 1:210:A:VAL:HG22 | 16       | 0.26          |
| (1,89)   | 1:206:A:MET:HB3  | 1:210:A:VAL:HG23 | 16       | 0.26          |
| (1,2834) | 1:163:A:TYR:HE1  | 1:221:A:GLU:HG2  | 10       | 0.25          |
| (1,2834) | 1:163:A:TYR:HE2  | 1:221:A:GLU:HG2  | 10       | 0.25          |
| (1,2474) | 1:168:A:GLN:HG2  | 1:169:A:TYR:HD1  | 18       | 0.25          |
| (1,2474) | 1:168:A:GLN:HG2  | 1:169:A:TYR:HD2  | 18       | 0.25          |
| (1,2445) | 1:122:A:VAL:HG21 | 1:124:A:GLY:H    | 2        | 0.25          |
| (1,2445) | 1:122:A:VAL:HG22 | 1:124:A:GLY:H    | 2        | 0.25          |
| (1,2445) | 1:122:A:VAL:HG23 | 1:124:A:GLY:H    | 2        | 0.25          |
| (1,2279) | 1:186:A:GLN:HB3  | 1:188:A:THR:H    | 6        | 0.25          |
| (1,2227) | 1:189:A:VAL:HG11 | 1:191:A:THR:H    | 11       | 0.25          |
| (1,2227) | 1:189:A:VAL:HG12 | 1:191:A:THR:H    | 11       | 0.25          |
| (1,2227) | 1:189:A:VAL:HG13 | 1:191:A:THR:H    | 11       | 0.25          |
| (1,1799) | 1:166:A:VAL:H    | 1:166:A:VAL:HG11 | 12       | 0.25          |
| (1,1799) | 1:166:A:VAL:H    | 1:166:A:VAL:HG12 | 12       | 0.25          |
| (1,1799) | 1:166:A:VAL:H    | 1:166:A:VAL:HG13 | 12       | 0.25          |
| (1,1584) | 1:122:A:VAL:H    | 1:122:A:VAL:HG11 | 1        | 0.25          |
| (1,1584) | 1:122:A:VAL:H    | 1:122:A:VAL:HG12 | 1        | 0.25          |
| (1,1584) | 1:122:A:VAL:H    | 1:122:A:VAL:HG13 | 1        | 0.25          |
| (1,1497) | 1:139:A:ILE:HD11 | 1:212:A:GLN:HB3  | 20       | 0.25          |
| (1,1497) | 1:139:A:ILE:HD12 | 1:212:A:GLN:HB3  | 20       | 0.25          |
| (1,1497) | 1:139:A:ILE:HD13 | 1:212:A:GLN:HB3  | 20       | 0.25          |
| (1,1392) | 1:133:A:ALA:HA   | 1:159:A:ASN:HB2  | 12       | 0.25          |
| (1,1340) | 1:160:A:GLN:HA   | 1:213:A:MET:HB2  | 1        | 0.25          |
| (1,1309) | 1:129:A:MET:HG2  | 1:164:A:ARG:HA   | 5        | 0.25          |
| (1,1231) | 1:209:A:VAL:HG21 | 1:213:A:MET:HG3  | 12       | 0.25          |
| (1,1231) | 1:209:A:VAL:HG22 | 1:213:A:MET:HG3  | 12       | 0.25          |
| (1,1231) | 1:209:A:VAL:HG23 | 1:213:A:MET:HG3  | 12       | 0.25          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1220) | 1:195:A:GLY:HA2  | 1:196:A:GLU:HA   | 1        | 0.25          |
| (1,1220) | 1:195:A:GLY:HA2  | 1:196:A:GLU:HA   | 13       | 0.25          |
| (1,1155) | 1:130:A:LEU:HB3  | 1:162:A:TYR:HA   | 3        | 0.25          |
| (1,1155) | 1:130:A:LEU:HB3  | 1:162:A:TYR:HA   | 13       | 0.25          |
| (1,1135) | 1:137:A:PRO:HB3  | 1:212:A:GLN:HG2  | 5        | 0.25          |
| (1,1101) | 1:160:A:GLN:H    | 1:213:A:MET:HB3  | 1        | 0.25          |
| (1,1101) | 1:160:A:GLN:H    | 1:213:A:MET:HB3  | 12       | 0.25          |
| (1,1055) | 1:203:A:VAL:HG21 | 1:207:A:GLU:HG2  | 2        | 0.25          |
| (1,1055) | 1:203:A:VAL:HG22 | 1:207:A:GLU:HG2  | 2        | 0.25          |
| (1,1055) | 1:203:A:VAL:HG23 | 1:207:A:GLU:HG2  | 2        | 0.25          |
| (1,1050) | 1:128:A:TYR:HA   | 1:129:A:MET:HG3  | 2        | 0.25          |
| (1,1050) | 1:128:A:TYR:HA   | 1:129:A:MET:HG3  | 19       | 0.25          |
| (1,1048) | 1:125:A:LEU:HB3  | 1:128:A:TYR:HA   | 16       | 0.25          |
| (1,774)  | 1:206:A:MET:HB2  | 1:206:A:MET:HE1  | 5        | 0.25          |
| (1,774)  | 1:206:A:MET:HB2  | 1:206:A:MET:HE2  | 5        | 0.25          |
| (1,774)  | 1:206:A:MET:HB2  | 1:206:A:MET:HE3  | 5        | 0.25          |
| (1,559)  | 1:162:A:TYR:HB3  | 1:182:A:ILE:HG21 | 2        | 0.25          |
| (1,559)  | 1:162:A:TYR:HB3  | 1:182:A:ILE:HG22 | 2        | 0.25          |
| (1,559)  | 1:162:A:TYR:HB3  | 1:182:A:ILE:HG23 | 2        | 0.25          |
| (1,501)  | 1:161:A:VAL:HA   | 1:162:A:TYR:HB3  | 16       | 0.25          |
| (1,501)  | 1:161:A:VAL:HA   | 1:162:A:TYR:HB3  | 17       | 0.25          |
| (1,435)  | 1:230:A:ARG:HA   | 1:230:A:ARG:HD2  | 15       | 0.25          |
| (1,362)  | 1:172:A:GLN:HG3  | 1:215:A:VAL:HG21 | 20       | 0.25          |
| (1,362)  | 1:172:A:GLN:HG3  | 1:215:A:VAL:HG22 | 20       | 0.25          |
| (1,362)  | 1:172:A:GLN:HG3  | 1:215:A:VAL:HG23 | 20       | 0.25          |
| (1,216)  | 1:216:A:THR:HG21 | 1:220:A:LYS:HG3  | 5        | 0.25          |
| (1,216)  | 1:216:A:THR:HG22 | 1:220:A:LYS:HG3  | 5        | 0.25          |
| (1,216)  | 1:216:A:THR:HG23 | 1:220:A:LYS:HG3  | 5        | 0.25          |
| (1,167)  | 1:203:A:VAL:H    | 1:203:A:VAL:HG11 | 12       | 0.25          |
| (1,167)  | 1:203:A:VAL:H    | 1:203:A:VAL:HG12 | 12       | 0.25          |
| (1,167)  | 1:203:A:VAL:H    | 1:203:A:VAL:HG13 | 12       | 0.25          |
| (1,107)  | 1:211:A:GLU:HG3  | 1:215:A:VAL:HG11 | 8        | 0.25          |
| (1,107)  | 1:211:A:GLU:HG3  | 1:215:A:VAL:HG12 | 8        | 0.25          |
| (1,107)  | 1:211:A:GLU:HG3  | 1:215:A:VAL:HG13 | 8        | 0.25          |
| (1,77)   | 1:208:A:ARG:H    | 1:209:A:VAL:HG11 | 10       | 0.25          |
| (1,77)   | 1:208:A:ARG:H    | 1:209:A:VAL:HG12 | 10       | 0.25          |
| (1,77)   | 1:208:A:ARG:H    | 1:209:A:VAL:HG13 | 10       | 0.25          |
| (1,77)   | 1:208:A:ARG:H    | 1:209:A:VAL:HG11 | 11       | 0.25          |
| (1,77)   | 1:208:A:ARG:H    | 1:209:A:VAL:HG12 | 11       | 0.25          |
| (1,77)   | 1:208:A:ARG:H    | 1:209:A:VAL:HG13 | 11       | 0.25          |
| (1,2807) | 1:149:A:TYR:HE1  | 1:153:A:ASN:HB3  | 3        | 0.24          |
| (1,2807) | 1:149:A:TYR:HE2  | 1:153:A:ASN:HB3  | 3        | 0.24          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2736) | 1:184:A:ILE:HG13 | 1:187:A:HIS:HD2  | 3        | 0.24          |
| (1,2657) | 1:141:A:PHE:HE1  | 1:208:A:ARG:HB3  | 9        | 0.24          |
| (1,2657) | 1:141:A:PHE:HE2  | 1:208:A:ARG:HB3  | 9        | 0.24          |
| (1,2501) | 1:149:A:TYR:HD1  | 1:205:A:MET:HG2  | 18       | 0.24          |
| (1,2501) | 1:149:A:TYR:HD2  | 1:205:A:MET:HG2  | 18       | 0.24          |
| (1,2354) | 1:170:A:SER:HB2  | 1:174:A:ASN:HD21 | 11       | 0.24          |
| (1,2314) | 1:133:A:ALA:HA   | 1:160:A:GLN:HE21 | 13       | 0.24          |
| (1,2314) | 1:133:A:ALA:HA   | 1:160:A:GLN:HE21 | 20       | 0.24          |
| (1,2237) | 1:166:A:VAL:HG11 | 1:222:A:SER:H    | 3        | 0.24          |
| (1,2237) | 1:166:A:VAL:HG12 | 1:222:A:SER:H    | 3        | 0.24          |
| (1,2237) | 1:166:A:VAL:HG13 | 1:222:A:SER:H    | 3        | 0.24          |
| (1,1847) | 1:197:A:ASN:H    | 1:197:A:ASN:HB3  | 8        | 0.24          |
| (1,1679) | 1:122:A:VAL:HG21 | 1:125:A:LEU:H    | 1        | 0.24          |
| (1,1679) | 1:122:A:VAL:HG22 | 1:125:A:LEU:H    | 1        | 0.24          |
| (1,1679) | 1:122:A:VAL:HG23 | 1:125:A:LEU:H    | 1        | 0.24          |
| (1,1575) | 1:136:A:ARG:H    | 1:136:A:ARG:HD3  | 15       | 0.24          |
| (1,1538) | 1:164:A:ARG:HD2  | 1:165:A:PRO:HD3  | 15       | 0.24          |
| (1,1459) | 1:136:A:ARG:HB3  | 1:159:A:ASN:HB3  | 14       | 0.24          |
| (1,1400) | 1:183:A:THR:HB   | 1:184:A:ILE:HG12 | 11       | 0.24          |
| (1,1309) | 1:129:A:MET:HG2  | 1:164:A:ARG:HA   | 2        | 0.24          |
| (1,1309) | 1:129:A:MET:HG2  | 1:164:A:ARG:HA   | 8        | 0.24          |
| (1,1309) | 1:129:A:MET:HG2  | 1:164:A:ARG:HA   | 12       | 0.24          |
| (1,1309) | 1:129:A:MET:HG2  | 1:164:A:ARG:HA   | 13       | 0.24          |
| (1,1309) | 1:129:A:MET:HG2  | 1:164:A:ARG:HA   | 20       | 0.24          |
| (1,1304) | 1:153:A:ASN:HA   | 1:156:A:ARG:HD3  | 12       | 0.24          |
| (1,1294) | 1:138:A:MET:HG3  | 1:139:A:ILE:H    | 17       | 0.24          |
| (1,1220) | 1:195:A:GLY:HA2  | 1:196:A:GLU:HA   | 12       | 0.24          |
| (1,1220) | 1:195:A:GLY:HA2  | 1:196:A:GLU:HA   | 20       | 0.24          |
| (1,1197) | 1:160:A:GLN:HB2  | 1:183:A:THR:HG21 | 3        | 0.24          |
| (1,1197) | 1:160:A:GLN:HB2  | 1:183:A:THR:HG22 | 3        | 0.24          |
| (1,1197) | 1:160:A:GLN:HB2  | 1:183:A:THR:HG23 | 3        | 0.24          |
| (1,1155) | 1:130:A:LEU:HB3  | 1:162:A:TYR:HA   | 8        | 0.24          |
| (1,1135) | 1:137:A:PRO:HB3  | 1:212:A:GLN:HG2  | 7        | 0.24          |
| (1,1070) | 1:152:A:GLU:HA   | 1:152:A:GLU:HG3  | 5        | 0.24          |
| (1,976)  | 1:148:A:ARG:HG3  | 1:152:A:GLU:HG2  | 8        | 0.24          |
| (1,893)  | 1:162:A:TYR:HB3  | 1:182:A:ILE:HB   | 4        | 0.24          |
| (1,864)  | 1:134:A:MET:HB3  | 1:135:A:SER:HB2  | 19       | 0.24          |
| (1,733)  | 1:222:A:SER:HB2  | 1:226:A:TYR:HD1  | 20       | 0.24          |
| (1,733)  | 1:222:A:SER:HB2  | 1:226:A:TYR:HD2  | 20       | 0.24          |
| (1,594)  | 1:160:A:GLN:HA   | 1:161:A:VAL:HG21 | 10       | 0.24          |
| (1,594)  | 1:160:A:GLN:HA   | 1:161:A:VAL:HG22 | 10       | 0.24          |
| (1,594)  | 1:160:A:GLN:HA   | 1:161:A:VAL:HG23 | 10       | 0.24          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,574)  | 1:153:A:ASN:HB2  | 1:155:A:TYR:HE1  | 1        | 0.24          |
| (1,574)  | 1:153:A:ASN:HB2  | 1:155:A:TYR:HE2  | 1        | 0.24          |
| (1,574)  | 1:153:A:ASN:HB2  | 1:155:A:TYR:HE1  | 8        | 0.24          |
| (1,574)  | 1:153:A:ASN:HB2  | 1:155:A:TYR:HE2  | 8        | 0.24          |
| (1,569)  | 1:128:A:TYR:HE1  | 1:179:A:CYS:HB3  | 9        | 0.24          |
| (1,569)  | 1:128:A:TYR:HE2  | 1:179:A:CYS:HB3  | 9        | 0.24          |
| (1,525)  | 1:132:A:SER:HB2  | 1:160:A:GLN:HE21 | 14       | 0.24          |
| (1,506)  | 1:179:A:CYS:HB2  | 1:214:A:CYS:HB2  | 7        | 0.24          |
| (1,496)  | 1:130:A:LEU:HA   | 1:162:A:TYR:HB2  | 17       | 0.24          |
| (1,467)  | 1:122:A:VAL:HG21 | 1:125:A:LEU:HB3  | 2        | 0.24          |
| (1,467)  | 1:122:A:VAL:HG22 | 1:125:A:LEU:HB3  | 2        | 0.24          |
| (1,467)  | 1:122:A:VAL:HG23 | 1:125:A:LEU:HB3  | 2        | 0.24          |
| (1,260)  | 1:186:A:GLN:HB2  | 1:190:A:THR:HG21 | 15       | 0.24          |
| (1,260)  | 1:186:A:GLN:HB2  | 1:190:A:THR:HG22 | 15       | 0.24          |
| (1,260)  | 1:186:A:GLN:HB2  | 1:190:A:THR:HG23 | 15       | 0.24          |
| (1,258)  | 1:122:A:VAL:HG11 | 1:190:A:THR:HG21 | 8        | 0.24          |
| (1,258)  | 1:122:A:VAL:HG11 | 1:190:A:THR:HG22 | 8        | 0.24          |
| (1,258)  | 1:122:A:VAL:HG11 | 1:190:A:THR:HG23 | 8        | 0.24          |
| (1,258)  | 1:122:A:VAL:HG12 | 1:190:A:THR:HG21 | 8        | 0.24          |
| (1,258)  | 1:122:A:VAL:HG12 | 1:190:A:THR:HG22 | 8        | 0.24          |
| (1,258)  | 1:122:A:VAL:HG12 | 1:190:A:THR:HG23 | 8        | 0.24          |
| (1,258)  | 1:122:A:VAL:HG13 | 1:190:A:THR:HG21 | 8        | 0.24          |
| (1,258)  | 1:122:A:VAL:HG13 | 1:190:A:THR:HG22 | 8        | 0.24          |
| (1,258)  | 1:122:A:VAL:HG13 | 1:190:A:THR:HG23 | 8        | 0.24          |
| (1,162)  | 1:226:A:TYR:HB2  | 1:228:A:GLY:HA2  | 4        | 0.24          |
| (1,162)  | 1:226:A:TYR:HB2  | 1:228:A:GLY:HA3  | 4        | 0.24          |
| (1,151)  | 1:126:A:GLY:HA3  | 1:164:A:ARG:HD3  | 2        | 0.24          |
| (1,2657) | 1:141:A:PHE:HE1  | 1:208:A:ARG:HB3  | 7        | 0.23          |
| (1,2657) | 1:141:A:PHE:HE2  | 1:208:A:ARG:HB3  | 7        | 0.23          |
| (1,2501) | 1:149:A:TYR:HD1  | 1:205:A:MET:HG2  | 2        | 0.23          |
| (1,2501) | 1:149:A:TYR:HD2  | 1:205:A:MET:HG2  | 2        | 0.23          |
| (1,2364) | 1:171:A:ASN:HD22 | 1:174:A:ASN:HD22 | 8        | 0.23          |
| (1,2322) | 1:130:A:LEU:HG   | 1:160:A:GLN:HE22 | 9        | 0.23          |
| (1,2322) | 1:130:A:LEU:HG   | 1:160:A:GLN:HE22 | 11       | 0.23          |
| (1,2054) | 1:166:A:VAL:HG11 | 1:221:A:GLU:H    | 1        | 0.23          |
| (1,2054) | 1:166:A:VAL:HG12 | 1:221:A:GLU:H    | 1        | 0.23          |
| (1,2054) | 1:166:A:VAL:HG13 | 1:221:A:GLU:H    | 1        | 0.23          |
| (1,1847) | 1:197:A:ASN:H    | 1:197:A:ASN:HB3  | 6        | 0.23          |
| (1,1799) | 1:166:A:VAL:H    | 1:166:A:VAL:HG11 | 3        | 0.23          |
| (1,1799) | 1:166:A:VAL:H    | 1:166:A:VAL:HG12 | 3        | 0.23          |
| (1,1799) | 1:166:A:VAL:H    | 1:166:A:VAL:HG13 | 3        | 0.23          |
| (1,1668) | 1:139:A:ILE:HG12 | 1:140:A:HIS:H    | 15       | 0.23          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1535) | 1:165:A:PRO:HD2  | 1:166:A:VAL:H    | 7        | 0.23          |
| (1,1497) | 1:139:A:ILE:HD11 | 1:212:A:GLN:HB3  | 3        | 0.23          |
| (1,1497) | 1:139:A:ILE:HD12 | 1:212:A:GLN:HB3  | 3        | 0.23          |
| (1,1497) | 1:139:A:ILE:HD13 | 1:212:A:GLN:HB3  | 3        | 0.23          |
| (1,1495) | 1:212:A:GLN:HB2  | 1:216:A:THR:H    | 4        | 0.23          |
| (1,1495) | 1:212:A:GLN:HB2  | 1:216:A:THR:H    | 15       | 0.23          |
| (1,1309) | 1:129:A:MET:HG2  | 1:164:A:ARG:HA   | 11       | 0.23          |
| (1,1294) | 1:138:A:MET:HG3  | 1:139:A:ILE:H    | 4        | 0.23          |
| (1,1220) | 1:195:A:GLY:HA2  | 1:196:A:GLU:HA   | 3        | 0.23          |
| (1,1220) | 1:195:A:GLY:HA2  | 1:196:A:GLU:HA   | 4        | 0.23          |
| (1,1220) | 1:195:A:GLY:HA2  | 1:196:A:GLU:HA   | 7        | 0.23          |
| (1,1220) | 1:195:A:GLY:HA2  | 1:196:A:GLU:HA   | 10       | 0.23          |
| (1,1220) | 1:195:A:GLY:HA2  | 1:196:A:GLU:HA   | 11       | 0.23          |
| (1,1220) | 1:195:A:GLY:HA2  | 1:196:A:GLU:HA   | 16       | 0.23          |
| (1,1207) | 1:168:A:GLN:HA   | 1:168:A:GLN:HE22 | 2        | 0.23          |
| (1,1155) | 1:130:A:LEU:HB3  | 1:162:A:TYR:HA   | 2        | 0.23          |
| (1,1023) | 1:206:A:MET:HG3  | 1:207:A:GLU:HG3  | 8        | 0.23          |
| (1,993)  | 1:211:A:GLU:HG3  | 1:215:A:VAL:H    | 7        | 0.23          |
| (1,976)  | 1:148:A:ARG:HG3  | 1:152:A:GLU:HG2  | 13       | 0.23          |
| (1,944)  | 1:171:A:ASN:HB3  | 1:172:A:GLN:HA   | 9        | 0.23          |
| (1,862)  | 1:143:A:ASN:HD22 | 1:146:A:GLU:HG2  | 10       | 0.23          |
| (1,527)  | 1:202:A:ASP:HB2  | 1:203:A:VAL:HG11 | 2        | 0.23          |
| (1,527)  | 1:202:A:ASP:HB2  | 1:203:A:VAL:HG12 | 2        | 0.23          |
| (1,527)  | 1:202:A:ASP:HB2  | 1:203:A:VAL:HG13 | 2        | 0.23          |
| (1,507)  | 1:211:A:GLU:HG3  | 1:214:A:CYS:HB2  | 1        | 0.23          |
| (1,501)  | 1:161:A:VAL:HA   | 1:162:A:TYR:HB3  | 15       | 0.23          |
| (1,445)  | 1:180:A:VAL:HA   | 1:184:A:ILE:HG12 | 14       | 0.23          |
| (1,350)  | 1:122:A:VAL:HG21 | 1:123:A:GLY:H    | 2        | 0.23          |
| (1,350)  | 1:122:A:VAL:HG22 | 1:123:A:GLY:H    | 2        | 0.23          |
| (1,350)  | 1:122:A:VAL:HG23 | 1:123:A:GLY:H    | 2        | 0.23          |
| (1,339)  | 1:209:A:VAL:HG21 | 1:210:A:VAL:HG21 | 11       | 0.23          |
| (1,339)  | 1:209:A:VAL:HG21 | 1:210:A:VAL:HG22 | 11       | 0.23          |
| (1,339)  | 1:209:A:VAL:HG21 | 1:210:A:VAL:HG23 | 11       | 0.23          |
| (1,339)  | 1:209:A:VAL:HG22 | 1:210:A:VAL:HG21 | 11       | 0.23          |
| (1,339)  | 1:209:A:VAL:HG22 | 1:210:A:VAL:HG22 | 11       | 0.23          |
| (1,339)  | 1:209:A:VAL:HG22 | 1:210:A:VAL:HG23 | 11       | 0.23          |
| (1,339)  | 1:209:A:VAL:HG23 | 1:210:A:VAL:HG21 | 11       | 0.23          |
| (1,339)  | 1:209:A:VAL:HG23 | 1:210:A:VAL:HG22 | 11       | 0.23          |
| (1,339)  | 1:209:A:VAL:HG23 | 1:210:A:VAL:HG23 | 11       | 0.23          |
| (1,240)  | 1:166:A:VAL:HG21 | 1:169:A:TYR:HB2  | 3        | 0.23          |
| (1,240)  | 1:166:A:VAL:HG22 | 1:169:A:TYR:HB2  | 3        | 0.23          |
| (1,240)  | 1:166:A:VAL:HG23 | 1:169:A:TYR:HB2  | 3        | 0.23          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,162)  | 1:226:A:TYR:HB2  | 1:228:A:GLY:HA2  | 9        | 0.23          |
| (1,162)  | 1:226:A:TYR:HB2  | 1:228:A:GLY:HA3  | 9        | 0.23          |
| (1,68)   | 1:172:A:GLN:HE22 | 1:176:A:VAL:HG21 | 12       | 0.23          |
| (1,68)   | 1:172:A:GLN:HE22 | 1:176:A:VAL:HG22 | 12       | 0.23          |
| (1,68)   | 1:172:A:GLN:HE22 | 1:176:A:VAL:HG23 | 12       | 0.23          |
| (1,2834) | 1:163:A:TYR:HE1  | 1:221:A:GLU:HG2  | 3        | 0.22          |
| (1,2834) | 1:163:A:TYR:HE2  | 1:221:A:GLU:HG2  | 3        | 0.22          |
| (1,2807) | 1:149:A:TYR:HE1  | 1:153:A:ASN:HB3  | 18       | 0.22          |
| (1,2807) | 1:149:A:TYR:HE2  | 1:153:A:ASN:HB3  | 18       | 0.22          |
| (1,2763) | 1:155:A:TYR:HE1  | 1:156:A:ARG:HD2  | 8        | 0.22          |
| (1,2763) | 1:155:A:TYR:HE2  | 1:156:A:ARG:HD2  | 8        | 0.22          |
| (1,2756) | 1:150:A:TYR:HE1  | 1:205:A:MET:HG2  | 8        | 0.22          |
| (1,2756) | 1:150:A:TYR:HE2  | 1:205:A:MET:HG2  | 8        | 0.22          |
| (1,2657) | 1:141:A:PHE:HE1  | 1:208:A:ARG:HB3  | 14       | 0.22          |
| (1,2657) | 1:141:A:PHE:HE2  | 1:208:A:ARG:HB3  | 14       | 0.22          |
| (1,2507) | 1:150:A:TYR:HD1  | 1:151:A:ARG:HG3  | 13       | 0.22          |
| (1,2507) | 1:150:A:TYR:HD2  | 1:151:A:ARG:HG3  | 13       | 0.22          |
| (1,2322) | 1:130:A:LEU:HG   | 1:160:A:GLN:HE22 | 5        | 0.22          |
| (1,2313) | 1:159:A:ASN:HD22 | 1:160:A:GLN:HE21 | 8        | 0.22          |
| (1,1746) | 1:184:A:ILE:H    | 1:184:A:ILE:HG12 | 1        | 0.22          |
| (1,1746) | 1:184:A:ILE:H    | 1:184:A:ILE:HG12 | 10       | 0.22          |
| (1,1746) | 1:184:A:ILE:H    | 1:184:A:ILE:HG12 | 13       | 0.22          |
| (1,1340) | 1:160:A:GLN:HA   | 1:213:A:MET:HB2  | 9        | 0.22          |
| (1,1304) | 1:153:A:ASN:HA   | 1:156:A:ARG:HD3  | 16       | 0.22          |
| (1,1256) | 1:184:A:ILE:HG13 | 1:206:A:MET:HG3  | 20       | 0.22          |
| (1,1220) | 1:195:A:GLY:HA2  | 1:196:A:GLU:HA   | 2        | 0.22          |
| (1,1220) | 1:195:A:GLY:HA2  | 1:196:A:GLU:HA   | 5        | 0.22          |
| (1,1101) | 1:160:A:GLN:H    | 1:213:A:MET:HB3  | 6        | 0.22          |
| (1,1097) | 1:165:A:PRO:HB3  | 1:168:A:GLN:HG2  | 17       | 0.22          |
| (1,1081) | 1:164:A:ARG:HD2  | 1:168:A:GLN:HG2  | 3        | 0.22          |
| (1,1070) | 1:152:A:GLU:HA   | 1:152:A:GLU:HG3  | 3        | 0.22          |
| (1,1070) | 1:152:A:GLU:HA   | 1:152:A:GLU:HG3  | 20       | 0.22          |
| (1,983)  | 1:149:A:TYR:H    | 1:152:A:GLU:HG2  | 11       | 0.22          |
| (1,967)  | 1:135:A:SER:HA   | 1:136:A:ARG:HB2  | 1        | 0.22          |
| (1,957)  | 1:184:A:ILE:HD11 | 1:207:A:GLU:HG3  | 11       | 0.22          |
| (1,957)  | 1:184:A:ILE:HD12 | 1:207:A:GLU:HG3  | 11       | 0.22          |
| (1,957)  | 1:184:A:ILE:HD13 | 1:207:A:GLU:HG3  | 11       | 0.22          |
| (1,873)  | 1:146:A:GLU:HA   | 1:150:A:TYR:HB3  | 19       | 0.22          |
| (1,774)  | 1:206:A:MET:HB2  | 1:206:A:MET:HE1  | 20       | 0.22          |
| (1,774)  | 1:206:A:MET:HB2  | 1:206:A:MET:HE2  | 20       | 0.22          |
| (1,774)  | 1:206:A:MET:HB2  | 1:206:A:MET:HE3  | 20       | 0.22          |
| (1,733)  | 1:222:A:SER:HB2  | 1:226:A:TYR:HD1  | 6        | 0.22          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,733)  | 1:222:A:SER:HB2  | 1:226:A:TYR:HD2  | 6        | 0.22          |
| (1,510)  | 1:211:A:GLU:HG3  | 1:214:A:CYS:HB3  | 18       | 0.22          |
| (1,501)  | 1:161:A:VAL:HA   | 1:162:A:TYR:HB3  | 6        | 0.22          |
| (1,501)  | 1:161:A:VAL:HA   | 1:162:A:TYR:HB3  | 7        | 0.22          |
| (1,496)  | 1:130:A:LEU:HA   | 1:162:A:TYR:HB2  | 4        | 0.22          |
| (1,467)  | 1:122:A:VAL:HG21 | 1:125:A:LEU:HB3  | 16       | 0.22          |
| (1,467)  | 1:122:A:VAL:HG22 | 1:125:A:LEU:HB3  | 16       | 0.22          |
| (1,467)  | 1:122:A:VAL:HG23 | 1:125:A:LEU:HB3  | 16       | 0.22          |
| (1,445)  | 1:180:A:VAL:HA   | 1:184:A:ILE:HG12 | 2        | 0.22          |
| (1,167)  | 1:203:A:VAL:H    | 1:203:A:VAL:HG11 | 18       | 0.22          |
| (1,167)  | 1:203:A:VAL:H    | 1:203:A:VAL:HG12 | 18       | 0.22          |
| (1,167)  | 1:203:A:VAL:H    | 1:203:A:VAL:HG13 | 18       | 0.22          |
| (1,151)  | 1:126:A:GLY:HA3  | 1:164:A:ARG:HD3  | 10       | 0.22          |
| (1,79)   | 1:138:A:MET:H    | 1:209:A:VAL:HG11 | 20       | 0.22          |
| (1,79)   | 1:138:A:MET:H    | 1:209:A:VAL:HG12 | 20       | 0.22          |
| (1,79)   | 1:138:A:MET:H    | 1:209:A:VAL:HG13 | 20       | 0.22          |
| (1,2791) | 1:126:A:GLY:HA2  | 1:128:A:TYR:HE1  | 19       | 0.21          |
| (1,2791) | 1:126:A:GLY:HA2  | 1:128:A:TYR:HE2  | 19       | 0.21          |
| (1,2657) | 1:141:A:PHE:HE1  | 1:208:A:ARG:HB3  | 17       | 0.21          |
| (1,2657) | 1:141:A:PHE:HE2  | 1:208:A:ARG:HB3  | 17       | 0.21          |
| (1,2501) | 1:149:A:TYR:HD1  | 1:205:A:MET:HG2  | 5        | 0.21          |
| (1,2501) | 1:149:A:TYR:HD2  | 1:205:A:MET:HG2  | 5        | 0.21          |
| (1,2314) | 1:133:A:ALA:HA   | 1:160:A:GLN:HE21 | 19       | 0.21          |
| (1,1937) | 1:220:A:LYS:H    | 1:221:A:GLU:HG3  | 16       | 0.21          |
| (1,1799) | 1:166:A:VAL:H    | 1:166:A:VAL:HG11 | 17       | 0.21          |
| (1,1799) | 1:166:A:VAL:H    | 1:166:A:VAL:HG12 | 17       | 0.21          |
| (1,1799) | 1:166:A:VAL:H    | 1:166:A:VAL:HG13 | 17       | 0.21          |
| (1,1678) | 1:125:A:LEU:H    | 1:125:A:LEU:HB2  | 2        | 0.21          |
| (1,1632) | 1:231:A:SER:HB3  | 1:232:A:SER:H    | 2        | 0.21          |
| (1,1632) | 1:231:A:SER:HB3  | 1:232:A:SER:H    | 8        | 0.21          |
| (1,1546) | 1:158:A:PRO:HD2  | 1:209:A:VAL:HG21 | 17       | 0.21          |
| (1,1546) | 1:158:A:PRO:HD2  | 1:209:A:VAL:HG22 | 17       | 0.21          |
| (1,1546) | 1:158:A:PRO:HD2  | 1:209:A:VAL:HG23 | 17       | 0.21          |
| (1,1392) | 1:133:A:ALA:HA   | 1:159:A:ASN:HB2  | 4        | 0.21          |
| (1,1340) | 1:160:A:GLN:HA   | 1:213:A:MET:HB2  | 12       | 0.21          |
| (1,1309) | 1:129:A:MET:HG2  | 1:164:A:ARG:HA   | 17       | 0.21          |
| (1,1280) | 1:202:A:ASP:HB2  | 1:206:A:MET:HG2  | 2        | 0.21          |
| (1,1256) | 1:184:A:ILE:HG13 | 1:206:A:MET:HG3  | 13       | 0.21          |
| (1,1207) | 1:168:A:GLN:HA   | 1:168:A:GLN:HE22 | 16       | 0.21          |
| (1,1070) | 1:152:A:GLU:HA   | 1:152:A:GLU:HG3  | 7        | 0.21          |
| (1,1050) | 1:128:A:TYR:HA   | 1:129:A:MET:HG3  | 17       | 0.21          |
| (1,1044) | 1:128:A:TYR:HA   | 1:165:A:PRO:HD2  | 15       | 0.21          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,957)  | 1:184:A:ILE:HD11 | 1:207:A:GLU:HG3  | 15       | 0.21          |
| (1,957)  | 1:184:A:ILE:HD12 | 1:207:A:GLU:HG3  | 15       | 0.21          |
| (1,957)  | 1:184:A:ILE:HD13 | 1:207:A:GLU:HG3  | 15       | 0.21          |
| (1,828)  | 1:222:A:SER:HA   | 1:226:A:TYR:HB3  | 3        | 0.21          |
| (1,828)  | 1:222:A:SER:HA   | 1:226:A:TYR:HB3  | 4        | 0.21          |
| (1,525)  | 1:132:A:SER:HB2  | 1:160:A:GLN:HE21 | 10       | 0.21          |
| (1,521)  | 1:223:A:GLN:HG3  | 1:224:A:ALA:HB1  | 1        | 0.21          |
| (1,521)  | 1:223:A:GLN:HG3  | 1:224:A:ALA:HB2  | 1        | 0.21          |
| (1,521)  | 1:223:A:GLN:HG3  | 1:224:A:ALA:HB3  | 1        | 0.21          |
| (1,501)  | 1:161:A:VAL:HA   | 1:162:A:TYR:HB3  | 4        | 0.21          |
| (1,350)  | 1:122:A:VAL:HG21 | 1:123:A:GLY:H    | 16       | 0.21          |
| (1,350)  | 1:122:A:VAL:HG22 | 1:123:A:GLY:H    | 16       | 0.21          |
| (1,350)  | 1:122:A:VAL:HG23 | 1:123:A:GLY:H    | 16       | 0.21          |
| (1,182)  | 1:216:A:THR:HB   | 1:220:A:LYS:HG3  | 1        | 0.21          |
| (1,179)  | 1:201:A:THR:HB   | 1:205:A:MET:HG3  | 16       | 0.21          |
| (1,96)   | 1:139:A:ILE:HG13 | 1:209:A:VAL:HG11 | 18       | 0.21          |
| (1,96)   | 1:139:A:ILE:HG13 | 1:209:A:VAL:HG12 | 18       | 0.21          |
| (1,96)   | 1:139:A:ILE:HG13 | 1:209:A:VAL:HG13 | 18       | 0.21          |
| (1,2830) | 1:172:A:GLN:HG2  | 1:218:A:TYR:HE1  | 10       | 0.2           |
| (1,2830) | 1:172:A:GLN:HG2  | 1:218:A:TYR:HE2  | 10       | 0.2           |
| (1,2771) | 1:130:A:LEU:HB3  | 1:162:A:TYR:HE1  | 8        | 0.2           |
| (1,2771) | 1:130:A:LEU:HB3  | 1:162:A:TYR:HE2  | 8        | 0.2           |
| (1,2756) | 1:150:A:TYR:HE1  | 1:205:A:MET:HG2  | 14       | 0.2           |
| (1,2756) | 1:150:A:TYR:HE2  | 1:205:A:MET:HG2  | 14       | 0.2           |
| (1,2736) | 1:184:A:ILE:HG13 | 1:187:A:HIS:HD2  | 1        | 0.2           |
| (1,2674) | 1:175:A:PHE:HZ   | 1:221:A:GLU:HG2  | 3        | 0.2           |
| (1,2642) | 1:157:A:TYR:HD1  | 1:209:A:VAL:HG11 | 16       | 0.2           |
| (1,2642) | 1:157:A:TYR:HD1  | 1:209:A:VAL:HG12 | 16       | 0.2           |
| (1,2642) | 1:157:A:TYR:HD1  | 1:209:A:VAL:HG13 | 16       | 0.2           |
| (1,2642) | 1:157:A:TYR:HD2  | 1:209:A:VAL:HG11 | 16       | 0.2           |
| (1,2642) | 1:157:A:TYR:HD2  | 1:209:A:VAL:HG12 | 16       | 0.2           |
| (1,2642) | 1:157:A:TYR:HD2  | 1:209:A:VAL:HG13 | 16       | 0.2           |
| (1,2356) | 1:169:A:TYR:HB2  | 1:174:A:ASN:HD21 | 10       | 0.2           |
| (1,2322) | 1:130:A:LEU:HG   | 1:160:A:GLN:HE22 | 19       | 0.2           |
| (1,2311) | 1:131:A:GLY:H    | 1:160:A:GLN:HE21 | 3        | 0.2           |
| (1,2092) | 1:169:A:TYR:H    | 1:169:A:TYR:HB3  | 6        | 0.2           |
| (1,1678) | 1:125:A:LEU:H    | 1:125:A:LEU:HB2  | 20       | 0.2           |
| (1,1309) | 1:129:A:MET:HG2  | 1:164:A:ARG:HA   | 6        | 0.2           |
| (1,1220) | 1:195:A:GLY:HA2  | 1:196:A:GLU:HA   | 9        | 0.2           |
| (1,1220) | 1:195:A:GLY:HA2  | 1:196:A:GLU:HA   | 15       | 0.2           |
| (1,1220) | 1:195:A:GLY:HA2  | 1:196:A:GLU:HA   | 18       | 0.2           |
| (1,1212) | 1:184:A:ILE:HD11 | 1:206:A:MET:HB3  | 18       | 0.2           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1212) | 1:184:A:ILE:HD12 | 1:206:A:MET:HB3  | 18       | 0.2           |
| (1,1212) | 1:184:A:ILE:HD13 | 1:206:A:MET:HB3  | 18       | 0.2           |
| (1,1197) | 1:160:A:GLN:HB2  | 1:183:A:THR:HG21 | 13       | 0.2           |
| (1,1197) | 1:160:A:GLN:HB2  | 1:183:A:THR:HG22 | 13       | 0.2           |
| (1,1197) | 1:160:A:GLN:HB2  | 1:183:A:THR:HG23 | 13       | 0.2           |
| (1,1197) | 1:160:A:GLN:HB2  | 1:183:A:THR:HG21 | 16       | 0.2           |
| (1,1197) | 1:160:A:GLN:HB2  | 1:183:A:THR:HG22 | 16       | 0.2           |
| (1,1197) | 1:160:A:GLN:HB2  | 1:183:A:THR:HG23 | 16       | 0.2           |
| (1,1155) | 1:130:A:LEU:HB3  | 1:162:A:TYR:HA   | 20       | 0.2           |
| (1,1101) | 1:160:A:GLN:H    | 1:213:A:MET:HB3  | 3        | 0.2           |
| (1,1097) | 1:165:A:PRO:HB3  | 1:168:A:GLN:HG2  | 14       | 0.2           |
| (1,1070) | 1:152:A:GLU:HA   | 1:152:A:GLU:HG3  | 1        | 0.2           |
| (1,1070) | 1:152:A:GLU:HA   | 1:152:A:GLU:HG3  | 9        | 0.2           |
| (1,1070) | 1:152:A:GLU:HA   | 1:152:A:GLU:HG3  | 18       | 0.2           |
| (1,873)  | 1:146:A:GLU:HA   | 1:150:A:TYR:HB3  | 20       | 0.2           |
| (1,864)  | 1:134:A:MET:HB3  | 1:135:A:SER:HB2  | 16       | 0.2           |
| (1,862)  | 1:143:A:ASN:HD22 | 1:146:A:GLU:HG2  | 11       | 0.2           |
| (1,828)  | 1:222:A:SER:HA   | 1:226:A:TYR:HB3  | 9        | 0.2           |
| (1,735)  | 1:222:A:SER:HB2  | 1:223:A:GLN:HB2  | 7        | 0.2           |
| (1,735)  | 1:222:A:SER:HB2  | 1:223:A:GLN:HB3  | 7        | 0.2           |
| (1,735)  | 1:222:A:SER:HB2  | 1:223:A:GLN:HB2  | 10       | 0.2           |
| (1,735)  | 1:222:A:SER:HB2  | 1:223:A:GLN:HB3  | 10       | 0.2           |
| (1,735)  | 1:222:A:SER:HB2  | 1:223:A:GLN:HB2  | 12       | 0.2           |
| (1,735)  | 1:222:A:SER:HB2  | 1:223:A:GLN:HB3  | 12       | 0.2           |
| (1,735)  | 1:222:A:SER:HB2  | 1:223:A:GLN:HB2  | 13       | 0.2           |
| (1,735)  | 1:222:A:SER:HB2  | 1:223:A:GLN:HB3  | 13       | 0.2           |
| (1,730)  | 1:166:A:VAL:HG11 | 1:167:A:SER:HB3  | 17       | 0.2           |
| (1,730)  | 1:166:A:VAL:HG12 | 1:167:A:SER:HB3  | 17       | 0.2           |
| (1,730)  | 1:166:A:VAL:HG13 | 1:167:A:SER:HB3  | 17       | 0.2           |
| (1,574)  | 1:153:A:ASN:HB2  | 1:155:A:TYR:HE1  | 17       | 0.2           |
| (1,574)  | 1:153:A:ASN:HB2  | 1:155:A:TYR:HE2  | 17       | 0.2           |
| (1,538)  | 1:146:A:GLU:HG3  | 1:205:A:MET:HE1  | 7        | 0.2           |
| (1,538)  | 1:146:A:GLU:HG3  | 1:205:A:MET:HE2  | 7        | 0.2           |
| (1,538)  | 1:146:A:GLU:HG3  | 1:205:A:MET:HE3  | 7        | 0.2           |
| (1,525)  | 1:132:A:SER:HB2  | 1:160:A:GLN:HE21 | 4        | 0.2           |
| (1,501)  | 1:161:A:VAL:HA   | 1:162:A:TYR:HB3  | 11       | 0.2           |
| (1,501)  | 1:161:A:VAL:HA   | 1:162:A:TYR:HB3  | 13       | 0.2           |
| (1,501)  | 1:161:A:VAL:HA   | 1:162:A:TYR:HB3  | 20       | 0.2           |
| (1,350)  | 1:122:A:VAL:HG21 | 1:123:A:GLY:H    | 18       | 0.2           |
| (1,350)  | 1:122:A:VAL:HG22 | 1:123:A:GLY:H    | 18       | 0.2           |
| (1,350)  | 1:122:A:VAL:HG23 | 1:123:A:GLY:H    | 18       | 0.2           |
| (1,260)  | 1:186:A:GLN:HB2  | 1:190:A:THR:HG21 | 8        | 0.2           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,260)  | 1:186:A:GLN:HB2  | 1:190:A:THR:HG22 | 8        | 0.2           |
| (1,260)  | 1:186:A:GLN:HB2  | 1:190:A:THR:HG23 | 8        | 0.2           |
| (1,216)  | 1:216:A:THR:HG21 | 1:220:A:LYS:HG3  | 8        | 0.2           |
| (1,216)  | 1:216:A:THR:HG22 | 1:220:A:LYS:HG3  | 8        | 0.2           |
| (1,216)  | 1:216:A:THR:HG23 | 1:220:A:LYS:HG3  | 8        | 0.2           |
| (1,216)  | 1:216:A:THR:HG21 | 1:220:A:LYS:HG3  | 14       | 0.2           |
| (1,216)  | 1:216:A:THR:HG22 | 1:220:A:LYS:HG3  | 14       | 0.2           |
| (1,216)  | 1:216:A:THR:HG23 | 1:220:A:LYS:HG3  | 14       | 0.2           |
| (1,111)  | 1:215:A:VAL:HG11 | 1:216:A:THR:HB   | 12       | 0.2           |
| (1,111)  | 1:215:A:VAL:HG12 | 1:216:A:THR:HB   | 12       | 0.2           |
| (1,111)  | 1:215:A:VAL:HG13 | 1:216:A:THR:HB   | 12       | 0.2           |
| (1,79)   | 1:138:A:MET:H    | 1:209:A:VAL:HG11 | 14       | 0.2           |
| (1,79)   | 1:138:A:MET:H    | 1:209:A:VAL:HG12 | 14       | 0.2           |
| (1,79)   | 1:138:A:MET:H    | 1:209:A:VAL:HG13 | 14       | 0.2           |
| (1,77)   | 1:208:A:ARG:H    | 1:209:A:VAL:HG11 | 18       | 0.2           |
| (1,77)   | 1:208:A:ARG:H    | 1:209:A:VAL:HG12 | 18       | 0.2           |
| (1,77)   | 1:208:A:ARG:H    | 1:209:A:VAL:HG13 | 18       | 0.2           |
| (1,2657) | 1:141:A:PHE:HE1  | 1:208:A:ARG:HB3  | 8        | 0.19          |
| (1,2657) | 1:141:A:PHE:HE2  | 1:208:A:ARG:HB3  | 8        | 0.19          |
| (1,2657) | 1:141:A:PHE:HE1  | 1:208:A:ARG:HB3  | 13       | 0.19          |
| (1,2657) | 1:141:A:PHE:HE2  | 1:208:A:ARG:HB3  | 13       | 0.19          |
| (1,2537) | 1:166:A:VAL:HG11 | 1:225:A:TYR:HD1  | 12       | 0.19          |
| (1,2537) | 1:166:A:VAL:HG11 | 1:225:A:TYR:HD2  | 12       | 0.19          |
| (1,2537) | 1:166:A:VAL:HG12 | 1:225:A:TYR:HD1  | 12       | 0.19          |
| (1,2537) | 1:166:A:VAL:HG12 | 1:225:A:TYR:HD2  | 12       | 0.19          |
| (1,2537) | 1:166:A:VAL:HG13 | 1:225:A:TYR:HD1  | 12       | 0.19          |
| (1,2537) | 1:166:A:VAL:HG13 | 1:225:A:TYR:HD2  | 12       | 0.19          |
| (1,1847) | 1:197:A:ASN:H    | 1:197:A:ASN:HB3  | 13       | 0.19          |
| (1,1678) | 1:125:A:LEU:H    | 1:125:A:LEU:HB2  | 14       | 0.19          |
| (1,1501) | 1:137:A:PRO:HD3  | 1:209:A:VAL:HG21 | 12       | 0.19          |
| (1,1501) | 1:137:A:PRO:HD3  | 1:209:A:VAL:HG22 | 12       | 0.19          |
| (1,1501) | 1:137:A:PRO:HD3  | 1:209:A:VAL:HG23 | 12       | 0.19          |
| (1,1495) | 1:212:A:GLN:HB2  | 1:216:A:THR:H    | 14       | 0.19          |
| (1,1466) | 1:210:A:VAL:H    | 1:211:A:GLU:HB3  | 14       | 0.19          |
| (1,1340) | 1:160:A:GLN:HA   | 1:213:A:MET:HB2  | 8        | 0.19          |
| (1,1309) | 1:129:A:MET:HG2  | 1:164:A:ARG:HA   | 9        | 0.19          |
| (1,1155) | 1:130:A:LEU:HB3  | 1:162:A:TYR:HA   | 5        | 0.19          |
| (1,1097) | 1:165:A:PRO:HB3  | 1:168:A:GLN:HG2  | 1        | 0.19          |
| (1,1070) | 1:152:A:GLU:HA   | 1:152:A:GLU:HG3  | 4        | 0.19          |
| (1,1070) | 1:152:A:GLU:HA   | 1:152:A:GLU:HG3  | 6        | 0.19          |
| (1,1070) | 1:152:A:GLU:HA   | 1:152:A:GLU:HG3  | 11       | 0.19          |
| (1,864)  | 1:134:A:MET:HB3  | 1:135:A:SER:HB2  | 18       | 0.19          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,752)  | 1:138:A:MET:HE1  | 1:139:A:ILE:HG12 | 5        | 0.19          |
| (1,752)  | 1:138:A:MET:HE2  | 1:139:A:ILE:HG12 | 5        | 0.19          |
| (1,752)  | 1:138:A:MET:HE3  | 1:139:A:ILE:HG12 | 5        | 0.19          |
| (1,735)  | 1:222:A:SER:HB2  | 1:223:A:GLN:HB2  | 1        | 0.19          |
| (1,735)  | 1:222:A:SER:HB2  | 1:223:A:GLN:HB3  | 1        | 0.19          |
| (1,735)  | 1:222:A:SER:HB2  | 1:223:A:GLN:HB2  | 17       | 0.19          |
| (1,735)  | 1:222:A:SER:HB2  | 1:223:A:GLN:HB3  | 17       | 0.19          |
| (1,734)  | 1:219:A:GLN:HA   | 1:222:A:SER:HB2  | 13       | 0.19          |
| (1,630)  | 1:165:A:PRO:HA   | 1:166:A:VAL:HG11 | 1        | 0.19          |
| (1,630)  | 1:165:A:PRO:HA   | 1:166:A:VAL:HG12 | 1        | 0.19          |
| (1,630)  | 1:165:A:PRO:HA   | 1:166:A:VAL:HG13 | 1        | 0.19          |
| (1,569)  | 1:128:A:TYR:HE1  | 1:179:A:CYS:HB3  | 17       | 0.19          |
| (1,569)  | 1:128:A:TYR:HE2  | 1:179:A:CYS:HB3  | 17       | 0.19          |
| (1,528)  | 1:143:A:ASN:HB2  | 1:147:A:ASP:HB3  | 6        | 0.19          |
| (1,528)  | 1:143:A:ASN:HB3  | 1:147:A:ASP:HB3  | 6        | 0.19          |
| (1,528)  | 1:143:A:ASN:HB2  | 1:147:A:ASP:HB3  | 15       | 0.19          |
| (1,528)  | 1:143:A:ASN:HB3  | 1:147:A:ASP:HB3  | 15       | 0.19          |
| (1,445)  | 1:180:A:VAL:HA   | 1:184:A:ILE:HG12 | 19       | 0.19          |
| (1,350)  | 1:122:A:VAL:HG21 | 1:123:A:GLY:H    | 12       | 0.19          |
| (1,350)  | 1:122:A:VAL:HG22 | 1:123:A:GLY:H    | 12       | 0.19          |
| (1,350)  | 1:122:A:VAL:HG23 | 1:123:A:GLY:H    | 12       | 0.19          |
| (1,333)  | 1:172:A:GLN:HE22 | 1:215:A:VAL:HG21 | 14       | 0.19          |
| (1,333)  | 1:172:A:GLN:HE22 | 1:215:A:VAL:HG22 | 14       | 0.19          |
| (1,333)  | 1:172:A:GLN:HE22 | 1:215:A:VAL:HG23 | 14       | 0.19          |
| (1,150)  | 1:126:A:GLY:HA3  | 1:127:A:GLY:H    | 14       | 0.19          |
| (1,111)  | 1:215:A:VAL:HG11 | 1:216:A:THR:HB   | 19       | 0.19          |
| (1,111)  | 1:215:A:VAL:HG12 | 1:216:A:THR:HB   | 19       | 0.19          |
| (1,111)  | 1:215:A:VAL:HG13 | 1:216:A:THR:HB   | 19       | 0.19          |
| (1,89)   | 1:206:A:MET:HB3  | 1:210:A:VAL:HG21 | 6        | 0.19          |
| (1,89)   | 1:206:A:MET:HB3  | 1:210:A:VAL:HG22 | 6        | 0.19          |
| (1,89)   | 1:206:A:MET:HB3  | 1:210:A:VAL:HG23 | 6        | 0.19          |
| (1,2807) | 1:149:A:TYR:HE1  | 1:153:A:ASN:HB3  | 20       | 0.18          |
| (1,2807) | 1:149:A:TYR:HE2  | 1:153:A:ASN:HB3  | 20       | 0.18          |
| (1,2683) | 1:139:A:ILE:HG12 | 1:141:A:PHE:HZ   | 12       | 0.18          |
| (1,2593) | 1:175:A:PHE:HE1  | 1:221:A:GLU:HG2  | 13       | 0.18          |
| (1,2593) | 1:175:A:PHE:HE2  | 1:221:A:GLU:HG2  | 13       | 0.18          |
| (1,2553) | 1:126:A:GLY:HA2  | 1:128:A:TYR:HD1  | 1        | 0.18          |
| (1,2553) | 1:126:A:GLY:HA2  | 1:128:A:TYR:HD2  | 1        | 0.18          |
| (1,2474) | 1:168:A:GLN:HG2  | 1:169:A:TYR:HD1  | 17       | 0.18          |
| (1,2474) | 1:168:A:GLN:HG2  | 1:169:A:TYR:HD2  | 17       | 0.18          |
| (1,2328) | 1:223:A:GLN:HE21 | 1:227:A:ASP:HB2  | 19       | 0.18          |
| (1,2328) | 1:223:A:GLN:HE21 | 1:227:A:ASP:HB3  | 19       | 0.18          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2322) | 1:130:A:LEU:HG   | 1:160:A:GLN:HE22 | 8        | 0.18          |
| (1,2322) | 1:130:A:LEU:HG   | 1:160:A:GLN:HE22 | 20       | 0.18          |
| (1,2270) | 1:132:A:SER:H    | 1:132:A:SER:HB2  | 4        | 0.18          |
| (1,2095) | 1:166:A:VAL:HG21 | 1:169:A:TYR:H    | 1        | 0.18          |
| (1,2095) | 1:166:A:VAL:HG22 | 1:169:A:TYR:H    | 1        | 0.18          |
| (1,2095) | 1:166:A:VAL:HG23 | 1:169:A:TYR:H    | 1        | 0.18          |
| (1,2050) | 1:221:A:GLU:H    | 1:221:A:GLU:HG3  | 7        | 0.18          |
| (1,1968) | 1:205:A:MET:H    | 1:205:A:MET:HG3  | 8        | 0.18          |
| (1,1746) | 1:184:A:ILE:H    | 1:184:A:ILE:HG12 | 12       | 0.18          |
| (1,1678) | 1:125:A:LEU:H    | 1:125:A:LEU:HB2  | 5        | 0.18          |
| (1,1678) | 1:125:A:LEU:H    | 1:125:A:LEU:HB2  | 9        | 0.18          |
| (1,1678) | 1:125:A:LEU:H    | 1:125:A:LEU:HB2  | 15       | 0.18          |
| (1,1535) | 1:165:A:PRO:HD2  | 1:166:A:VAL:H    | 13       | 0.18          |
| (1,1497) | 1:139:A:ILE:HD11 | 1:212:A:GLN:HB3  | 2        | 0.18          |
| (1,1497) | 1:139:A:ILE:HD12 | 1:212:A:GLN:HB3  | 2        | 0.18          |
| (1,1497) | 1:139:A:ILE:HD13 | 1:212:A:GLN:HB3  | 2        | 0.18          |
| (1,1231) | 1:209:A:VAL:HG21 | 1:213:A:MET:HG3  | 7        | 0.18          |
| (1,1231) | 1:209:A:VAL:HG22 | 1:213:A:MET:HG3  | 7        | 0.18          |
| (1,1231) | 1:209:A:VAL:HG23 | 1:213:A:MET:HG3  | 7        | 0.18          |
| (1,1227) | 1:210:A:VAL:HA   | 1:213:A:MET:HG2  | 7        | 0.18          |
| (1,1089) | 1:182:A:ILE:HD11 | 1:186:A:GLN:HE21 | 12       | 0.18          |
| (1,1089) | 1:182:A:ILE:HD12 | 1:186:A:GLN:HE21 | 12       | 0.18          |
| (1,1089) | 1:182:A:ILE:HD13 | 1:186:A:GLN:HE21 | 12       | 0.18          |
| (1,1070) | 1:152:A:GLU:HA   | 1:152:A:GLU:HG3  | 2        | 0.18          |
| (1,1060) | 1:207:A:GLU:HG3  | 1:208:A:ARG:H    | 12       | 0.18          |
| (1,1050) | 1:128:A:TYR:HA   | 1:129:A:MET:HG3  | 8        | 0.18          |
| (1,1033) | 1:205:A:MET:H    | 1:207:A:GLU:HG3  | 17       | 0.18          |
| (1,957)  | 1:184:A:ILE:HD11 | 1:207:A:GLU:HG3  | 13       | 0.18          |
| (1,957)  | 1:184:A:ILE:HD12 | 1:207:A:GLU:HG3  | 13       | 0.18          |
| (1,957)  | 1:184:A:ILE:HD13 | 1:207:A:GLU:HG3  | 13       | 0.18          |
| (1,873)  | 1:146:A:GLU:HA   | 1:150:A:TYR:HB3  | 9        | 0.18          |
| (1,862)  | 1:143:A:ASN:HD22 | 1:146:A:GLU:HG2  | 13       | 0.18          |
| (1,775)  | 1:203:A:VAL:HG11 | 1:206:A:MET:HE1  | 12       | 0.18          |
| (1,775)  | 1:203:A:VAL:HG11 | 1:206:A:MET:HE2  | 12       | 0.18          |
| (1,775)  | 1:203:A:VAL:HG11 | 1:206:A:MET:HE3  | 12       | 0.18          |
| (1,775)  | 1:203:A:VAL:HG12 | 1:206:A:MET:HE1  | 12       | 0.18          |
| (1,775)  | 1:203:A:VAL:HG12 | 1:206:A:MET:HE2  | 12       | 0.18          |
| (1,775)  | 1:203:A:VAL:HG12 | 1:206:A:MET:HE3  | 12       | 0.18          |
| (1,775)  | 1:203:A:VAL:HG13 | 1:206:A:MET:HE1  | 12       | 0.18          |
| (1,775)  | 1:203:A:VAL:HG13 | 1:206:A:MET:HE2  | 12       | 0.18          |
| (1,775)  | 1:203:A:VAL:HG13 | 1:206:A:MET:HE3  | 12       | 0.18          |
| (1,735)  | 1:222:A:SER:HB2  | 1:223:A:GLN:HB2  | 8        | 0.18          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,735)  | 1:222:A:SER:HB2  | 1:223:A:GLN:HB3  | 8        | 0.18          |
| (1,735)  | 1:222:A:SER:HB2  | 1:223:A:GLN:HB2  | 16       | 0.18          |
| (1,735)  | 1:222:A:SER:HB2  | 1:223:A:GLN:HB3  | 16       | 0.18          |
| (1,574)  | 1:153:A:ASN:HB2  | 1:155:A:TYR:HE1  | 2        | 0.18          |
| (1,574)  | 1:153:A:ASN:HB2  | 1:155:A:TYR:HE2  | 2        | 0.18          |
| (1,527)  | 1:202:A:ASP:HB2  | 1:203:A:VAL:HG11 | 7        | 0.18          |
| (1,527)  | 1:202:A:ASP:HB2  | 1:203:A:VAL:HG12 | 7        | 0.18          |
| (1,527)  | 1:202:A:ASP:HB2  | 1:203:A:VAL:HG13 | 7        | 0.18          |
| (1,506)  | 1:179:A:CYS:HB2  | 1:214:A:CYS:HB2  | 17       | 0.18          |
| (1,501)  | 1:161:A:VAL:HA   | 1:162:A:TYR:HB3  | 2        | 0.18          |
| (1,501)  | 1:161:A:VAL:HA   | 1:162:A:TYR:HB3  | 18       | 0.18          |
| (1,150)  | 1:126:A:GLY:HA3  | 1:127:A:GLY:H    | 7        | 0.18          |
| (1,89)   | 1:206:A:MET:HB3  | 1:210:A:VAL:HG21 | 2        | 0.18          |
| (1,89)   | 1:206:A:MET:HB3  | 1:210:A:VAL:HG22 | 2        | 0.18          |
| (1,89)   | 1:206:A:MET:HB3  | 1:210:A:VAL:HG23 | 2        | 0.18          |
| (1,2834) | 1:163:A:TYR:HE1  | 1:221:A:GLU:HG2  | 17       | 0.17          |
| (1,2834) | 1:163:A:TYR:HE2  | 1:221:A:GLU:HG2  | 17       | 0.17          |
| (1,2736) | 1:184:A:ILE:HG13 | 1:187:A:HIS:HD2  | 18       | 0.17          |
| (1,2466) | 1:169:A:TYR:HD1  | 1:174:A:ASN:HB3  | 18       | 0.17          |
| (1,2466) | 1:169:A:TYR:HD2  | 1:174:A:ASN:HB3  | 18       | 0.17          |
| (1,2445) | 1:122:A:VAL:HG21 | 1:124:A:GLY:H    | 16       | 0.17          |
| (1,2445) | 1:122:A:VAL:HG22 | 1:124:A:GLY:H    | 16       | 0.17          |
| (1,2445) | 1:122:A:VAL:HG23 | 1:124:A:GLY:H    | 16       | 0.17          |
| (1,2405) | 1:125:A:LEU:HD21 | 1:126:A:GLY:H    | 6        | 0.17          |
| (1,2405) | 1:125:A:LEU:HD22 | 1:126:A:GLY:H    | 6        | 0.17          |
| (1,2405) | 1:125:A:LEU:HD23 | 1:126:A:GLY:H    | 6        | 0.17          |
| (1,2328) | 1:223:A:GLN:HE21 | 1:227:A:ASP:HB2  | 12       | 0.17          |
| (1,2328) | 1:223:A:GLN:HE21 | 1:227:A:ASP:HB3  | 12       | 0.17          |
| (1,2214) | 1:151:A:ARG:HB3  | 1:153:A:ASN:H    | 13       | 0.17          |
| (1,2050) | 1:221:A:GLU:H    | 1:221:A:GLU:HG3  | 6        | 0.17          |
| (1,1968) | 1:205:A:MET:H    | 1:205:A:MET:HG3  | 5        | 0.17          |
| (1,1847) | 1:197:A:ASN:H    | 1:197:A:ASN:HB3  | 2        | 0.17          |
| (1,1495) | 1:212:A:GLN:HB2  | 1:216:A:THR:H    | 1        | 0.17          |
| (1,1495) | 1:212:A:GLN:HB2  | 1:216:A:THR:H    | 11       | 0.17          |
| (1,1479) | 1:145:A:TRP:HB2  | 1:146:A:GLU:HG2  | 19       | 0.17          |
| (1,1479) | 1:145:A:TRP:HB3  | 1:146:A:GLU:HG2  | 19       | 0.17          |
| (1,1466) | 1:210:A:VAL:H    | 1:211:A:GLU:HB3  | 1        | 0.17          |
| (1,1227) | 1:210:A:VAL:HA   | 1:213:A:MET:HG2  | 6        | 0.17          |
| (1,1220) | 1:195:A:GLY:HA2  | 1:196:A:GLU:HA   | 17       | 0.17          |
| (1,1155) | 1:130:A:LEU:HB3  | 1:162:A:TYR:HA   | 18       | 0.17          |
| (1,1152) | 1:205:A:MET:HA   | 1:205:A:MET:HG3  | 15       | 0.17          |
| (1,1152) | 1:205:A:MET:HA   | 1:205:A:MET:HG3  | 18       | 0.17          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1096) | 1:165:A:PRO:HD3  | 1:168:A:GLN:HG2  | 7        | 0.17          |
| (1,1070) | 1:152:A:GLU:HA   | 1:152:A:GLU:HG3  | 14       | 0.17          |
| (1,1070) | 1:152:A:GLU:HA   | 1:152:A:GLU:HG3  | 16       | 0.17          |
| (1,902)  | 1:147:A:ASP:HB2  | 1:148:A:ARG:HA   | 12       | 0.17          |
| (1,902)  | 1:147:A:ASP:HB2  | 1:148:A:ARG:HA   | 17       | 0.17          |
| (1,735)  | 1:222:A:SER:HB2  | 1:223:A:GLN:HB2  | 5        | 0.17          |
| (1,735)  | 1:222:A:SER:HB2  | 1:223:A:GLN:HB3  | 5        | 0.17          |
| (1,677)  | 1:135:A:SER:HB2  | 1:213:A:MET:HA   | 15       | 0.17          |
| (1,552)  | 1:153:A:ASN:HB2  | 1:156:A:ARG:HD2  | 5        | 0.17          |
| (1,544)  | 1:182:A:ILE:HG21 | 1:186:A:GLN:HB3  | 11       | 0.17          |
| (1,544)  | 1:182:A:ILE:HG22 | 1:186:A:GLN:HB3  | 11       | 0.17          |
| (1,544)  | 1:182:A:ILE:HG23 | 1:186:A:GLN:HB3  | 11       | 0.17          |
| (1,497)  | 1:128:A:TYR:HB2  | 1:162:A:TYR:HB2  | 16       | 0.17          |
| (1,379)  | 1:139:A:ILE:HG13 | 1:209:A:VAL:HG21 | 5        | 0.17          |
| (1,379)  | 1:139:A:ILE:HG13 | 1:209:A:VAL:HG22 | 5        | 0.17          |
| (1,379)  | 1:139:A:ILE:HG13 | 1:209:A:VAL:HG23 | 5        | 0.17          |
| (1,374)  | 1:209:A:VAL:HG21 | 1:210:A:VAL:H    | 16       | 0.17          |
| (1,374)  | 1:209:A:VAL:HG22 | 1:210:A:VAL:H    | 16       | 0.17          |
| (1,374)  | 1:209:A:VAL:HG23 | 1:210:A:VAL:H    | 16       | 0.17          |
| (1,359)  | 1:122:A:VAL:HG21 | 1:182:A:ILE:HG21 | 9        | 0.17          |
| (1,359)  | 1:122:A:VAL:HG21 | 1:182:A:ILE:HG22 | 9        | 0.17          |
| (1,359)  | 1:122:A:VAL:HG21 | 1:182:A:ILE:HG23 | 9        | 0.17          |
| (1,359)  | 1:122:A:VAL:HG22 | 1:182:A:ILE:HG21 | 9        | 0.17          |
| (1,359)  | 1:122:A:VAL:HG22 | 1:182:A:ILE:HG22 | 9        | 0.17          |
| (1,359)  | 1:122:A:VAL:HG22 | 1:182:A:ILE:HG23 | 9        | 0.17          |
| (1,359)  | 1:122:A:VAL:HG23 | 1:182:A:ILE:HG21 | 9        | 0.17          |
| (1,359)  | 1:122:A:VAL:HG23 | 1:182:A:ILE:HG22 | 9        | 0.17          |
| (1,359)  | 1:122:A:VAL:HG23 | 1:182:A:ILE:HG23 | 9        | 0.17          |
| (1,309)  | 1:186:A:GLN:HE21 | 1:189:A:VAL:HG11 | 13       | 0.17          |
| (1,309)  | 1:186:A:GLN:HE21 | 1:189:A:VAL:HG12 | 13       | 0.17          |
| (1,309)  | 1:186:A:GLN:HE21 | 1:189:A:VAL:HG13 | 13       | 0.17          |
| (1,174)  | 1:202:A:ASP:HB3  | 1:203:A:VAL:HG11 | 7        | 0.17          |
| (1,174)  | 1:202:A:ASP:HB3  | 1:203:A:VAL:HG12 | 7        | 0.17          |
| (1,174)  | 1:202:A:ASP:HB3  | 1:203:A:VAL:HG13 | 7        | 0.17          |
| (1,162)  | 1:226:A:TYR:HB2  | 1:228:A:GLY:HA2  | 14       | 0.17          |
| (1,162)  | 1:226:A:TYR:HB2  | 1:228:A:GLY:HA3  | 14       | 0.17          |
| (1,162)  | 1:226:A:TYR:HB2  | 1:228:A:GLY:HA2  | 19       | 0.17          |
| (1,162)  | 1:226:A:TYR:HB2  | 1:228:A:GLY:HA3  | 19       | 0.17          |
| (1,150)  | 1:126:A:GLY:HA3  | 1:127:A:GLY:H    | 4        | 0.17          |
| (1,150)  | 1:126:A:GLY:HA3  | 1:127:A:GLY:H    | 15       | 0.17          |
| (1,150)  | 1:126:A:GLY:HA3  | 1:127:A:GLY:H    | 20       | 0.17          |
| (1,77)   | 1:208:A:ARG:H    | 1:209:A:VAL:HG11 | 13       | 0.17          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,77)   | 1:208:A:ARG:H    | 1:209:A:VAL:HG12 | 13       | 0.17          |
| (1,77)   | 1:208:A:ARG:H    | 1:209:A:VAL:HG13 | 13       | 0.17          |
| (1,31)   | 1:219:A:GLN:HA   | 1:220:A:LYS:HG3  | 16       | 0.17          |
| (1,31)   | 1:219:A:GLN:HA   | 1:220:A:LYS:HG3  | 18       | 0.17          |
| (1,2830) | 1:172:A:GLN:HG2  | 1:218:A:TYR:HE1  | 7        | 0.16          |
| (1,2830) | 1:172:A:GLN:HG2  | 1:218:A:TYR:HE2  | 7        | 0.16          |
| (1,2736) | 1:184:A:ILE:HG13 | 1:187:A:HIS:HD2  | 11       | 0.16          |
| (1,2553) | 1:126:A:GLY:HA2  | 1:128:A:TYR:HD1  | 14       | 0.16          |
| (1,2553) | 1:126:A:GLY:HA2  | 1:128:A:TYR:HD2  | 14       | 0.16          |
| (1,2537) | 1:166:A:VAL:HG11 | 1:225:A:TYR:HD1  | 1        | 0.16          |
| (1,2537) | 1:166:A:VAL:HG11 | 1:225:A:TYR:HD2  | 1        | 0.16          |
| (1,2537) | 1:166:A:VAL:HG12 | 1:225:A:TYR:HD1  | 1        | 0.16          |
| (1,2537) | 1:166:A:VAL:HG12 | 1:225:A:TYR:HD2  | 1        | 0.16          |
| (1,2537) | 1:166:A:VAL:HG13 | 1:225:A:TYR:HD1  | 1        | 0.16          |
| (1,2537) | 1:166:A:VAL:HG13 | 1:225:A:TYR:HD2  | 1        | 0.16          |
| (1,2414) | 1:136:A:ARG:HB3  | 1:159:A:ASN:HD21 | 20       | 0.16          |
| (1,1893) | 1:208:A:ARG:HB3  | 1:209:A:VAL:H    | 16       | 0.16          |
| (1,1535) | 1:165:A:PRO:HD2  | 1:166:A:VAL:H    | 18       | 0.16          |
| (1,1227) | 1:210:A:VAL:HA   | 1:213:A:MET:HG2  | 20       | 0.16          |
| (1,1207) | 1:168:A:GLN:HA   | 1:168:A:GLN:HE22 | 17       | 0.16          |
| (1,1135) | 1:137:A:PRO:HB3  | 1:212:A:GLN:HG2  | 12       | 0.16          |
| (1,1097) | 1:165:A:PRO:HB3  | 1:168:A:GLN:HG2  | 19       | 0.16          |
| (1,1015) | 1:152:A:GLU:HG2  | 1:153:A:ASN:HD22 | 5        | 0.16          |
| (1,1012) | 1:208:A:ARG:HA   | 1:212:A:GLN:HE22 | 18       | 0.16          |
| (1,957)  | 1:184:A:ILE:HD11 | 1:207:A:GLU:HG3  | 17       | 0.16          |
| (1,957)  | 1:184:A:ILE:HD12 | 1:207:A:GLU:HG3  | 17       | 0.16          |
| (1,957)  | 1:184:A:ILE:HD13 | 1:207:A:GLU:HG3  | 17       | 0.16          |
| (1,902)  | 1:147:A:ASP:HB2  | 1:148:A:ARG:HA   | 16       | 0.16          |
| (1,774)  | 1:206:A:MET:HB2  | 1:206:A:MET:HE1  | 15       | 0.16          |
| (1,774)  | 1:206:A:MET:HB2  | 1:206:A:MET:HE2  | 15       | 0.16          |
| (1,774)  | 1:206:A:MET:HB2  | 1:206:A:MET:HE3  | 15       | 0.16          |
| (1,574)  | 1:153:A:ASN:HB2  | 1:155:A:TYR:HE1  | 16       | 0.16          |
| (1,574)  | 1:153:A:ASN:HB2  | 1:155:A:TYR:HE2  | 16       | 0.16          |
| (1,501)  | 1:161:A:VAL:HA   | 1:162:A:TYR:HB3  | 3        | 0.16          |
| (1,496)  | 1:130:A:LEU:HA   | 1:162:A:TYR:HB2  | 7        | 0.16          |
| (1,392)  | 1:122:A:VAL:HG11 | 1:190:A:THR:HB   | 12       | 0.16          |
| (1,392)  | 1:122:A:VAL:HG12 | 1:190:A:THR:HB   | 12       | 0.16          |
| (1,392)  | 1:122:A:VAL:HG13 | 1:190:A:THR:HB   | 12       | 0.16          |
| (1,374)  | 1:209:A:VAL:HG21 | 1:210:A:VAL:H    | 10       | 0.16          |
| (1,374)  | 1:209:A:VAL:HG22 | 1:210:A:VAL:H    | 10       | 0.16          |
| (1,374)  | 1:209:A:VAL:HG23 | 1:210:A:VAL:H    | 10       | 0.16          |
| (1,244)  | 1:166:A:VAL:HG21 | 1:175:A:PHE:HB2  | 1        | 0.16          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,244)  | 1:166:A:VAL:HG22 | 1:175:A:PHE:HB2  | 1        | 0.16          |
| (1,244)  | 1:166:A:VAL:HG23 | 1:175:A:PHE:HB2  | 1        | 0.16          |
| (1,216)  | 1:216:A:THR:HG21 | 1:220:A:LYS:HG3  | 17       | 0.16          |
| (1,216)  | 1:216:A:THR:HG22 | 1:220:A:LYS:HG3  | 17       | 0.16          |
| (1,216)  | 1:216:A:THR:HG23 | 1:220:A:LYS:HG3  | 17       | 0.16          |
| (1,216)  | 1:216:A:THR:HG21 | 1:220:A:LYS:HG3  | 20       | 0.16          |
| (1,216)  | 1:216:A:THR:HG22 | 1:220:A:LYS:HG3  | 20       | 0.16          |
| (1,216)  | 1:216:A:THR:HG23 | 1:220:A:LYS:HG3  | 20       | 0.16          |
| (1,182)  | 1:216:A:THR:HB   | 1:220:A:LYS:HG3  | 3        | 0.16          |
| (1,150)  | 1:126:A:GLY:HA3  | 1:127:A:GLY:H    | 12       | 0.16          |
| (1,150)  | 1:126:A:GLY:HA3  | 1:127:A:GLY:H    | 16       | 0.16          |
| (1,89)   | 1:206:A:MET:HB3  | 1:210:A:VAL:HG21 | 11       | 0.16          |
| (1,89)   | 1:206:A:MET:HB3  | 1:210:A:VAL:HG22 | 11       | 0.16          |
| (1,89)   | 1:206:A:MET:HB3  | 1:210:A:VAL:HG23 | 11       | 0.16          |
| (1,77)   | 1:208:A:ARG:H    | 1:209:A:VAL:HG11 | 14       | 0.16          |
| (1,77)   | 1:208:A:ARG:H    | 1:209:A:VAL:HG12 | 14       | 0.16          |
| (1,77)   | 1:208:A:ARG:H    | 1:209:A:VAL:HG13 | 14       | 0.16          |
| (1,11)   | 1:139:A:ILE:HG13 | 1:209:A:VAL:H    | 12       | 0.16          |
| (1,2843) | 1:157:A:TYR:HE1  | 1:206:A:MET:HE1  | 16       | 0.15          |
| (1,2843) | 1:157:A:TYR:HE1  | 1:206:A:MET:HE2  | 16       | 0.15          |
| (1,2843) | 1:157:A:TYR:HE1  | 1:206:A:MET:HE3  | 16       | 0.15          |
| (1,2843) | 1:157:A:TYR:HE2  | 1:206:A:MET:HE1  | 16       | 0.15          |
| (1,2843) | 1:157:A:TYR:HE2  | 1:206:A:MET:HE2  | 16       | 0.15          |
| (1,2843) | 1:157:A:TYR:HE2  | 1:206:A:MET:HE3  | 16       | 0.15          |
| (1,2834) | 1:163:A:TYR:HE1  | 1:221:A:GLU:HG2  | 9        | 0.15          |
| (1,2834) | 1:163:A:TYR:HE2  | 1:221:A:GLU:HG2  | 9        | 0.15          |
| (1,2831) | 1:166:A:VAL:HG21 | 1:218:A:TYR:HE1  | 12       | 0.15          |
| (1,2831) | 1:166:A:VAL:HG21 | 1:218:A:TYR:HE2  | 12       | 0.15          |
| (1,2831) | 1:166:A:VAL:HG22 | 1:218:A:TYR:HE1  | 12       | 0.15          |
| (1,2831) | 1:166:A:VAL:HG22 | 1:218:A:TYR:HE2  | 12       | 0.15          |
| (1,2831) | 1:166:A:VAL:HG23 | 1:218:A:TYR:HE1  | 12       | 0.15          |
| (1,2831) | 1:166:A:VAL:HG23 | 1:218:A:TYR:HE2  | 12       | 0.15          |
| (1,2756) | 1:150:A:TYR:HE1  | 1:205:A:MET:HG2  | 7        | 0.15          |
| (1,2756) | 1:150:A:TYR:HE2  | 1:205:A:MET:HG2  | 7        | 0.15          |
| (1,2657) | 1:141:A:PHE:HE1  | 1:208:A:ARG:HB3  | 18       | 0.15          |
| (1,2657) | 1:141:A:PHE:HE2  | 1:208:A:ARG:HB3  | 18       | 0.15          |
| (1,2644) | 1:157:A:TYR:HD1  | 1:206:A:MET:HB2  | 3        | 0.15          |
| (1,2644) | 1:157:A:TYR:HD2  | 1:206:A:MET:HB2  | 3        | 0.15          |
| (1,2501) | 1:149:A:TYR:HD1  | 1:205:A:MET:HG2  | 8        | 0.15          |
| (1,2501) | 1:149:A:TYR:HD2  | 1:205:A:MET:HG2  | 8        | 0.15          |
| (1,2445) | 1:122:A:VAL:HG21 | 1:124:A:GLY:H    | 12       | 0.15          |
| (1,2445) | 1:122:A:VAL:HG22 | 1:124:A:GLY:H    | 12       | 0.15          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2445) | 1:122:A:VAL:HG23 | 1:124:A:GLY:H    | 12       | 0.15          |
| (1,1893) | 1:208:A:ARG:HB3  | 1:209:A:VAL:H    | 5        | 0.15          |
| (1,1746) | 1:184:A:ILE:H    | 1:184:A:ILE:HG12 | 3        | 0.15          |
| (1,1746) | 1:184:A:ILE:H    | 1:184:A:ILE:HG12 | 16       | 0.15          |
| (1,1717) | 1:222:A:SER:HB2  | 1:224:A:ALA:H    | 8        | 0.15          |
| (1,1501) | 1:137:A:PRO:HD3  | 1:209:A:VAL:HG21 | 4        | 0.15          |
| (1,1501) | 1:137:A:PRO:HD3  | 1:209:A:VAL:HG22 | 4        | 0.15          |
| (1,1501) | 1:137:A:PRO:HD3  | 1:209:A:VAL:HG23 | 4        | 0.15          |
| (1,1501) | 1:137:A:PRO:HD3  | 1:209:A:VAL:HG21 | 10       | 0.15          |
| (1,1501) | 1:137:A:PRO:HD3  | 1:209:A:VAL:HG22 | 10       | 0.15          |
| (1,1501) | 1:137:A:PRO:HD3  | 1:209:A:VAL:HG23 | 10       | 0.15          |
| (1,1340) | 1:160:A:GLN:HA   | 1:213:A:MET:HB2  | 5        | 0.15          |
| (1,1340) | 1:160:A:GLN:HA   | 1:213:A:MET:HB2  | 14       | 0.15          |
| (1,1227) | 1:210:A:VAL:HA   | 1:213:A:MET:HG2  | 11       | 0.15          |
| (1,1197) | 1:160:A:GLN:HB2  | 1:183:A:THR:HG21 | 10       | 0.15          |
| (1,1197) | 1:160:A:GLN:HB2  | 1:183:A:THR:HG22 | 10       | 0.15          |
| (1,1197) | 1:160:A:GLN:HB2  | 1:183:A:THR:HG23 | 10       | 0.15          |
| (1,1155) | 1:130:A:LEU:HB3  | 1:162:A:TYR:HA   | 15       | 0.15          |
| (1,1050) | 1:128:A:TYR:HA   | 1:129:A:MET:HG3  | 6        | 0.15          |
| (1,1003) | 1:139:A:ILE:HD11 | 1:212:A:GLN:HG3  | 8        | 0.15          |
| (1,1003) | 1:139:A:ILE:HD12 | 1:212:A:GLN:HG3  | 8        | 0.15          |
| (1,1003) | 1:139:A:ILE:HD13 | 1:212:A:GLN:HG3  | 8        | 0.15          |
| (1,983)  | 1:149:A:TYR:H    | 1:152:A:GLU:HG2  | 7        | 0.15          |
| (1,814)  | 1:226:A:TYR:HB2  | 1:227:A:ASP:HA   | 1        | 0.15          |
| (1,814)  | 1:226:A:TYR:HB2  | 1:227:A:ASP:HA   | 9        | 0.15          |
| (1,745)  | 1:122:A:VAL:HA   | 1:190:A:THR:HG21 | 8        | 0.15          |
| (1,745)  | 1:122:A:VAL:HA   | 1:190:A:THR:HG22 | 8        | 0.15          |
| (1,745)  | 1:122:A:VAL:HA   | 1:190:A:THR:HG23 | 8        | 0.15          |
| (1,735)  | 1:222:A:SER:HB2  | 1:223:A:GLN:HB2  | 15       | 0.15          |
| (1,735)  | 1:222:A:SER:HB2  | 1:223:A:GLN:HB3  | 15       | 0.15          |
| (1,591)  | 1:139:A:ILE:HD11 | 1:205:A:MET:HE1  | 12       | 0.15          |
| (1,591)  | 1:139:A:ILE:HD11 | 1:205:A:MET:HE2  | 12       | 0.15          |
| (1,591)  | 1:139:A:ILE:HD11 | 1:205:A:MET:HE3  | 12       | 0.15          |
| (1,591)  | 1:139:A:ILE:HD12 | 1:205:A:MET:HE1  | 12       | 0.15          |
| (1,591)  | 1:139:A:ILE:HD12 | 1:205:A:MET:HE2  | 12       | 0.15          |
| (1,591)  | 1:139:A:ILE:HD12 | 1:205:A:MET:HE3  | 12       | 0.15          |
| (1,591)  | 1:139:A:ILE:HD13 | 1:205:A:MET:HE1  | 12       | 0.15          |
| (1,591)  | 1:139:A:ILE:HD13 | 1:205:A:MET:HE2  | 12       | 0.15          |
| (1,591)  | 1:139:A:ILE:HD13 | 1:205:A:MET:HE3  | 12       | 0.15          |
| (1,579)  | 1:152:A:GLU:HB2  | 1:153:A:ASN:HB3  | 2        | 0.15          |
| (1,579)  | 1:152:A:GLU:HB3  | 1:153:A:ASN:HB3  | 2        | 0.15          |
| (1,574)  | 1:153:A:ASN:HB2  | 1:155:A:TYR:HE1  | 7        | 0.15          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,574) | 1:153:A:ASN:HB2  | 1:155:A:TYR:HE2  | 7        | 0.15          |
| (1,569) | 1:128:A:TYR:HE1  | 1:179:A:CYS:HB3  | 20       | 0.15          |
| (1,569) | 1:128:A:TYR:HE2  | 1:179:A:CYS:HB3  | 20       | 0.15          |
| (1,525) | 1:132:A:SER:HB2  | 1:160:A:GLN:HE21 | 7        | 0.15          |
| (1,501) | 1:161:A:VAL:HA   | 1:162:A:TYR:HB3  | 1        | 0.15          |
| (1,362) | 1:172:A:GLN:HG3  | 1:215:A:VAL:HG21 | 15       | 0.15          |
| (1,362) | 1:172:A:GLN:HG3  | 1:215:A:VAL:HG22 | 15       | 0.15          |
| (1,362) | 1:172:A:GLN:HG3  | 1:215:A:VAL:HG23 | 15       | 0.15          |
| (1,359) | 1:122:A:VAL:HG21 | 1:182:A:ILE:HG21 | 13       | 0.15          |
| (1,359) | 1:122:A:VAL:HG21 | 1:182:A:ILE:HG22 | 13       | 0.15          |
| (1,359) | 1:122:A:VAL:HG21 | 1:182:A:ILE:HG23 | 13       | 0.15          |
| (1,359) | 1:122:A:VAL:HG22 | 1:182:A:ILE:HG21 | 13       | 0.15          |
| (1,359) | 1:122:A:VAL:HG22 | 1:182:A:ILE:HG22 | 13       | 0.15          |
| (1,359) | 1:122:A:VAL:HG22 | 1:182:A:ILE:HG23 | 13       | 0.15          |
| (1,359) | 1:122:A:VAL:HG23 | 1:182:A:ILE:HG21 | 13       | 0.15          |
| (1,359) | 1:122:A:VAL:HG23 | 1:182:A:ILE:HG22 | 13       | 0.15          |
| (1,359) | 1:122:A:VAL:HG23 | 1:182:A:ILE:HG23 | 13       | 0.15          |
| (1,359) | 1:122:A:VAL:HG21 | 1:182:A:ILE:HG21 | 17       | 0.15          |
| (1,359) | 1:122:A:VAL:HG21 | 1:182:A:ILE:HG22 | 17       | 0.15          |
| (1,359) | 1:122:A:VAL:HG21 | 1:182:A:ILE:HG23 | 17       | 0.15          |
| (1,359) | 1:122:A:VAL:HG22 | 1:182:A:ILE:HG21 | 17       | 0.15          |
| (1,359) | 1:122:A:VAL:HG22 | 1:182:A:ILE:HG22 | 17       | 0.15          |
| (1,359) | 1:122:A:VAL:HG22 | 1:182:A:ILE:HG23 | 17       | 0.15          |
| (1,359) | 1:122:A:VAL:HG23 | 1:182:A:ILE:HG21 | 17       | 0.15          |
| (1,359) | 1:122:A:VAL:HG23 | 1:182:A:ILE:HG22 | 17       | 0.15          |
| (1,359) | 1:122:A:VAL:HG23 | 1:182:A:ILE:HG23 | 17       | 0.15          |
| (1,333) | 1:172:A:GLN:HE22 | 1:215:A:VAL:HG21 | 8        | 0.15          |
| (1,333) | 1:172:A:GLN:HE22 | 1:215:A:VAL:HG22 | 8        | 0.15          |
| (1,333) | 1:172:A:GLN:HE22 | 1:215:A:VAL:HG23 | 8        | 0.15          |
| (1,307) | 1:176:A:VAL:HG11 | 1:215:A:VAL:HG21 | 9        | 0.15          |
| (1,307) | 1:176:A:VAL:HG11 | 1:215:A:VAL:HG22 | 9        | 0.15          |
| (1,307) | 1:176:A:VAL:HG11 | 1:215:A:VAL:HG23 | 9        | 0.15          |
| (1,307) | 1:176:A:VAL:HG12 | 1:215:A:VAL:HG21 | 9        | 0.15          |
| (1,307) | 1:176:A:VAL:HG12 | 1:215:A:VAL:HG22 | 9        | 0.15          |
| (1,307) | 1:176:A:VAL:HG12 | 1:215:A:VAL:HG23 | 9        | 0.15          |
| (1,307) | 1:176:A:VAL:HG13 | 1:215:A:VAL:HG21 | 9        | 0.15          |
| (1,307) | 1:176:A:VAL:HG13 | 1:215:A:VAL:HG22 | 9        | 0.15          |
| (1,307) | 1:176:A:VAL:HG13 | 1:215:A:VAL:HG23 | 9        | 0.15          |
| (1,288) | 1:192:A:THR:HG21 | 1:196:A:GLU:HB2  | 6        | 0.15          |
| (1,288) | 1:192:A:THR:HG21 | 1:196:A:GLU:HB3  | 6        | 0.15          |
| (1,288) | 1:192:A:THR:HG22 | 1:196:A:GLU:HB2  | 6        | 0.15          |
| (1,288) | 1:192:A:THR:HG22 | 1:196:A:GLU:HB3  | 6        | 0.15          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,288)  | 1:192:A:THR:HG23 | 1:196:A:GLU:HB2  | 6        | 0.15          |
| (1,288)  | 1:192:A:THR:HG23 | 1:196:A:GLU:HB3  | 6        | 0.15          |
| (1,288)  | 1:192:A:THR:HG21 | 1:196:A:GLU:HB2  | 11       | 0.15          |
| (1,288)  | 1:192:A:THR:HG21 | 1:196:A:GLU:HB3  | 11       | 0.15          |
| (1,288)  | 1:192:A:THR:HG22 | 1:196:A:GLU:HB2  | 11       | 0.15          |
| (1,288)  | 1:192:A:THR:HG22 | 1:196:A:GLU:HB3  | 11       | 0.15          |
| (1,288)  | 1:192:A:THR:HG23 | 1:196:A:GLU:HB2  | 11       | 0.15          |
| (1,288)  | 1:192:A:THR:HG23 | 1:196:A:GLU:HB3  | 11       | 0.15          |
| (1,288)  | 1:192:A:THR:HG21 | 1:196:A:GLU:HB2  | 12       | 0.15          |
| (1,288)  | 1:192:A:THR:HG21 | 1:196:A:GLU:HB3  | 12       | 0.15          |
| (1,288)  | 1:192:A:THR:HG22 | 1:196:A:GLU:HB2  | 12       | 0.15          |
| (1,288)  | 1:192:A:THR:HG22 | 1:196:A:GLU:HB3  | 12       | 0.15          |
| (1,288)  | 1:192:A:THR:HG23 | 1:196:A:GLU:HB2  | 12       | 0.15          |
| (1,288)  | 1:192:A:THR:HG23 | 1:196:A:GLU:HB3  | 12       | 0.15          |
| (1,196)  | 1:161:A:VAL:HG21 | 1:216:A:THR:HG21 | 15       | 0.15          |
| (1,196)  | 1:161:A:VAL:HG21 | 1:216:A:THR:HG22 | 15       | 0.15          |
| (1,196)  | 1:161:A:VAL:HG21 | 1:216:A:THR:HG23 | 15       | 0.15          |
| (1,196)  | 1:161:A:VAL:HG22 | 1:216:A:THR:HG21 | 15       | 0.15          |
| (1,196)  | 1:161:A:VAL:HG22 | 1:216:A:THR:HG22 | 15       | 0.15          |
| (1,196)  | 1:161:A:VAL:HG22 | 1:216:A:THR:HG23 | 15       | 0.15          |
| (1,196)  | 1:161:A:VAL:HG23 | 1:216:A:THR:HG21 | 15       | 0.15          |
| (1,196)  | 1:161:A:VAL:HG23 | 1:216:A:THR:HG22 | 15       | 0.15          |
| (1,196)  | 1:161:A:VAL:HG23 | 1:216:A:THR:HG23 | 15       | 0.15          |
| (1,150)  | 1:126:A:GLY:HA3  | 1:127:A:GLY:H    | 3        | 0.15          |
| (1,150)  | 1:126:A:GLY:HA3  | 1:127:A:GLY:H    | 9        | 0.15          |
| (1,150)  | 1:126:A:GLY:HA3  | 1:127:A:GLY:H    | 10       | 0.15          |
| (1,150)  | 1:126:A:GLY:HA3  | 1:127:A:GLY:H    | 11       | 0.15          |
| (1,150)  | 1:126:A:GLY:HA3  | 1:127:A:GLY:H    | 13       | 0.15          |
| (1,150)  | 1:126:A:GLY:HA3  | 1:127:A:GLY:H    | 18       | 0.15          |
| (1,89)   | 1:206:A:MET:HB3  | 1:210:A:VAL:HG21 | 12       | 0.15          |
| (1,89)   | 1:206:A:MET:HB3  | 1:210:A:VAL:HG22 | 12       | 0.15          |
| (1,89)   | 1:206:A:MET:HB3  | 1:210:A:VAL:HG23 | 12       | 0.15          |
| (1,79)   | 1:138:A:MET:H    | 1:209:A:VAL:HG11 | 16       | 0.15          |
| (1,79)   | 1:138:A:MET:H    | 1:209:A:VAL:HG12 | 16       | 0.15          |
| (1,79)   | 1:138:A:MET:H    | 1:209:A:VAL:HG13 | 16       | 0.15          |
| (1,32)   | 1:219:A:GLN:HB3  | 1:220:A:LYS:HG3  | 4        | 0.15          |
| (1,32)   | 1:219:A:GLN:HB3  | 1:220:A:LYS:HG3  | 8        | 0.15          |
| (1,32)   | 1:219:A:GLN:HB3  | 1:220:A:LYS:HG3  | 11       | 0.15          |
| (1,32)   | 1:219:A:GLN:HB3  | 1:220:A:LYS:HG3  | 16       | 0.15          |
| (1,31)   | 1:219:A:GLN:HA   | 1:220:A:LYS:HG3  | 15       | 0.15          |
| (1,31)   | 1:219:A:GLN:HA   | 1:220:A:LYS:HG3  | 19       | 0.15          |
| (1,2736) | 1:184:A:ILE:HG13 | 1:187:A:HIS:HD2  | 7        | 0.14          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2683) | 1:139:A:ILE:HG12 | 1:141:A:PHE:HZ   | 1        | 0.14          |
| (1,2593) | 1:175:A:PHE:HE1  | 1:221:A:GLU:HG2  | 10       | 0.14          |
| (1,2593) | 1:175:A:PHE:HE2  | 1:221:A:GLU:HG2  | 10       | 0.14          |
| (1,2553) | 1:126:A:GLY:HA2  | 1:128:A:TYR:HD1  | 6        | 0.14          |
| (1,2553) | 1:126:A:GLY:HA2  | 1:128:A:TYR:HD2  | 6        | 0.14          |
| (1,2553) | 1:126:A:GLY:HA2  | 1:128:A:TYR:HD1  | 13       | 0.14          |
| (1,2553) | 1:126:A:GLY:HA2  | 1:128:A:TYR:HD2  | 13       | 0.14          |
| (1,2520) | 1:154:A:MET:HE1  | 1:155:A:TYR:HD1  | 2        | 0.14          |
| (1,2520) | 1:154:A:MET:HE1  | 1:155:A:TYR:HD2  | 2        | 0.14          |
| (1,2520) | 1:154:A:MET:HE2  | 1:155:A:TYR:HD1  | 2        | 0.14          |
| (1,2520) | 1:154:A:MET:HE2  | 1:155:A:TYR:HD2  | 2        | 0.14          |
| (1,2520) | 1:154:A:MET:HE3  | 1:155:A:TYR:HD1  | 2        | 0.14          |
| (1,2520) | 1:154:A:MET:HE3  | 1:155:A:TYR:HD2  | 2        | 0.14          |
| (1,2520) | 1:154:A:MET:HE1  | 1:155:A:TYR:HD1  | 14       | 0.14          |
| (1,2520) | 1:154:A:MET:HE1  | 1:155:A:TYR:HD2  | 14       | 0.14          |
| (1,2520) | 1:154:A:MET:HE2  | 1:155:A:TYR:HD1  | 14       | 0.14          |
| (1,2520) | 1:154:A:MET:HE2  | 1:155:A:TYR:HD2  | 14       | 0.14          |
| (1,2520) | 1:154:A:MET:HE3  | 1:155:A:TYR:HD1  | 14       | 0.14          |
| (1,2520) | 1:154:A:MET:HE3  | 1:155:A:TYR:HD2  | 14       | 0.14          |
| (1,2474) | 1:168:A:GLN:HG2  | 1:169:A:TYR:HD1  | 1        | 0.14          |
| (1,2474) | 1:168:A:GLN:HG2  | 1:169:A:TYR:HD2  | 1        | 0.14          |
| (1,2474) | 1:168:A:GLN:HG2  | 1:169:A:TYR:HD1  | 8        | 0.14          |
| (1,2474) | 1:168:A:GLN:HG2  | 1:169:A:TYR:HD2  | 8        | 0.14          |
| (1,2234) | 1:221:A:GLU:HG3  | 1:222:A:SER:H    | 7        | 0.14          |
| (1,2234) | 1:221:A:GLU:HG3  | 1:222:A:SER:H    | 17       | 0.14          |
| (1,2160) | 1:189:A:VAL:HG11 | 1:193:A:THR:H    | 11       | 0.14          |
| (1,2160) | 1:189:A:VAL:HG12 | 1:193:A:THR:H    | 11       | 0.14          |
| (1,2160) | 1:189:A:VAL:HG13 | 1:193:A:THR:H    | 11       | 0.14          |
| (1,2095) | 1:166:A:VAL:HG21 | 1:169:A:TYR:H    | 17       | 0.14          |
| (1,2095) | 1:166:A:VAL:HG22 | 1:169:A:TYR:H    | 17       | 0.14          |
| (1,2095) | 1:166:A:VAL:HG23 | 1:169:A:TYR:H    | 17       | 0.14          |
| (1,1907) | 1:178:A:ASP:HB2  | 1:179:A:CYS:H    | 2        | 0.14          |
| (1,1746) | 1:184:A:ILE:H    | 1:184:A:ILE:HG12 | 2        | 0.14          |
| (1,1495) | 1:212:A:GLN:HB2  | 1:216:A:THR:H    | 16       | 0.14          |
| (1,1340) | 1:160:A:GLN:HA   | 1:213:A:MET:HB2  | 7        | 0.14          |
| (1,1340) | 1:160:A:GLN:HA   | 1:213:A:MET:HB2  | 16       | 0.14          |
| (1,1340) | 1:160:A:GLN:HA   | 1:213:A:MET:HB2  | 18       | 0.14          |
| (1,1155) | 1:130:A:LEU:HB3  | 1:162:A:TYR:HA   | 19       | 0.14          |
| (1,1152) | 1:205:A:MET:HA   | 1:205:A:MET:HG3  | 8        | 0.14          |
| (1,1101) | 1:160:A:GLN:H    | 1:213:A:MET:HB3  | 7        | 0.14          |
| (1,1095) | 1:165:A:PRO:HA   | 1:168:A:GLN:HG2  | 3        | 0.14          |
| (1,1026) | 1:186:A:GLN:HB2  | 1:187:A:HIS:HA   | 6        | 0.14          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1026) | 1:186:A:GLN:HB2  | 1:187:A:HIS:HA   | 16       | 0.14          |
| (1,1015) | 1:152:A:GLU:HG2  | 1:153:A:ASN:HD22 | 1        | 0.14          |
| (1,881)  | 1:145:A:TRP:HE3  | 1:146:A:GLU:HG3  | 8        | 0.14          |
| (1,873)  | 1:146:A:GLU:HA   | 1:150:A:TYR:HB3  | 8        | 0.14          |
| (1,784)  | 1:166:A:VAL:HG11 | 1:218:A:TYR:HA   | 12       | 0.14          |
| (1,784)  | 1:166:A:VAL:HG12 | 1:218:A:TYR:HA   | 12       | 0.14          |
| (1,784)  | 1:166:A:VAL:HG13 | 1:218:A:TYR:HA   | 12       | 0.14          |
| (1,745)  | 1:122:A:VAL:HA   | 1:190:A:THR:HG21 | 6        | 0.14          |
| (1,745)  | 1:122:A:VAL:HA   | 1:190:A:THR:HG22 | 6        | 0.14          |
| (1,745)  | 1:122:A:VAL:HA   | 1:190:A:THR:HG23 | 6        | 0.14          |
| (1,745)  | 1:122:A:VAL:HA   | 1:190:A:THR:HG21 | 15       | 0.14          |
| (1,745)  | 1:122:A:VAL:HA   | 1:190:A:THR:HG22 | 15       | 0.14          |
| (1,745)  | 1:122:A:VAL:HA   | 1:190:A:THR:HG23 | 15       | 0.14          |
| (1,658)  | 1:154:A:MET:HG3  | 1:154:A:MET:HE1  | 1        | 0.14          |
| (1,658)  | 1:154:A:MET:HG3  | 1:154:A:MET:HE2  | 1        | 0.14          |
| (1,658)  | 1:154:A:MET:HG3  | 1:154:A:MET:HE3  | 1        | 0.14          |
| (1,658)  | 1:154:A:MET:HG3  | 1:154:A:MET:HE1  | 13       | 0.14          |
| (1,658)  | 1:154:A:MET:HG3  | 1:154:A:MET:HE2  | 13       | 0.14          |
| (1,658)  | 1:154:A:MET:HG3  | 1:154:A:MET:HE3  | 13       | 0.14          |
| (1,497)  | 1:128:A:TYR:HB2  | 1:162:A:TYR:HB2  | 4        | 0.14          |
| (1,496)  | 1:130:A:LEU:HA   | 1:162:A:TYR:HB2  | 9        | 0.14          |
| (1,445)  | 1:180:A:VAL:HA   | 1:184:A:ILE:HG12 | 17       | 0.14          |
| (1,359)  | 1:122:A:VAL:HG21 | 1:182:A:ILE:HG21 | 20       | 0.14          |
| (1,359)  | 1:122:A:VAL:HG21 | 1:182:A:ILE:HG22 | 20       | 0.14          |
| (1,359)  | 1:122:A:VAL:HG21 | 1:182:A:ILE:HG23 | 20       | 0.14          |
| (1,359)  | 1:122:A:VAL:HG22 | 1:182:A:ILE:HG21 | 20       | 0.14          |
| (1,359)  | 1:122:A:VAL:HG22 | 1:182:A:ILE:HG22 | 20       | 0.14          |
| (1,359)  | 1:122:A:VAL:HG22 | 1:182:A:ILE:HG23 | 20       | 0.14          |
| (1,359)  | 1:122:A:VAL:HG23 | 1:182:A:ILE:HG21 | 20       | 0.14          |
| (1,359)  | 1:122:A:VAL:HG23 | 1:182:A:ILE:HG22 | 20       | 0.14          |
| (1,359)  | 1:122:A:VAL:HG23 | 1:182:A:ILE:HG23 | 20       | 0.14          |
| (1,350)  | 1:122:A:VAL:HG21 | 1:123:A:GLY:H    | 8        | 0.14          |
| (1,350)  | 1:122:A:VAL:HG22 | 1:123:A:GLY:H    | 8        | 0.14          |
| (1,350)  | 1:122:A:VAL:HG23 | 1:123:A:GLY:H    | 8        | 0.14          |
| (1,348)  | 1:122:A:VAL:HG21 | 1:124:A:GLY:HA2  | 13       | 0.14          |
| (1,348)  | 1:122:A:VAL:HG21 | 1:124:A:GLY:HA3  | 13       | 0.14          |
| (1,348)  | 1:122:A:VAL:HG22 | 1:124:A:GLY:HA2  | 13       | 0.14          |
| (1,348)  | 1:122:A:VAL:HG22 | 1:124:A:GLY:HA3  | 13       | 0.14          |
| (1,348)  | 1:122:A:VAL:HG23 | 1:124:A:GLY:HA2  | 13       | 0.14          |
| (1,348)  | 1:122:A:VAL:HG23 | 1:124:A:GLY:HA3  | 13       | 0.14          |
| (1,307)  | 1:176:A:VAL:HG11 | 1:215:A:VAL:HG21 | 15       | 0.14          |
| (1,307)  | 1:176:A:VAL:HG11 | 1:215:A:VAL:HG22 | 15       | 0.14          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,307) | 1:176:A:VAL:HG11 | 1:215:A:VAL:HG23 | 15       | 0.14          |
| (1,307) | 1:176:A:VAL:HG12 | 1:215:A:VAL:HG21 | 15       | 0.14          |
| (1,307) | 1:176:A:VAL:HG12 | 1:215:A:VAL:HG22 | 15       | 0.14          |
| (1,307) | 1:176:A:VAL:HG12 | 1:215:A:VAL:HG23 | 15       | 0.14          |
| (1,307) | 1:176:A:VAL:HG13 | 1:215:A:VAL:HG21 | 15       | 0.14          |
| (1,307) | 1:176:A:VAL:HG13 | 1:215:A:VAL:HG22 | 15       | 0.14          |
| (1,307) | 1:176:A:VAL:HG13 | 1:215:A:VAL:HG23 | 15       | 0.14          |
| (1,307) | 1:176:A:VAL:HG11 | 1:215:A:VAL:HG21 | 20       | 0.14          |
| (1,307) | 1:176:A:VAL:HG11 | 1:215:A:VAL:HG22 | 20       | 0.14          |
| (1,307) | 1:176:A:VAL:HG11 | 1:215:A:VAL:HG23 | 20       | 0.14          |
| (1,307) | 1:176:A:VAL:HG12 | 1:215:A:VAL:HG21 | 20       | 0.14          |
| (1,307) | 1:176:A:VAL:HG12 | 1:215:A:VAL:HG22 | 20       | 0.14          |
| (1,307) | 1:176:A:VAL:HG12 | 1:215:A:VAL:HG23 | 20       | 0.14          |
| (1,307) | 1:176:A:VAL:HG13 | 1:215:A:VAL:HG21 | 20       | 0.14          |
| (1,307) | 1:176:A:VAL:HG13 | 1:215:A:VAL:HG22 | 20       | 0.14          |
| (1,307) | 1:176:A:VAL:HG13 | 1:215:A:VAL:HG23 | 20       | 0.14          |
| (1,296) | 1:187:A:HIS:HB3  | 1:190:A:THR:HG21 | 8        | 0.14          |
| (1,296) | 1:187:A:HIS:HB3  | 1:190:A:THR:HG22 | 8        | 0.14          |
| (1,296) | 1:187:A:HIS:HB3  | 1:190:A:THR:HG23 | 8        | 0.14          |
| (1,288) | 1:192:A:THR:HG21 | 1:196:A:GLU:HB2  | 1        | 0.14          |
| (1,288) | 1:192:A:THR:HG21 | 1:196:A:GLU:HB3  | 1        | 0.14          |
| (1,288) | 1:192:A:THR:HG22 | 1:196:A:GLU:HB2  | 1        | 0.14          |
| (1,288) | 1:192:A:THR:HG22 | 1:196:A:GLU:HB3  | 1        | 0.14          |
| (1,288) | 1:192:A:THR:HG23 | 1:196:A:GLU:HB2  | 1        | 0.14          |
| (1,288) | 1:192:A:THR:HG23 | 1:196:A:GLU:HB3  | 1        | 0.14          |
| (1,288) | 1:192:A:THR:HG21 | 1:196:A:GLU:HB2  | 3        | 0.14          |
| (1,288) | 1:192:A:THR:HG21 | 1:196:A:GLU:HB3  | 3        | 0.14          |
| (1,288) | 1:192:A:THR:HG22 | 1:196:A:GLU:HB2  | 3        | 0.14          |
| (1,288) | 1:192:A:THR:HG22 | 1:196:A:GLU:HB3  | 3        | 0.14          |
| (1,288) | 1:192:A:THR:HG23 | 1:196:A:GLU:HB2  | 3        | 0.14          |
| (1,288) | 1:192:A:THR:HG23 | 1:196:A:GLU:HB3  | 3        | 0.14          |
| (1,288) | 1:192:A:THR:HG21 | 1:196:A:GLU:HB2  | 5        | 0.14          |
| (1,288) | 1:192:A:THR:HG21 | 1:196:A:GLU:HB3  | 5        | 0.14          |
| (1,288) | 1:192:A:THR:HG22 | 1:196:A:GLU:HB2  | 5        | 0.14          |
| (1,288) | 1:192:A:THR:HG22 | 1:196:A:GLU:HB3  | 5        | 0.14          |
| (1,288) | 1:192:A:THR:HG23 | 1:196:A:GLU:HB2  | 5        | 0.14          |
| (1,288) | 1:192:A:THR:HG23 | 1:196:A:GLU:HB3  | 5        | 0.14          |
| (1,288) | 1:192:A:THR:HG21 | 1:196:A:GLU:HB2  | 7        | 0.14          |
| (1,288) | 1:192:A:THR:HG21 | 1:196:A:GLU:HB3  | 7        | 0.14          |
| (1,288) | 1:192:A:THR:HG22 | 1:196:A:GLU:HB2  | 7        | 0.14          |
| (1,288) | 1:192:A:THR:HG22 | 1:196:A:GLU:HB3  | 7        | 0.14          |
| (1,288) | 1:192:A:THR:HG23 | 1:196:A:GLU:HB2  | 7        | 0.14          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,288)  | 1:192:A:THR:HG23 | 1:196:A:GLU:HB3  | 7        | 0.14          |
| (1,288)  | 1:192:A:THR:HG21 | 1:196:A:GLU:HB2  | 10       | 0.14          |
| (1,288)  | 1:192:A:THR:HG21 | 1:196:A:GLU:HB3  | 10       | 0.14          |
| (1,288)  | 1:192:A:THR:HG22 | 1:196:A:GLU:HB2  | 10       | 0.14          |
| (1,288)  | 1:192:A:THR:HG22 | 1:196:A:GLU:HB3  | 10       | 0.14          |
| (1,288)  | 1:192:A:THR:HG23 | 1:196:A:GLU:HB2  | 10       | 0.14          |
| (1,288)  | 1:192:A:THR:HG23 | 1:196:A:GLU:HB3  | 10       | 0.14          |
| (1,288)  | 1:192:A:THR:HG21 | 1:196:A:GLU:HB2  | 14       | 0.14          |
| (1,288)  | 1:192:A:THR:HG21 | 1:196:A:GLU:HB3  | 14       | 0.14          |
| (1,288)  | 1:192:A:THR:HG22 | 1:196:A:GLU:HB2  | 14       | 0.14          |
| (1,288)  | 1:192:A:THR:HG22 | 1:196:A:GLU:HB3  | 14       | 0.14          |
| (1,288)  | 1:192:A:THR:HG23 | 1:196:A:GLU:HB2  | 14       | 0.14          |
| (1,288)  | 1:192:A:THR:HG23 | 1:196:A:GLU:HB3  | 14       | 0.14          |
| (1,288)  | 1:192:A:THR:HG21 | 1:196:A:GLU:HB2  | 15       | 0.14          |
| (1,288)  | 1:192:A:THR:HG21 | 1:196:A:GLU:HB3  | 15       | 0.14          |
| (1,288)  | 1:192:A:THR:HG22 | 1:196:A:GLU:HB2  | 15       | 0.14          |
| (1,288)  | 1:192:A:THR:HG22 | 1:196:A:GLU:HB3  | 15       | 0.14          |
| (1,288)  | 1:192:A:THR:HG23 | 1:196:A:GLU:HB2  | 15       | 0.14          |
| (1,288)  | 1:192:A:THR:HG23 | 1:196:A:GLU:HB3  | 15       | 0.14          |
| (1,288)  | 1:192:A:THR:HG21 | 1:196:A:GLU:HB2  | 20       | 0.14          |
| (1,288)  | 1:192:A:THR:HG21 | 1:196:A:GLU:HB3  | 20       | 0.14          |
| (1,288)  | 1:192:A:THR:HG22 | 1:196:A:GLU:HB2  | 20       | 0.14          |
| (1,288)  | 1:192:A:THR:HG22 | 1:196:A:GLU:HB3  | 20       | 0.14          |
| (1,288)  | 1:192:A:THR:HG23 | 1:196:A:GLU:HB2  | 20       | 0.14          |
| (1,288)  | 1:192:A:THR:HG23 | 1:196:A:GLU:HB3  | 20       | 0.14          |
| (1,260)  | 1:186:A:GLN:HB2  | 1:190:A:THR:HG21 | 6        | 0.14          |
| (1,260)  | 1:186:A:GLN:HB2  | 1:190:A:THR:HG22 | 6        | 0.14          |
| (1,260)  | 1:186:A:GLN:HB2  | 1:190:A:THR:HG23 | 6        | 0.14          |
| (1,202)  | 1:183:A:THR:HG21 | 1:184:A:ILE:HG12 | 18       | 0.14          |
| (1,202)  | 1:183:A:THR:HG22 | 1:184:A:ILE:HG12 | 18       | 0.14          |
| (1,202)  | 1:183:A:THR:HG23 | 1:184:A:ILE:HG12 | 18       | 0.14          |
| (1,150)  | 1:126:A:GLY:HA3  | 1:127:A:GLY:H    | 1        | 0.14          |
| (1,150)  | 1:126:A:GLY:HA3  | 1:127:A:GLY:H    | 2        | 0.14          |
| (1,150)  | 1:126:A:GLY:HA3  | 1:127:A:GLY:H    | 5        | 0.14          |
| (1,89)   | 1:206:A:MET:HB3  | 1:210:A:VAL:HG21 | 15       | 0.14          |
| (1,89)   | 1:206:A:MET:HB3  | 1:210:A:VAL:HG22 | 15       | 0.14          |
| (1,89)   | 1:206:A:MET:HB3  | 1:210:A:VAL:HG23 | 15       | 0.14          |
| (1,32)   | 1:219:A:GLN:HB3  | 1:220:A:LYS:HG3  | 9        | 0.14          |
| (1,32)   | 1:219:A:GLN:HB3  | 1:220:A:LYS:HG3  | 12       | 0.14          |
| (1,32)   | 1:219:A:GLN:HB3  | 1:220:A:LYS:HG3  | 15       | 0.14          |
| (1,2843) | 1:157:A:TYR:HE1  | 1:206:A:MET:HE1  | 9        | 0.13          |
| (1,2843) | 1:157:A:TYR:HE1  | 1:206:A:MET:HE2  | 9        | 0.13          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2843) | 1:157:A:TYR:HE1 | 1:206:A:MET:HE3 | 9        | 0.13          |
| (1,2843) | 1:157:A:TYR:HE2 | 1:206:A:MET:HE1 | 9        | 0.13          |
| (1,2843) | 1:157:A:TYR:HE2 | 1:206:A:MET:HE2 | 9        | 0.13          |
| (1,2843) | 1:157:A:TYR:HE2 | 1:206:A:MET:HE3 | 9        | 0.13          |
| (1,2520) | 1:154:A:MET:HE1 | 1:155:A:TYR:HD1 | 6        | 0.13          |
| (1,2520) | 1:154:A:MET:HE1 | 1:155:A:TYR:HD2 | 6        | 0.13          |
| (1,2520) | 1:154:A:MET:HE2 | 1:155:A:TYR:HD1 | 6        | 0.13          |
| (1,2520) | 1:154:A:MET:HE2 | 1:155:A:TYR:HD2 | 6        | 0.13          |
| (1,2520) | 1:154:A:MET:HE3 | 1:155:A:TYR:HD1 | 6        | 0.13          |
| (1,2520) | 1:154:A:MET:HE3 | 1:155:A:TYR:HD2 | 6        | 0.13          |
| (1,2520) | 1:154:A:MET:HE1 | 1:155:A:TYR:HD1 | 9        | 0.13          |
| (1,2520) | 1:154:A:MET:HE1 | 1:155:A:TYR:HD2 | 9        | 0.13          |
| (1,2520) | 1:154:A:MET:HE2 | 1:155:A:TYR:HD1 | 9        | 0.13          |
| (1,2520) | 1:154:A:MET:HE2 | 1:155:A:TYR:HD2 | 9        | 0.13          |
| (1,2520) | 1:154:A:MET:HE3 | 1:155:A:TYR:HD1 | 9        | 0.13          |
| (1,2520) | 1:154:A:MET:HE3 | 1:155:A:TYR:HD2 | 9        | 0.13          |
| (1,2520) | 1:154:A:MET:HE1 | 1:155:A:TYR:HD1 | 12       | 0.13          |
| (1,2520) | 1:154:A:MET:HE1 | 1:155:A:TYR:HD2 | 12       | 0.13          |
| (1,2520) | 1:154:A:MET:HE2 | 1:155:A:TYR:HD1 | 12       | 0.13          |
| (1,2520) | 1:154:A:MET:HE2 | 1:155:A:TYR:HD2 | 12       | 0.13          |
| (1,2520) | 1:154:A:MET:HE3 | 1:155:A:TYR:HD1 | 12       | 0.13          |
| (1,2520) | 1:154:A:MET:HE3 | 1:155:A:TYR:HD2 | 12       | 0.13          |
| (1,2520) | 1:154:A:MET:HE1 | 1:155:A:TYR:HD1 | 15       | 0.13          |
| (1,2520) | 1:154:A:MET:HE1 | 1:155:A:TYR:HD2 | 15       | 0.13          |
| (1,2520) | 1:154:A:MET:HE2 | 1:155:A:TYR:HD1 | 15       | 0.13          |
| (1,2520) | 1:154:A:MET:HE2 | 1:155:A:TYR:HD2 | 15       | 0.13          |
| (1,2520) | 1:154:A:MET:HE3 | 1:155:A:TYR:HD1 | 15       | 0.13          |
| (1,2520) | 1:154:A:MET:HE3 | 1:155:A:TYR:HD2 | 15       | 0.13          |
| (1,2520) | 1:154:A:MET:HE1 | 1:155:A:TYR:HD1 | 18       | 0.13          |
| (1,2520) | 1:154:A:MET:HE1 | 1:155:A:TYR:HD2 | 18       | 0.13          |
| (1,2520) | 1:154:A:MET:HE2 | 1:155:A:TYR:HD1 | 18       | 0.13          |
| (1,2520) | 1:154:A:MET:HE2 | 1:155:A:TYR:HD2 | 18       | 0.13          |
| (1,2520) | 1:154:A:MET:HE3 | 1:155:A:TYR:HD1 | 18       | 0.13          |
| (1,2520) | 1:154:A:MET:HE3 | 1:155:A:TYR:HD2 | 18       | 0.13          |
| (1,2520) | 1:154:A:MET:HE1 | 1:155:A:TYR:HD1 | 19       | 0.13          |
| (1,2520) | 1:154:A:MET:HE1 | 1:155:A:TYR:HD2 | 19       | 0.13          |
| (1,2520) | 1:154:A:MET:HE2 | 1:155:A:TYR:HD1 | 19       | 0.13          |
| (1,2520) | 1:154:A:MET:HE2 | 1:155:A:TYR:HD2 | 19       | 0.13          |
| (1,2520) | 1:154:A:MET:HE3 | 1:155:A:TYR:HD1 | 19       | 0.13          |
| (1,2520) | 1:154:A:MET:HE3 | 1:155:A:TYR:HD2 | 19       | 0.13          |
| (1,2520) | 1:154:A:MET:HE1 | 1:155:A:TYR:HD1 | 20       | 0.13          |
| (1,2520) | 1:154:A:MET:HE1 | 1:155:A:TYR:HD2 | 20       | 0.13          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2520) | 1:154:A:MET:HE2  | 1:155:A:TYR:HD1  | 20       | 0.13          |
| (1,2520) | 1:154:A:MET:HE2  | 1:155:A:TYR:HD2  | 20       | 0.13          |
| (1,2520) | 1:154:A:MET:HE3  | 1:155:A:TYR:HD1  | 20       | 0.13          |
| (1,2520) | 1:154:A:MET:HE3  | 1:155:A:TYR:HD2  | 20       | 0.13          |
| (1,2474) | 1:168:A:GLN:HG2  | 1:169:A:TYR:HD1  | 16       | 0.13          |
| (1,2474) | 1:168:A:GLN:HG2  | 1:169:A:TYR:HD2  | 16       | 0.13          |
| (1,2464) | 1:169:A:TYR:HD1  | 1:218:A:TYR:HE1  | 12       | 0.13          |
| (1,2464) | 1:169:A:TYR:HD1  | 1:218:A:TYR:HE2  | 12       | 0.13          |
| (1,2464) | 1:169:A:TYR:HD2  | 1:218:A:TYR:HE1  | 12       | 0.13          |
| (1,2464) | 1:169:A:TYR:HD2  | 1:218:A:TYR:HE2  | 12       | 0.13          |
| (1,2322) | 1:130:A:LEU:HG   | 1:160:A:GLN:HE22 | 13       | 0.13          |
| (1,2152) | 1:134:A:MET:HB3  | 1:135:A:SER:H    | 17       | 0.13          |
| (1,1968) | 1:205:A:MET:H    | 1:205:A:MET:HG3  | 7        | 0.13          |
| (1,1968) | 1:205:A:MET:H    | 1:205:A:MET:HG3  | 10       | 0.13          |
| (1,1746) | 1:184:A:ILE:H    | 1:184:A:ILE:HG12 | 6        | 0.13          |
| (1,1679) | 1:122:A:VAL:HG21 | 1:125:A:LEU:H    | 2        | 0.13          |
| (1,1679) | 1:122:A:VAL:HG22 | 1:125:A:LEU:H    | 2        | 0.13          |
| (1,1679) | 1:122:A:VAL:HG23 | 1:125:A:LEU:H    | 2        | 0.13          |
| (1,1535) | 1:165:A:PRO:HD2  | 1:166:A:VAL:H    | 4        | 0.13          |
| (1,1535) | 1:165:A:PRO:HD2  | 1:166:A:VAL:H    | 6        | 0.13          |
| (1,1495) | 1:212:A:GLN:HB2  | 1:216:A:THR:H    | 20       | 0.13          |
| (1,1479) | 1:145:A:TRP:HB2  | 1:146:A:GLU:HG2  | 10       | 0.13          |
| (1,1479) | 1:145:A:TRP:HB3  | 1:146:A:GLU:HG2  | 10       | 0.13          |
| (1,1466) | 1:210:A:VAL:H    | 1:211:A:GLU:HB3  | 18       | 0.13          |
| (1,1303) | 1:137:A:PRO:HB2  | 1:213:A:MET:HG2  | 13       | 0.13          |
| (1,1212) | 1:184:A:ILE:HD11 | 1:206:A:MET:HB3  | 16       | 0.13          |
| (1,1212) | 1:184:A:ILE:HD12 | 1:206:A:MET:HB3  | 16       | 0.13          |
| (1,1212) | 1:184:A:ILE:HD13 | 1:206:A:MET:HB3  | 16       | 0.13          |
| (1,1152) | 1:205:A:MET:HA   | 1:205:A:MET:HG3  | 20       | 0.13          |
| (1,1053) | 1:204:A:LYS:HA   | 1:207:A:GLU:HG2  | 18       | 0.13          |
| (1,1026) | 1:186:A:GLN:HB2  | 1:187:A:HIS:HA   | 8        | 0.13          |
| (1,963)  | 1:184:A:ILE:HD11 | 1:185:A:LYS:HA   | 6        | 0.13          |
| (1,963)  | 1:184:A:ILE:HD12 | 1:185:A:LYS:HA   | 6        | 0.13          |
| (1,963)  | 1:184:A:ILE:HD13 | 1:185:A:LYS:HA   | 6        | 0.13          |
| (1,963)  | 1:184:A:ILE:HD11 | 1:185:A:LYS:HA   | 8        | 0.13          |
| (1,963)  | 1:184:A:ILE:HD12 | 1:185:A:LYS:HA   | 8        | 0.13          |
| (1,963)  | 1:184:A:ILE:HD13 | 1:185:A:LYS:HA   | 8        | 0.13          |
| (1,963)  | 1:184:A:ILE:HD11 | 1:185:A:LYS:HA   | 15       | 0.13          |
| (1,963)  | 1:184:A:ILE:HD12 | 1:185:A:LYS:HA   | 15       | 0.13          |
| (1,963)  | 1:184:A:ILE:HD13 | 1:185:A:LYS:HA   | 15       | 0.13          |
| (1,963)  | 1:184:A:ILE:HD11 | 1:185:A:LYS:HA   | 16       | 0.13          |
| (1,963)  | 1:184:A:ILE:HD12 | 1:185:A:LYS:HA   | 16       | 0.13          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,963) | 1:184:A:ILE:HD13 | 1:185:A:LYS:HA   | 16       | 0.13          |
| (1,963) | 1:184:A:ILE:HD11 | 1:185:A:LYS:HA   | 18       | 0.13          |
| (1,963) | 1:184:A:ILE:HD12 | 1:185:A:LYS:HA   | 18       | 0.13          |
| (1,963) | 1:184:A:ILE:HD13 | 1:185:A:LYS:HA   | 18       | 0.13          |
| (1,960) | 1:180:A:VAL:HG21 | 1:184:A:ILE:HD11 | 10       | 0.13          |
| (1,960) | 1:180:A:VAL:HG21 | 1:184:A:ILE:HD12 | 10       | 0.13          |
| (1,960) | 1:180:A:VAL:HG21 | 1:184:A:ILE:HD13 | 10       | 0.13          |
| (1,960) | 1:180:A:VAL:HG22 | 1:184:A:ILE:HD11 | 10       | 0.13          |
| (1,960) | 1:180:A:VAL:HG22 | 1:184:A:ILE:HD12 | 10       | 0.13          |
| (1,960) | 1:180:A:VAL:HG22 | 1:184:A:ILE:HD13 | 10       | 0.13          |
| (1,960) | 1:180:A:VAL:HG23 | 1:184:A:ILE:HD11 | 10       | 0.13          |
| (1,960) | 1:180:A:VAL:HG23 | 1:184:A:ILE:HD12 | 10       | 0.13          |
| (1,960) | 1:180:A:VAL:HG23 | 1:184:A:ILE:HD13 | 10       | 0.13          |
| (1,960) | 1:180:A:VAL:HG21 | 1:184:A:ILE:HD11 | 11       | 0.13          |
| (1,960) | 1:180:A:VAL:HG21 | 1:184:A:ILE:HD12 | 11       | 0.13          |
| (1,960) | 1:180:A:VAL:HG21 | 1:184:A:ILE:HD13 | 11       | 0.13          |
| (1,960) | 1:180:A:VAL:HG22 | 1:184:A:ILE:HD11 | 11       | 0.13          |
| (1,960) | 1:180:A:VAL:HG22 | 1:184:A:ILE:HD12 | 11       | 0.13          |
| (1,960) | 1:180:A:VAL:HG22 | 1:184:A:ILE:HD13 | 11       | 0.13          |
| (1,960) | 1:180:A:VAL:HG23 | 1:184:A:ILE:HD11 | 11       | 0.13          |
| (1,960) | 1:180:A:VAL:HG23 | 1:184:A:ILE:HD12 | 11       | 0.13          |
| (1,960) | 1:180:A:VAL:HG23 | 1:184:A:ILE:HD13 | 11       | 0.13          |
| (1,944) | 1:171:A:ASN:HB3  | 1:172:A:GLN:HA   | 14       | 0.13          |
| (1,902) | 1:147:A:ASP:HB2  | 1:148:A:ARG:HA   | 11       | 0.13          |
| (1,902) | 1:147:A:ASP:HB2  | 1:148:A:ARG:HA   | 15       | 0.13          |
| (1,881) | 1:145:A:TRP:HE3  | 1:146:A:GLU:HG3  | 10       | 0.13          |
| (1,828) | 1:222:A:SER:HA   | 1:226:A:TYR:HB3  | 19       | 0.13          |
| (1,814) | 1:226:A:TYR:HB2  | 1:227:A:ASP:HA   | 6        | 0.13          |
| (1,814) | 1:226:A:TYR:HB2  | 1:227:A:ASP:HA   | 18       | 0.13          |
| (1,774) | 1:206:A:MET:HB2  | 1:206:A:MET:HE1  | 9        | 0.13          |
| (1,774) | 1:206:A:MET:HB2  | 1:206:A:MET:HE2  | 9        | 0.13          |
| (1,774) | 1:206:A:MET:HB2  | 1:206:A:MET:HE3  | 9        | 0.13          |
| (1,760) | 1:184:A:ILE:HB   | 1:206:A:MET:HE1  | 16       | 0.13          |
| (1,760) | 1:184:A:ILE:HB   | 1:206:A:MET:HE2  | 16       | 0.13          |
| (1,760) | 1:184:A:ILE:HB   | 1:206:A:MET:HE3  | 16       | 0.13          |
| (1,733) | 1:222:A:SER:HB2  | 1:226:A:TYR:HD1  | 16       | 0.13          |
| (1,733) | 1:222:A:SER:HB2  | 1:226:A:TYR:HD2  | 16       | 0.13          |
| (1,667) | 1:138:A:MET:HE1  | 1:154:A:MET:HE1  | 15       | 0.13          |
| (1,667) | 1:138:A:MET:HE1  | 1:154:A:MET:HE2  | 15       | 0.13          |
| (1,667) | 1:138:A:MET:HE1  | 1:154:A:MET:HE3  | 15       | 0.13          |
| (1,667) | 1:138:A:MET:HE2  | 1:154:A:MET:HE1  | 15       | 0.13          |
| (1,667) | 1:138:A:MET:HE2  | 1:154:A:MET:HE2  | 15       | 0.13          |

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| Key     | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,667) | 1:138:A:MET:HE2 | 1:154:A:MET:HE3  | 15       | 0.13          |
| (1,667) | 1:138:A:MET:HE3 | 1:154:A:MET:HE1  | 15       | 0.13          |
| (1,667) | 1:138:A:MET:HE3 | 1:154:A:MET:HE2  | 15       | 0.13          |
| (1,667) | 1:138:A:MET:HE3 | 1:154:A:MET:HE3  | 15       | 0.13          |
| (1,659) | 1:136:A:ARG:HG2 | 1:154:A:MET:HE1  | 11       | 0.13          |
| (1,659) | 1:136:A:ARG:HG2 | 1:154:A:MET:HE2  | 11       | 0.13          |
| (1,659) | 1:136:A:ARG:HG2 | 1:154:A:MET:HE3  | 11       | 0.13          |
| (1,659) | 1:136:A:ARG:HG3 | 1:154:A:MET:HE1  | 11       | 0.13          |
| (1,659) | 1:136:A:ARG:HG3 | 1:154:A:MET:HE2  | 11       | 0.13          |
| (1,659) | 1:136:A:ARG:HG3 | 1:154:A:MET:HE3  | 11       | 0.13          |
| (1,658) | 1:154:A:MET:HG3 | 1:154:A:MET:HE1  | 10       | 0.13          |
| (1,658) | 1:154:A:MET:HG3 | 1:154:A:MET:HE2  | 10       | 0.13          |
| (1,658) | 1:154:A:MET:HG3 | 1:154:A:MET:HE3  | 10       | 0.13          |
| (1,656) | 1:138:A:MET:HG3 | 1:154:A:MET:HE1  | 7        | 0.13          |
| (1,656) | 1:138:A:MET:HG3 | 1:154:A:MET:HE2  | 7        | 0.13          |
| (1,656) | 1:138:A:MET:HG3 | 1:154:A:MET:HE3  | 7        | 0.13          |
| (1,656) | 1:138:A:MET:HG3 | 1:154:A:MET:HE1  | 14       | 0.13          |
| (1,656) | 1:138:A:MET:HG3 | 1:154:A:MET:HE2  | 14       | 0.13          |
| (1,656) | 1:138:A:MET:HG3 | 1:154:A:MET:HE3  | 14       | 0.13          |
| (1,656) | 1:138:A:MET:HG3 | 1:154:A:MET:HE1  | 18       | 0.13          |
| (1,656) | 1:138:A:MET:HG3 | 1:154:A:MET:HE2  | 18       | 0.13          |
| (1,656) | 1:138:A:MET:HG3 | 1:154:A:MET:HE3  | 18       | 0.13          |
| (1,611) | 1:134:A:MET:HE1 | 1:218:A:TYR:H    | 2        | 0.13          |
| (1,611) | 1:134:A:MET:HE2 | 1:218:A:TYR:H    | 2        | 0.13          |
| (1,611) | 1:134:A:MET:HE3 | 1:218:A:TYR:H    | 2        | 0.13          |
| (1,611) | 1:134:A:MET:HE1 | 1:218:A:TYR:H    | 15       | 0.13          |
| (1,611) | 1:134:A:MET:HE2 | 1:218:A:TYR:H    | 15       | 0.13          |
| (1,611) | 1:134:A:MET:HE3 | 1:218:A:TYR:H    | 15       | 0.13          |
| (1,611) | 1:134:A:MET:HE1 | 1:218:A:TYR:H    | 16       | 0.13          |
| (1,611) | 1:134:A:MET:HE2 | 1:218:A:TYR:H    | 16       | 0.13          |
| (1,611) | 1:134:A:MET:HE3 | 1:218:A:TYR:H    | 16       | 0.13          |
| (1,602) | 1:230:A:ARG:H   | 1:231:A:SER:HB3  | 14       | 0.13          |
| (1,569) | 1:128:A:TYR:HE1 | 1:179:A:CYS:HB3  | 12       | 0.13          |
| (1,569) | 1:128:A:TYR:HE2 | 1:179:A:CYS:HB3  | 12       | 0.13          |
| (1,559) | 1:162:A:TYR:HB3 | 1:182:A:ILE:HG21 | 18       | 0.13          |
| (1,559) | 1:162:A:TYR:HB3 | 1:182:A:ILE:HG22 | 18       | 0.13          |
| (1,559) | 1:162:A:TYR:HB3 | 1:182:A:ILE:HG23 | 18       | 0.13          |
| (1,501) | 1:161:A:VAL:HA  | 1:162:A:TYR:HB3  | 9        | 0.13          |
| (1,497) | 1:128:A:TYR:HB2 | 1:162:A:TYR:HB2  | 1        | 0.13          |
| (1,497) | 1:128:A:TYR:HB2 | 1:162:A:TYR:HB2  | 11       | 0.13          |
| (1,496) | 1:130:A:LEU:HA  | 1:162:A:TYR:HB2  | 15       | 0.13          |
| (1,425) | 1:148:A:ARG:HD3 | 1:149:A:TYR:HB2  | 9        | 0.13          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,391) | 1:122:A:VAL:HG21 | 1:125:A:LEU:HD21 | 1        | 0.13          |
| (1,391) | 1:122:A:VAL:HG21 | 1:125:A:LEU:HD22 | 1        | 0.13          |
| (1,391) | 1:122:A:VAL:HG21 | 1:125:A:LEU:HD23 | 1        | 0.13          |
| (1,391) | 1:122:A:VAL:HG22 | 1:125:A:LEU:HD21 | 1        | 0.13          |
| (1,391) | 1:122:A:VAL:HG22 | 1:125:A:LEU:HD22 | 1        | 0.13          |
| (1,391) | 1:122:A:VAL:HG22 | 1:125:A:LEU:HD23 | 1        | 0.13          |
| (1,391) | 1:122:A:VAL:HG23 | 1:125:A:LEU:HD21 | 1        | 0.13          |
| (1,391) | 1:122:A:VAL:HG23 | 1:125:A:LEU:HD22 | 1        | 0.13          |
| (1,391) | 1:122:A:VAL:HG23 | 1:125:A:LEU:HD23 | 1        | 0.13          |
| (1,359) | 1:122:A:VAL:HG21 | 1:182:A:ILE:HG21 | 3        | 0.13          |
| (1,359) | 1:122:A:VAL:HG21 | 1:182:A:ILE:HG22 | 3        | 0.13          |
| (1,359) | 1:122:A:VAL:HG21 | 1:182:A:ILE:HG23 | 3        | 0.13          |
| (1,359) | 1:122:A:VAL:HG22 | 1:182:A:ILE:HG21 | 3        | 0.13          |
| (1,359) | 1:122:A:VAL:HG22 | 1:182:A:ILE:HG22 | 3        | 0.13          |
| (1,359) | 1:122:A:VAL:HG22 | 1:182:A:ILE:HG23 | 3        | 0.13          |
| (1,359) | 1:122:A:VAL:HG23 | 1:182:A:ILE:HG21 | 3        | 0.13          |
| (1,359) | 1:122:A:VAL:HG23 | 1:182:A:ILE:HG22 | 3        | 0.13          |
| (1,359) | 1:122:A:VAL:HG23 | 1:182:A:ILE:HG23 | 3        | 0.13          |
| (1,359) | 1:122:A:VAL:HG21 | 1:182:A:ILE:HG21 | 5        | 0.13          |
| (1,359) | 1:122:A:VAL:HG21 | 1:182:A:ILE:HG22 | 5        | 0.13          |
| (1,359) | 1:122:A:VAL:HG21 | 1:182:A:ILE:HG23 | 5        | 0.13          |
| (1,359) | 1:122:A:VAL:HG22 | 1:182:A:ILE:HG21 | 5        | 0.13          |
| (1,359) | 1:122:A:VAL:HG22 | 1:182:A:ILE:HG22 | 5        | 0.13          |
| (1,359) | 1:122:A:VAL:HG22 | 1:182:A:ILE:HG23 | 5        | 0.13          |
| (1,359) | 1:122:A:VAL:HG23 | 1:182:A:ILE:HG21 | 5        | 0.13          |
| (1,359) | 1:122:A:VAL:HG23 | 1:182:A:ILE:HG22 | 5        | 0.13          |
| (1,359) | 1:122:A:VAL:HG23 | 1:182:A:ILE:HG23 | 5        | 0.13          |
| (1,359) | 1:122:A:VAL:HG21 | 1:182:A:ILE:HG21 | 10       | 0.13          |
| (1,359) | 1:122:A:VAL:HG21 | 1:182:A:ILE:HG22 | 10       | 0.13          |
| (1,359) | 1:122:A:VAL:HG21 | 1:182:A:ILE:HG23 | 10       | 0.13          |
| (1,359) | 1:122:A:VAL:HG22 | 1:182:A:ILE:HG21 | 10       | 0.13          |
| (1,359) | 1:122:A:VAL:HG22 | 1:182:A:ILE:HG22 | 10       | 0.13          |
| (1,359) | 1:122:A:VAL:HG22 | 1:182:A:ILE:HG23 | 10       | 0.13          |
| (1,359) | 1:122:A:VAL:HG23 | 1:182:A:ILE:HG21 | 10       | 0.13          |
| (1,359) | 1:122:A:VAL:HG23 | 1:182:A:ILE:HG22 | 10       | 0.13          |
| (1,359) | 1:122:A:VAL:HG23 | 1:182:A:ILE:HG23 | 10       | 0.13          |
| (1,300) | 1:191:A:THR:HG21 | 1:194:A:LYS:HB2  | 4        | 0.13          |
| (1,300) | 1:191:A:THR:HG22 | 1:194:A:LYS:HB2  | 4        | 0.13          |
| (1,300) | 1:191:A:THR:HG23 | 1:194:A:LYS:HB2  | 4        | 0.13          |
| (1,300) | 1:191:A:THR:HG21 | 1:194:A:LYS:HB2  | 17       | 0.13          |
| (1,300) | 1:191:A:THR:HG22 | 1:194:A:LYS:HB2  | 17       | 0.13          |
| (1,300) | 1:191:A:THR:HG23 | 1:194:A:LYS:HB2  | 17       | 0.13          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,296) | 1:187:A:HIS:HB3  | 1:190:A:THR:HG21 | 15       | 0.13          |
| (1,296) | 1:187:A:HIS:HB3  | 1:190:A:THR:HG22 | 15       | 0.13          |
| (1,296) | 1:187:A:HIS:HB3  | 1:190:A:THR:HG23 | 15       | 0.13          |
| (1,289) | 1:189:A:VAL:HG21 | 1:192:A:THR:HG21 | 8        | 0.13          |
| (1,289) | 1:189:A:VAL:HG21 | 1:192:A:THR:HG22 | 8        | 0.13          |
| (1,289) | 1:189:A:VAL:HG21 | 1:192:A:THR:HG23 | 8        | 0.13          |
| (1,289) | 1:189:A:VAL:HG22 | 1:192:A:THR:HG21 | 8        | 0.13          |
| (1,289) | 1:189:A:VAL:HG22 | 1:192:A:THR:HG22 | 8        | 0.13          |
| (1,289) | 1:189:A:VAL:HG22 | 1:192:A:THR:HG23 | 8        | 0.13          |
| (1,289) | 1:189:A:VAL:HG23 | 1:192:A:THR:HG21 | 8        | 0.13          |
| (1,289) | 1:189:A:VAL:HG23 | 1:192:A:THR:HG22 | 8        | 0.13          |
| (1,289) | 1:189:A:VAL:HG23 | 1:192:A:THR:HG23 | 8        | 0.13          |
| (1,288) | 1:192:A:THR:HG21 | 1:196:A:GLU:HB2  | 2        | 0.13          |
| (1,288) | 1:192:A:THR:HG21 | 1:196:A:GLU:HB3  | 2        | 0.13          |
| (1,288) | 1:192:A:THR:HG22 | 1:196:A:GLU:HB2  | 2        | 0.13          |
| (1,288) | 1:192:A:THR:HG22 | 1:196:A:GLU:HB3  | 2        | 0.13          |
| (1,288) | 1:192:A:THR:HG23 | 1:196:A:GLU:HB2  | 2        | 0.13          |
| (1,288) | 1:192:A:THR:HG23 | 1:196:A:GLU:HB3  | 2        | 0.13          |
| (1,288) | 1:192:A:THR:HG21 | 1:196:A:GLU:HB2  | 4        | 0.13          |
| (1,288) | 1:192:A:THR:HG21 | 1:196:A:GLU:HB3  | 4        | 0.13          |
| (1,288) | 1:192:A:THR:HG22 | 1:196:A:GLU:HB2  | 4        | 0.13          |
| (1,288) | 1:192:A:THR:HG22 | 1:196:A:GLU:HB3  | 4        | 0.13          |
| (1,288) | 1:192:A:THR:HG23 | 1:196:A:GLU:HB2  | 4        | 0.13          |
| (1,288) | 1:192:A:THR:HG23 | 1:196:A:GLU:HB3  | 4        | 0.13          |
| (1,288) | 1:192:A:THR:HG21 | 1:196:A:GLU:HB2  | 9        | 0.13          |
| (1,288) | 1:192:A:THR:HG21 | 1:196:A:GLU:HB3  | 9        | 0.13          |
| (1,288) | 1:192:A:THR:HG22 | 1:196:A:GLU:HB2  | 9        | 0.13          |
| (1,288) | 1:192:A:THR:HG22 | 1:196:A:GLU:HB3  | 9        | 0.13          |
| (1,288) | 1:192:A:THR:HG23 | 1:196:A:GLU:HB2  | 9        | 0.13          |
| (1,288) | 1:192:A:THR:HG23 | 1:196:A:GLU:HB3  | 9        | 0.13          |
| (1,288) | 1:192:A:THR:HG21 | 1:196:A:GLU:HB2  | 16       | 0.13          |
| (1,288) | 1:192:A:THR:HG21 | 1:196:A:GLU:HB3  | 16       | 0.13          |
| (1,288) | 1:192:A:THR:HG22 | 1:196:A:GLU:HB2  | 16       | 0.13          |
| (1,288) | 1:192:A:THR:HG22 | 1:196:A:GLU:HB3  | 16       | 0.13          |
| (1,288) | 1:192:A:THR:HG23 | 1:196:A:GLU:HB2  | 16       | 0.13          |
| (1,288) | 1:192:A:THR:HG23 | 1:196:A:GLU:HB3  | 16       | 0.13          |
| (1,261) | 1:185:A:LYS:HD2  | 1:188:A:THR:HG21 | 18       | 0.13          |
| (1,261) | 1:185:A:LYS:HD2  | 1:188:A:THR:HG22 | 18       | 0.13          |
| (1,261) | 1:185:A:LYS:HD2  | 1:188:A:THR:HG23 | 18       | 0.13          |
| (1,261) | 1:185:A:LYS:HD3  | 1:188:A:THR:HG21 | 18       | 0.13          |
| (1,261) | 1:185:A:LYS:HD3  | 1:188:A:THR:HG22 | 18       | 0.13          |
| (1,261) | 1:185:A:LYS:HD3  | 1:188:A:THR:HG23 | 18       | 0.13          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,224) | 1:127:A:GLY:HA3  | 1:128:A:TYR:HB2  | 11       | 0.13          |
| (1,217) | 1:193:A:THR:HG21 | 1:196:A:GLU:HB2  | 3        | 0.13          |
| (1,217) | 1:193:A:THR:HG21 | 1:196:A:GLU:HB3  | 3        | 0.13          |
| (1,217) | 1:193:A:THR:HG22 | 1:196:A:GLU:HB2  | 3        | 0.13          |
| (1,217) | 1:193:A:THR:HG22 | 1:196:A:GLU:HB3  | 3        | 0.13          |
| (1,217) | 1:193:A:THR:HG23 | 1:196:A:GLU:HB2  | 3        | 0.13          |
| (1,217) | 1:193:A:THR:HG23 | 1:196:A:GLU:HB3  | 3        | 0.13          |
| (1,217) | 1:193:A:THR:HG21 | 1:196:A:GLU:HB2  | 8        | 0.13          |
| (1,217) | 1:193:A:THR:HG21 | 1:196:A:GLU:HB3  | 8        | 0.13          |
| (1,217) | 1:193:A:THR:HG22 | 1:196:A:GLU:HB2  | 8        | 0.13          |
| (1,217) | 1:193:A:THR:HG22 | 1:196:A:GLU:HB3  | 8        | 0.13          |
| (1,217) | 1:193:A:THR:HG23 | 1:196:A:GLU:HB2  | 8        | 0.13          |
| (1,217) | 1:193:A:THR:HG23 | 1:196:A:GLU:HB3  | 8        | 0.13          |
| (1,217) | 1:193:A:THR:HG21 | 1:196:A:GLU:HB2  | 13       | 0.13          |
| (1,217) | 1:193:A:THR:HG21 | 1:196:A:GLU:HB3  | 13       | 0.13          |
| (1,217) | 1:193:A:THR:HG22 | 1:196:A:GLU:HB2  | 13       | 0.13          |
| (1,217) | 1:193:A:THR:HG22 | 1:196:A:GLU:HB3  | 13       | 0.13          |
| (1,217) | 1:193:A:THR:HG23 | 1:196:A:GLU:HB2  | 13       | 0.13          |
| (1,217) | 1:193:A:THR:HG23 | 1:196:A:GLU:HB3  | 13       | 0.13          |
| (1,216) | 1:216:A:THR:HG21 | 1:220:A:LYS:HG3  | 4        | 0.13          |
| (1,216) | 1:216:A:THR:HG22 | 1:220:A:LYS:HG3  | 4        | 0.13          |
| (1,216) | 1:216:A:THR:HG23 | 1:220:A:LYS:HG3  | 4        | 0.13          |
| (1,216) | 1:216:A:THR:HG21 | 1:220:A:LYS:HG3  | 16       | 0.13          |
| (1,216) | 1:216:A:THR:HG22 | 1:220:A:LYS:HG3  | 16       | 0.13          |
| (1,216) | 1:216:A:THR:HG23 | 1:220:A:LYS:HG3  | 16       | 0.13          |
| (1,189) | 1:123:A:GLY:HA2  | 1:125:A:LEU:HD21 | 12       | 0.13          |
| (1,189) | 1:123:A:GLY:HA2  | 1:125:A:LEU:HD22 | 12       | 0.13          |
| (1,189) | 1:123:A:GLY:HA2  | 1:125:A:LEU:HD23 | 12       | 0.13          |
| (1,189) | 1:123:A:GLY:HA3  | 1:125:A:LEU:HD21 | 12       | 0.13          |
| (1,189) | 1:123:A:GLY:HA3  | 1:125:A:LEU:HD22 | 12       | 0.13          |
| (1,189) | 1:123:A:GLY:HA3  | 1:125:A:LEU:HD23 | 12       | 0.13          |
| (1,162) | 1:226:A:TYR:HB2  | 1:228:A:GLY:HA2  | 7        | 0.13          |
| (1,162) | 1:226:A:TYR:HB2  | 1:228:A:GLY:HA3  | 7        | 0.13          |
| (1,150) | 1:126:A:GLY:HA3  | 1:127:A:GLY:H    | 8        | 0.13          |
| (1,150) | 1:126:A:GLY:HA3  | 1:127:A:GLY:H    | 19       | 0.13          |
| (1,112) | 1:214:A:CYS:HA   | 1:215:A:VAL:HG11 | 5        | 0.13          |
| (1,112) | 1:214:A:CYS:HA   | 1:215:A:VAL:HG12 | 5        | 0.13          |
| (1,112) | 1:214:A:CYS:HA   | 1:215:A:VAL:HG13 | 5        | 0.13          |
| (1,112) | 1:214:A:CYS:HA   | 1:215:A:VAL:HG11 | 10       | 0.13          |
| (1,112) | 1:214:A:CYS:HA   | 1:215:A:VAL:HG12 | 10       | 0.13          |
| (1,112) | 1:214:A:CYS:HA   | 1:215:A:VAL:HG13 | 10       | 0.13          |
| (1,111) | 1:215:A:VAL:HG11 | 1:216:A:THR:HB   | 13       | 0.13          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,111)  | 1:215:A:VAL:HG12 | 1:216:A:THR:HB  | 13       | 0.13          |
| (1,111)  | 1:215:A:VAL:HG13 | 1:216:A:THR:HB  | 13       | 0.13          |
| (1,32)   | 1:219:A:GLN:HB3  | 1:220:A:LYS:HG3 | 18       | 0.13          |
| (1,32)   | 1:219:A:GLN:HB3  | 1:220:A:LYS:HG3 | 19       | 0.13          |
| (1,31)   | 1:219:A:GLN:HA   | 1:220:A:LYS:HG3 | 14       | 0.13          |
| (1,2843) | 1:157:A:TYR:HE1  | 1:206:A:MET:HE1 | 6        | 0.12          |
| (1,2843) | 1:157:A:TYR:HE1  | 1:206:A:MET:HE2 | 6        | 0.12          |
| (1,2843) | 1:157:A:TYR:HE1  | 1:206:A:MET:HE3 | 6        | 0.12          |
| (1,2843) | 1:157:A:TYR:HE2  | 1:206:A:MET:HE1 | 6        | 0.12          |
| (1,2843) | 1:157:A:TYR:HE2  | 1:206:A:MET:HE2 | 6        | 0.12          |
| (1,2843) | 1:157:A:TYR:HE2  | 1:206:A:MET:HE3 | 6        | 0.12          |
| (1,2843) | 1:157:A:TYR:HE1  | 1:206:A:MET:HE1 | 7        | 0.12          |
| (1,2843) | 1:157:A:TYR:HE1  | 1:206:A:MET:HE2 | 7        | 0.12          |
| (1,2843) | 1:157:A:TYR:HE1  | 1:206:A:MET:HE3 | 7        | 0.12          |
| (1,2843) | 1:157:A:TYR:HE2  | 1:206:A:MET:HE1 | 7        | 0.12          |
| (1,2843) | 1:157:A:TYR:HE2  | 1:206:A:MET:HE2 | 7        | 0.12          |
| (1,2843) | 1:157:A:TYR:HE2  | 1:206:A:MET:HE3 | 7        | 0.12          |
| (1,2843) | 1:157:A:TYR:HE1  | 1:206:A:MET:HE1 | 12       | 0.12          |
| (1,2843) | 1:157:A:TYR:HE1  | 1:206:A:MET:HE2 | 12       | 0.12          |
| (1,2843) | 1:157:A:TYR:HE1  | 1:206:A:MET:HE3 | 12       | 0.12          |
| (1,2843) | 1:157:A:TYR:HE2  | 1:206:A:MET:HE1 | 12       | 0.12          |
| (1,2843) | 1:157:A:TYR:HE2  | 1:206:A:MET:HE2 | 12       | 0.12          |
| (1,2843) | 1:157:A:TYR:HE2  | 1:206:A:MET:HE3 | 12       | 0.12          |
| (1,2829) | 1:166:A:VAL:HB   | 1:218:A:TYR:HE1 | 1        | 0.12          |
| (1,2829) | 1:166:A:VAL:HB   | 1:218:A:TYR:HE2 | 1        | 0.12          |
| (1,2825) | 1:176:A:VAL:HG21 | 1:218:A:TYR:HE1 | 7        | 0.12          |
| (1,2825) | 1:176:A:VAL:HG21 | 1:218:A:TYR:HE2 | 7        | 0.12          |
| (1,2825) | 1:176:A:VAL:HG22 | 1:218:A:TYR:HE1 | 7        | 0.12          |
| (1,2825) | 1:176:A:VAL:HG22 | 1:218:A:TYR:HE2 | 7        | 0.12          |
| (1,2825) | 1:176:A:VAL:HG23 | 1:218:A:TYR:HE1 | 7        | 0.12          |
| (1,2825) | 1:176:A:VAL:HG23 | 1:218:A:TYR:HE2 | 7        | 0.12          |
| (1,2650) | 1:139:A:ILE:HG12 | 1:141:A:PHE:HE1 | 18       | 0.12          |
| (1,2650) | 1:139:A:ILE:HG12 | 1:141:A:PHE:HE2 | 18       | 0.12          |
| (1,2631) | 1:198:A:PHE:HD1  | 1:203:A:VAL:HA  | 16       | 0.12          |
| (1,2631) | 1:198:A:PHE:HD2  | 1:203:A:VAL:HA  | 16       | 0.12          |
| (1,2593) | 1:175:A:PHE:HE1  | 1:221:A:GLU:HG2 | 8        | 0.12          |
| (1,2593) | 1:175:A:PHE:HE2  | 1:221:A:GLU:HG2 | 8        | 0.12          |
| (1,2575) | 1:166:A:VAL:HG21 | 1:218:A:TYR:HD1 | 1        | 0.12          |
| (1,2575) | 1:166:A:VAL:HG21 | 1:218:A:TYR:HD2 | 1        | 0.12          |
| (1,2575) | 1:166:A:VAL:HG22 | 1:218:A:TYR:HD1 | 1        | 0.12          |
| (1,2575) | 1:166:A:VAL:HG22 | 1:218:A:TYR:HD2 | 1        | 0.12          |
| (1,2575) | 1:166:A:VAL:HG23 | 1:218:A:TYR:HD1 | 1        | 0.12          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2575) | 1:166:A:VAL:HG23 | 1:218:A:TYR:HD2  | 1        | 0.12          |
| (1,2520) | 1:154:A:MET:HE1  | 1:155:A:TYR:HD1  | 5        | 0.12          |
| (1,2520) | 1:154:A:MET:HE1  | 1:155:A:TYR:HD2  | 5        | 0.12          |
| (1,2520) | 1:154:A:MET:HE2  | 1:155:A:TYR:HD1  | 5        | 0.12          |
| (1,2520) | 1:154:A:MET:HE2  | 1:155:A:TYR:HD2  | 5        | 0.12          |
| (1,2520) | 1:154:A:MET:HE3  | 1:155:A:TYR:HD1  | 5        | 0.12          |
| (1,2520) | 1:154:A:MET:HE3  | 1:155:A:TYR:HD2  | 5        | 0.12          |
| (1,2500) | 1:149:A:TYR:HD1  | 1:201:A:THR:HG21 | 4        | 0.12          |
| (1,2500) | 1:149:A:TYR:HD1  | 1:201:A:THR:HG22 | 4        | 0.12          |
| (1,2500) | 1:149:A:TYR:HD1  | 1:201:A:THR:HG23 | 4        | 0.12          |
| (1,2500) | 1:149:A:TYR:HD2  | 1:201:A:THR:HG21 | 4        | 0.12          |
| (1,2500) | 1:149:A:TYR:HD2  | 1:201:A:THR:HG22 | 4        | 0.12          |
| (1,2500) | 1:149:A:TYR:HD2  | 1:201:A:THR:HG23 | 4        | 0.12          |
| (1,2464) | 1:169:A:TYR:HD1  | 1:218:A:TYR:HE1  | 3        | 0.12          |
| (1,2464) | 1:169:A:TYR:HD1  | 1:218:A:TYR:HE2  | 3        | 0.12          |
| (1,2464) | 1:169:A:TYR:HD2  | 1:218:A:TYR:HE1  | 3        | 0.12          |
| (1,2464) | 1:169:A:TYR:HD2  | 1:218:A:TYR:HE2  | 3        | 0.12          |
| (1,2464) | 1:169:A:TYR:HD1  | 1:218:A:TYR:HE1  | 17       | 0.12          |
| (1,2464) | 1:169:A:TYR:HD1  | 1:218:A:TYR:HE2  | 17       | 0.12          |
| (1,2464) | 1:169:A:TYR:HD2  | 1:218:A:TYR:HE1  | 17       | 0.12          |
| (1,2464) | 1:169:A:TYR:HD2  | 1:218:A:TYR:HE2  | 17       | 0.12          |
| (1,2456) | 1:139:A:ILE:HG21 | 1:208:A:ARG:HE   | 12       | 0.12          |
| (1,2456) | 1:139:A:ILE:HG22 | 1:208:A:ARG:HE   | 12       | 0.12          |
| (1,2456) | 1:139:A:ILE:HG23 | 1:208:A:ARG:HE   | 12       | 0.12          |
| (1,2445) | 1:122:A:VAL:HG21 | 1:124:A:GLY:H    | 9        | 0.12          |
| (1,2445) | 1:122:A:VAL:HG22 | 1:124:A:GLY:H    | 9        | 0.12          |
| (1,2445) | 1:122:A:VAL:HG23 | 1:124:A:GLY:H    | 9        | 0.12          |
| (1,2397) | 1:185:A:LYS:HB2  | 1:186:A:GLN:HE22 | 15       | 0.12          |
| (1,2397) | 1:185:A:LYS:HB3  | 1:186:A:GLN:HE22 | 15       | 0.12          |
| (1,2092) | 1:169:A:TYR:H    | 1:169:A:TYR:HB3  | 5        | 0.12          |
| (1,2092) | 1:169:A:TYR:H    | 1:169:A:TYR:HB3  | 7        | 0.12          |
| (1,2045) | 1:230:A:ARG:HG3  | 1:231:A:SER:H    | 18       | 0.12          |
| (1,1968) | 1:205:A:MET:H    | 1:205:A:MET:HG3  | 16       | 0.12          |
| (1,1926) | 1:134:A:MET:HE1  | 1:214:A:CYS:H    | 20       | 0.12          |
| (1,1926) | 1:134:A:MET:HE2  | 1:214:A:CYS:H    | 20       | 0.12          |
| (1,1926) | 1:134:A:MET:HE3  | 1:214:A:CYS:H    | 20       | 0.12          |
| (1,1893) | 1:208:A:ARG:HB3  | 1:209:A:VAL:H    | 17       | 0.12          |
| (1,1847) | 1:197:A:ASN:H    | 1:197:A:ASN:HB3  | 20       | 0.12          |
| (1,1679) | 1:122:A:VAL:HG21 | 1:125:A:LEU:H    | 15       | 0.12          |
| (1,1679) | 1:122:A:VAL:HG22 | 1:125:A:LEU:H    | 15       | 0.12          |
| (1,1679) | 1:122:A:VAL:HG23 | 1:125:A:LEU:H    | 15       | 0.12          |
| (1,1558) | 1:208:A:ARG:HG3  | 1:209:A:VAL:H    | 6        | 0.12          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1546) | 1:158:A:PRO:HD2  | 1:209:A:VAL:HG21 | 2        | 0.12          |
| (1,1546) | 1:158:A:PRO:HD2  | 1:209:A:VAL:HG22 | 2        | 0.12          |
| (1,1546) | 1:158:A:PRO:HD2  | 1:209:A:VAL:HG23 | 2        | 0.12          |
| (1,1535) | 1:165:A:PRO:HD2  | 1:166:A:VAL:H    | 10       | 0.12          |
| (1,1535) | 1:165:A:PRO:HD2  | 1:166:A:VAL:H    | 15       | 0.12          |
| (1,1479) | 1:145:A:TRP:HB2  | 1:146:A:GLU:HG2  | 9        | 0.12          |
| (1,1479) | 1:145:A:TRP:HB3  | 1:146:A:GLU:HG2  | 9        | 0.12          |
| (1,1466) | 1:210:A:VAL:H    | 1:211:A:GLU:HB3  | 13       | 0.12          |
| (1,1459) | 1:136:A:ARG:HB3  | 1:159:A:ASN:HB3  | 16       | 0.12          |
| (1,1400) | 1:183:A:THR:HB   | 1:184:A:ILE:HG12 | 1        | 0.12          |
| (1,1392) | 1:133:A:ALA:HA   | 1:159:A:ASN:HB2  | 19       | 0.12          |
| (1,1385) | 1:183:A:THR:HG21 | 1:187:A:HIS:HB2  | 18       | 0.12          |
| (1,1385) | 1:183:A:THR:HG22 | 1:187:A:HIS:HB2  | 18       | 0.12          |
| (1,1385) | 1:183:A:THR:HG23 | 1:187:A:HIS:HB2  | 18       | 0.12          |
| (1,1253) | 1:203:A:VAL:HA   | 1:204:A:LYS:HB2  | 7        | 0.12          |
| (1,1253) | 1:203:A:VAL:HA   | 1:204:A:LYS:HB3  | 7        | 0.12          |
| (1,1253) | 1:203:A:VAL:HA   | 1:204:A:LYS:HB2  | 8        | 0.12          |
| (1,1253) | 1:203:A:VAL:HA   | 1:204:A:LYS:HB3  | 8        | 0.12          |
| (1,1234) | 1:122:A:VAL:HB   | 1:123:A:GLY:HA2  | 3        | 0.12          |
| (1,1234) | 1:122:A:VAL:HB   | 1:123:A:GLY:HA3  | 3        | 0.12          |
| (1,1234) | 1:122:A:VAL:HB   | 1:123:A:GLY:HA2  | 4        | 0.12          |
| (1,1234) | 1:122:A:VAL:HB   | 1:123:A:GLY:HA3  | 4        | 0.12          |
| (1,1234) | 1:122:A:VAL:HB   | 1:123:A:GLY:HA2  | 10       | 0.12          |
| (1,1234) | 1:122:A:VAL:HB   | 1:123:A:GLY:HA3  | 10       | 0.12          |
| (1,1234) | 1:122:A:VAL:HB   | 1:123:A:GLY:HA2  | 17       | 0.12          |
| (1,1234) | 1:122:A:VAL:HB   | 1:123:A:GLY:HA3  | 17       | 0.12          |
| (1,1234) | 1:122:A:VAL:HB   | 1:123:A:GLY:HA2  | 20       | 0.12          |
| (1,1234) | 1:122:A:VAL:HB   | 1:123:A:GLY:HA3  | 20       | 0.12          |
| (1,1230) | 1:137:A:PRO:HD2  | 1:213:A:MET:HG3  | 14       | 0.12          |
| (1,1097) | 1:165:A:PRO:HB3  | 1:168:A:GLN:HG2  | 13       | 0.12          |
| (1,1070) | 1:152:A:GLU:HA   | 1:152:A:GLU:HG3  | 19       | 0.12          |
| (1,1026) | 1:186:A:GLN:HB2  | 1:187:A:HIS:HA   | 18       | 0.12          |
| (1,1015) | 1:152:A:GLU:HG2  | 1:153:A:ASN:HD22 | 7        | 0.12          |
| (1,1007) | 1:137:A:PRO:HA   | 1:139:A:ILE:HD11 | 5        | 0.12          |
| (1,1007) | 1:137:A:PRO:HA   | 1:139:A:ILE:HD12 | 5        | 0.12          |
| (1,1007) | 1:137:A:PRO:HA   | 1:139:A:ILE:HD13 | 5        | 0.12          |
| (1,1007) | 1:137:A:PRO:HA   | 1:139:A:ILE:HD11 | 6        | 0.12          |
| (1,1007) | 1:137:A:PRO:HA   | 1:139:A:ILE:HD12 | 6        | 0.12          |
| (1,1007) | 1:137:A:PRO:HA   | 1:139:A:ILE:HD13 | 6        | 0.12          |
| (1,1007) | 1:137:A:PRO:HA   | 1:139:A:ILE:HD11 | 9        | 0.12          |
| (1,1007) | 1:137:A:PRO:HA   | 1:139:A:ILE:HD12 | 9        | 0.12          |
| (1,1007) | 1:137:A:PRO:HA   | 1:139:A:ILE:HD13 | 9        | 0.12          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1007) | 1:137:A:PRO:HA   | 1:139:A:ILE:HD11 | 15       | 0.12          |
| (1,1007) | 1:137:A:PRO:HA   | 1:139:A:ILE:HD12 | 15       | 0.12          |
| (1,1007) | 1:137:A:PRO:HA   | 1:139:A:ILE:HD13 | 15       | 0.12          |
| (1,1007) | 1:137:A:PRO:HA   | 1:139:A:ILE:HD11 | 20       | 0.12          |
| (1,1007) | 1:137:A:PRO:HA   | 1:139:A:ILE:HD12 | 20       | 0.12          |
| (1,1007) | 1:137:A:PRO:HA   | 1:139:A:ILE:HD13 | 20       | 0.12          |
| (1,967)  | 1:135:A:SER:HA   | 1:136:A:ARG:HB2  | 10       | 0.12          |
| (1,963)  | 1:184:A:ILE:HD11 | 1:185:A:LYS:HA   | 1        | 0.12          |
| (1,963)  | 1:184:A:ILE:HD12 | 1:185:A:LYS:HA   | 1        | 0.12          |
| (1,963)  | 1:184:A:ILE:HD13 | 1:185:A:LYS:HA   | 1        | 0.12          |
| (1,963)  | 1:184:A:ILE:HD11 | 1:185:A:LYS:HA   | 2        | 0.12          |
| (1,963)  | 1:184:A:ILE:HD12 | 1:185:A:LYS:HA   | 2        | 0.12          |
| (1,963)  | 1:184:A:ILE:HD13 | 1:185:A:LYS:HA   | 2        | 0.12          |
| (1,963)  | 1:184:A:ILE:HD11 | 1:185:A:LYS:HA   | 3        | 0.12          |
| (1,963)  | 1:184:A:ILE:HD12 | 1:185:A:LYS:HA   | 3        | 0.12          |
| (1,963)  | 1:184:A:ILE:HD13 | 1:185:A:LYS:HA   | 3        | 0.12          |
| (1,963)  | 1:184:A:ILE:HD11 | 1:185:A:LYS:HA   | 4        | 0.12          |
| (1,963)  | 1:184:A:ILE:HD12 | 1:185:A:LYS:HA   | 4        | 0.12          |
| (1,963)  | 1:184:A:ILE:HD13 | 1:185:A:LYS:HA   | 4        | 0.12          |
| (1,963)  | 1:184:A:ILE:HD11 | 1:185:A:LYS:HA   | 5        | 0.12          |
| (1,963)  | 1:184:A:ILE:HD12 | 1:185:A:LYS:HA   | 5        | 0.12          |
| (1,963)  | 1:184:A:ILE:HD13 | 1:185:A:LYS:HA   | 5        | 0.12          |
| (1,963)  | 1:184:A:ILE:HD11 | 1:185:A:LYS:HA   | 7        | 0.12          |
| (1,963)  | 1:184:A:ILE:HD12 | 1:185:A:LYS:HA   | 7        | 0.12          |
| (1,963)  | 1:184:A:ILE:HD13 | 1:185:A:LYS:HA   | 7        | 0.12          |
| (1,963)  | 1:184:A:ILE:HD11 | 1:185:A:LYS:HA   | 9        | 0.12          |
| (1,963)  | 1:184:A:ILE:HD12 | 1:185:A:LYS:HA   | 9        | 0.12          |
| (1,963)  | 1:184:A:ILE:HD13 | 1:185:A:LYS:HA   | 9        | 0.12          |
| (1,963)  | 1:184:A:ILE:HD11 | 1:185:A:LYS:HA   | 10       | 0.12          |
| (1,963)  | 1:184:A:ILE:HD12 | 1:185:A:LYS:HA   | 10       | 0.12          |
| (1,963)  | 1:184:A:ILE:HD13 | 1:185:A:LYS:HA   | 10       | 0.12          |
| (1,963)  | 1:184:A:ILE:HD11 | 1:185:A:LYS:HA   | 13       | 0.12          |
| (1,963)  | 1:184:A:ILE:HD12 | 1:185:A:LYS:HA   | 13       | 0.12          |
| (1,963)  | 1:184:A:ILE:HD13 | 1:185:A:LYS:HA   | 13       | 0.12          |
| (1,963)  | 1:184:A:ILE:HD11 | 1:185:A:LYS:HA   | 17       | 0.12          |
| (1,963)  | 1:184:A:ILE:HD12 | 1:185:A:LYS:HA   | 17       | 0.12          |
| (1,963)  | 1:184:A:ILE:HD13 | 1:185:A:LYS:HA   | 17       | 0.12          |
| (1,963)  | 1:184:A:ILE:HD11 | 1:185:A:LYS:HA   | 19       | 0.12          |
| (1,963)  | 1:184:A:ILE:HD12 | 1:185:A:LYS:HA   | 19       | 0.12          |
| (1,963)  | 1:184:A:ILE:HD13 | 1:185:A:LYS:HA   | 19       | 0.12          |
| (1,963)  | 1:184:A:ILE:HD11 | 1:185:A:LYS:HA   | 20       | 0.12          |
| (1,963)  | 1:184:A:ILE:HD12 | 1:185:A:LYS:HA   | 20       | 0.12          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,963) | 1:184:A:ILE:HD13 | 1:185:A:LYS:HA   | 20       | 0.12          |
| (1,939) | 1:169:A:TYR:HA   | 1:170:A:SER:HA   | 1        | 0.12          |
| (1,902) | 1:147:A:ASP:HB2  | 1:148:A:ARG:HA   | 4        | 0.12          |
| (1,902) | 1:147:A:ASP:HB2  | 1:148:A:ARG:HA   | 6        | 0.12          |
| (1,902) | 1:147:A:ASP:HB2  | 1:148:A:ARG:HA   | 18       | 0.12          |
| (1,864) | 1:134:A:MET:HB3  | 1:135:A:SER:HB2  | 1        | 0.12          |
| (1,862) | 1:143:A:ASN:HD22 | 1:146:A:GLU:HG2  | 19       | 0.12          |
| (1,828) | 1:222:A:SER:HA   | 1:226:A:TYR:HB3  | 18       | 0.12          |
| (1,814) | 1:226:A:TYR:HB2  | 1:227:A:ASP:HA   | 2        | 0.12          |
| (1,814) | 1:226:A:TYR:HB2  | 1:227:A:ASP:HA   | 20       | 0.12          |
| (1,807) | 1:181:A:ASN:HB3  | 1:184:A:ILE:HG21 | 6        | 0.12          |
| (1,807) | 1:181:A:ASN:HB3  | 1:184:A:ILE:HG22 | 6        | 0.12          |
| (1,807) | 1:181:A:ASN:HB3  | 1:184:A:ILE:HG23 | 6        | 0.12          |
| (1,807) | 1:181:A:ASN:HB3  | 1:184:A:ILE:HG21 | 8        | 0.12          |
| (1,807) | 1:181:A:ASN:HB3  | 1:184:A:ILE:HG22 | 8        | 0.12          |
| (1,807) | 1:181:A:ASN:HB3  | 1:184:A:ILE:HG23 | 8        | 0.12          |
| (1,807) | 1:181:A:ASN:HB3  | 1:184:A:ILE:HG21 | 13       | 0.12          |
| (1,807) | 1:181:A:ASN:HB3  | 1:184:A:ILE:HG22 | 13       | 0.12          |
| (1,807) | 1:181:A:ASN:HB3  | 1:184:A:ILE:HG23 | 13       | 0.12          |
| (1,807) | 1:181:A:ASN:HB3  | 1:184:A:ILE:HG21 | 16       | 0.12          |
| (1,807) | 1:181:A:ASN:HB3  | 1:184:A:ILE:HG22 | 16       | 0.12          |
| (1,807) | 1:181:A:ASN:HB3  | 1:184:A:ILE:HG23 | 16       | 0.12          |
| (1,807) | 1:181:A:ASN:HB3  | 1:184:A:ILE:HG21 | 18       | 0.12          |
| (1,807) | 1:181:A:ASN:HB3  | 1:184:A:ILE:HG22 | 18       | 0.12          |
| (1,807) | 1:181:A:ASN:HB3  | 1:184:A:ILE:HG23 | 18       | 0.12          |
| (1,784) | 1:166:A:VAL:HG11 | 1:218:A:TYR:HA   | 3        | 0.12          |
| (1,784) | 1:166:A:VAL:HG12 | 1:218:A:TYR:HA   | 3        | 0.12          |
| (1,784) | 1:166:A:VAL:HG13 | 1:218:A:TYR:HA   | 3        | 0.12          |
| (1,760) | 1:184:A:ILE:HB   | 1:206:A:MET:HE1  | 18       | 0.12          |
| (1,760) | 1:184:A:ILE:HB   | 1:206:A:MET:HE2  | 18       | 0.12          |
| (1,760) | 1:184:A:ILE:HB   | 1:206:A:MET:HE3  | 18       | 0.12          |
| (1,735) | 1:222:A:SER:HB2  | 1:223:A:GLN:HB2  | 20       | 0.12          |
| (1,735) | 1:222:A:SER:HB2  | 1:223:A:GLN:HB3  | 20       | 0.12          |
| (1,667) | 1:138:A:MET:HE1  | 1:154:A:MET:HE1  | 9        | 0.12          |
| (1,667) | 1:138:A:MET:HE1  | 1:154:A:MET:HE2  | 9        | 0.12          |
| (1,667) | 1:138:A:MET:HE1  | 1:154:A:MET:HE3  | 9        | 0.12          |
| (1,667) | 1:138:A:MET:HE2  | 1:154:A:MET:HE1  | 9        | 0.12          |
| (1,667) | 1:138:A:MET:HE2  | 1:154:A:MET:HE2  | 9        | 0.12          |
| (1,667) | 1:138:A:MET:HE2  | 1:154:A:MET:HE3  | 9        | 0.12          |
| (1,667) | 1:138:A:MET:HE3  | 1:154:A:MET:HE1  | 9        | 0.12          |
| (1,667) | 1:138:A:MET:HE3  | 1:154:A:MET:HE2  | 9        | 0.12          |
| (1,667) | 1:138:A:MET:HE3  | 1:154:A:MET:HE3  | 9        | 0.12          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,667) | 1:138:A:MET:HE1 | 1:154:A:MET:HE1 | 17       | 0.12          |
| (1,667) | 1:138:A:MET:HE1 | 1:154:A:MET:HE2 | 17       | 0.12          |
| (1,667) | 1:138:A:MET:HE1 | 1:154:A:MET:HE3 | 17       | 0.12          |
| (1,667) | 1:138:A:MET:HE2 | 1:154:A:MET:HE1 | 17       | 0.12          |
| (1,667) | 1:138:A:MET:HE2 | 1:154:A:MET:HE2 | 17       | 0.12          |
| (1,667) | 1:138:A:MET:HE2 | 1:154:A:MET:HE3 | 17       | 0.12          |
| (1,667) | 1:138:A:MET:HE3 | 1:154:A:MET:HE1 | 17       | 0.12          |
| (1,667) | 1:138:A:MET:HE3 | 1:154:A:MET:HE2 | 17       | 0.12          |
| (1,667) | 1:138:A:MET:HE3 | 1:154:A:MET:HE3 | 17       | 0.12          |
| (1,659) | 1:136:A:ARG:HG2 | 1:154:A:MET:HE1 | 1        | 0.12          |
| (1,659) | 1:136:A:ARG:HG2 | 1:154:A:MET:HE2 | 1        | 0.12          |
| (1,659) | 1:136:A:ARG:HG2 | 1:154:A:MET:HE3 | 1        | 0.12          |
| (1,659) | 1:136:A:ARG:HG3 | 1:154:A:MET:HE1 | 1        | 0.12          |
| (1,659) | 1:136:A:ARG:HG3 | 1:154:A:MET:HE2 | 1        | 0.12          |
| (1,659) | 1:136:A:ARG:HG3 | 1:154:A:MET:HE3 | 1        | 0.12          |
| (1,659) | 1:136:A:ARG:HG2 | 1:154:A:MET:HE1 | 20       | 0.12          |
| (1,659) | 1:136:A:ARG:HG2 | 1:154:A:MET:HE2 | 20       | 0.12          |
| (1,659) | 1:136:A:ARG:HG2 | 1:154:A:MET:HE3 | 20       | 0.12          |
| (1,659) | 1:136:A:ARG:HG3 | 1:154:A:MET:HE1 | 20       | 0.12          |
| (1,659) | 1:136:A:ARG:HG3 | 1:154:A:MET:HE2 | 20       | 0.12          |
| (1,659) | 1:136:A:ARG:HG3 | 1:154:A:MET:HE3 | 20       | 0.12          |
| (1,656) | 1:138:A:MET:HG3 | 1:154:A:MET:HE1 | 1        | 0.12          |
| (1,656) | 1:138:A:MET:HG3 | 1:154:A:MET:HE2 | 1        | 0.12          |
| (1,656) | 1:138:A:MET:HG3 | 1:154:A:MET:HE3 | 1        | 0.12          |
| (1,656) | 1:138:A:MET:HG3 | 1:154:A:MET:HE1 | 13       | 0.12          |
| (1,656) | 1:138:A:MET:HG3 | 1:154:A:MET:HE2 | 13       | 0.12          |
| (1,656) | 1:138:A:MET:HG3 | 1:154:A:MET:HE3 | 13       | 0.12          |
| (1,656) | 1:138:A:MET:HG3 | 1:154:A:MET:HE1 | 16       | 0.12          |
| (1,656) | 1:138:A:MET:HG3 | 1:154:A:MET:HE2 | 16       | 0.12          |
| (1,656) | 1:138:A:MET:HG3 | 1:154:A:MET:HE3 | 16       | 0.12          |
| (1,656) | 1:138:A:MET:HG3 | 1:154:A:MET:HE1 | 17       | 0.12          |
| (1,656) | 1:138:A:MET:HG3 | 1:154:A:MET:HE2 | 17       | 0.12          |
| (1,656) | 1:138:A:MET:HG3 | 1:154:A:MET:HE3 | 17       | 0.12          |
| (1,653) | 1:139:A:ILE:H   | 1:154:A:MET:HE1 | 8        | 0.12          |
| (1,653) | 1:139:A:ILE:H   | 1:154:A:MET:HE2 | 8        | 0.12          |
| (1,653) | 1:139:A:ILE:H   | 1:154:A:MET:HE3 | 8        | 0.12          |
| (1,612) | 1:134:A:MET:HE1 | 1:213:A:MET:H   | 3        | 0.12          |
| (1,612) | 1:134:A:MET:HE2 | 1:213:A:MET:H   | 3        | 0.12          |
| (1,612) | 1:134:A:MET:HE3 | 1:213:A:MET:H   | 3        | 0.12          |
| (1,612) | 1:134:A:MET:HE1 | 1:213:A:MET:H   | 4        | 0.12          |
| (1,612) | 1:134:A:MET:HE2 | 1:213:A:MET:H   | 4        | 0.12          |
| (1,612) | 1:134:A:MET:HE3 | 1:213:A:MET:H   | 4        | 0.12          |

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| Key     | Atom-1          | Atom-2        | Model ID | Violation (Å) |
|---------|-----------------|---------------|----------|---------------|
| (1,612) | 1:134:A:MET:HE1 | 1:213:A:MET:H | 15       | 0.12          |
| (1,612) | 1:134:A:MET:HE2 | 1:213:A:MET:H | 15       | 0.12          |
| (1,612) | 1:134:A:MET:HE3 | 1:213:A:MET:H | 15       | 0.12          |
| (1,612) | 1:134:A:MET:HE1 | 1:213:A:MET:H | 18       | 0.12          |
| (1,612) | 1:134:A:MET:HE2 | 1:213:A:MET:H | 18       | 0.12          |
| (1,612) | 1:134:A:MET:HE3 | 1:213:A:MET:H | 18       | 0.12          |
| (1,611) | 1:134:A:MET:HE1 | 1:218:A:TYR:H | 1        | 0.12          |
| (1,611) | 1:134:A:MET:HE2 | 1:218:A:TYR:H | 1        | 0.12          |
| (1,611) | 1:134:A:MET:HE3 | 1:218:A:TYR:H | 1        | 0.12          |
| (1,611) | 1:134:A:MET:HE1 | 1:218:A:TYR:H | 3        | 0.12          |
| (1,611) | 1:134:A:MET:HE2 | 1:218:A:TYR:H | 3        | 0.12          |
| (1,611) | 1:134:A:MET:HE3 | 1:218:A:TYR:H | 3        | 0.12          |
| (1,611) | 1:134:A:MET:HE1 | 1:218:A:TYR:H | 4        | 0.12          |
| (1,611) | 1:134:A:MET:HE2 | 1:218:A:TYR:H | 4        | 0.12          |
| (1,611) | 1:134:A:MET:HE3 | 1:218:A:TYR:H | 4        | 0.12          |
| (1,611) | 1:134:A:MET:HE1 | 1:218:A:TYR:H | 6        | 0.12          |
| (1,611) | 1:134:A:MET:HE2 | 1:218:A:TYR:H | 6        | 0.12          |
| (1,611) | 1:134:A:MET:HE3 | 1:218:A:TYR:H | 6        | 0.12          |
| (1,611) | 1:134:A:MET:HE1 | 1:218:A:TYR:H | 7        | 0.12          |
| (1,611) | 1:134:A:MET:HE2 | 1:218:A:TYR:H | 7        | 0.12          |
| (1,611) | 1:134:A:MET:HE3 | 1:218:A:TYR:H | 7        | 0.12          |
| (1,611) | 1:134:A:MET:HE1 | 1:218:A:TYR:H | 8        | 0.12          |
| (1,611) | 1:134:A:MET:HE2 | 1:218:A:TYR:H | 8        | 0.12          |
| (1,611) | 1:134:A:MET:HE3 | 1:218:A:TYR:H | 8        | 0.12          |
| (1,611) | 1:134:A:MET:HE1 | 1:218:A:TYR:H | 9        | 0.12          |
| (1,611) | 1:134:A:MET:HE2 | 1:218:A:TYR:H | 9        | 0.12          |
| (1,611) | 1:134:A:MET:HE3 | 1:218:A:TYR:H | 9        | 0.12          |
| (1,611) | 1:134:A:MET:HE1 | 1:218:A:TYR:H | 10       | 0.12          |
| (1,611) | 1:134:A:MET:HE2 | 1:218:A:TYR:H | 10       | 0.12          |
| (1,611) | 1:134:A:MET:HE3 | 1:218:A:TYR:H | 10       | 0.12          |
| (1,611) | 1:134:A:MET:HE1 | 1:218:A:TYR:H | 13       | 0.12          |
| (1,611) | 1:134:A:MET:HE2 | 1:218:A:TYR:H | 13       | 0.12          |
| (1,611) | 1:134:A:MET:HE3 | 1:218:A:TYR:H | 13       | 0.12          |
| (1,611) | 1:134:A:MET:HE1 | 1:218:A:TYR:H | 14       | 0.12          |
| (1,611) | 1:134:A:MET:HE2 | 1:218:A:TYR:H | 14       | 0.12          |
| (1,611) | 1:134:A:MET:HE3 | 1:218:A:TYR:H | 14       | 0.12          |
| (1,611) | 1:134:A:MET:HE1 | 1:218:A:TYR:H | 17       | 0.12          |
| (1,611) | 1:134:A:MET:HE2 | 1:218:A:TYR:H | 17       | 0.12          |
| (1,611) | 1:134:A:MET:HE3 | 1:218:A:TYR:H | 17       | 0.12          |
| (1,611) | 1:134:A:MET:HE1 | 1:218:A:TYR:H | 19       | 0.12          |
| (1,611) | 1:134:A:MET:HE2 | 1:218:A:TYR:H | 19       | 0.12          |
| (1,611) | 1:134:A:MET:HE3 | 1:218:A:TYR:H | 19       | 0.12          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,611) | 1:134:A:MET:HE1  | 1:218:A:TYR:H    | 20       | 0.12          |
| (1,611) | 1:134:A:MET:HE2  | 1:218:A:TYR:H    | 20       | 0.12          |
| (1,611) | 1:134:A:MET:HE3  | 1:218:A:TYR:H    | 20       | 0.12          |
| (1,601) | 1:166:A:VAL:HG21 | 1:170:A:SER:HB2  | 20       | 0.12          |
| (1,601) | 1:166:A:VAL:HG22 | 1:170:A:SER:HB2  | 20       | 0.12          |
| (1,601) | 1:166:A:VAL:HG23 | 1:170:A:SER:HB2  | 20       | 0.12          |
| (1,582) | 1:139:A:ILE:HG21 | 1:205:A:MET:HE1  | 12       | 0.12          |
| (1,582) | 1:139:A:ILE:HG21 | 1:205:A:MET:HE2  | 12       | 0.12          |
| (1,582) | 1:139:A:ILE:HG21 | 1:205:A:MET:HE3  | 12       | 0.12          |
| (1,582) | 1:139:A:ILE:HG22 | 1:205:A:MET:HE1  | 12       | 0.12          |
| (1,582) | 1:139:A:ILE:HG22 | 1:205:A:MET:HE2  | 12       | 0.12          |
| (1,582) | 1:139:A:ILE:HG22 | 1:205:A:MET:HE3  | 12       | 0.12          |
| (1,582) | 1:139:A:ILE:HG23 | 1:205:A:MET:HE1  | 12       | 0.12          |
| (1,582) | 1:139:A:ILE:HG23 | 1:205:A:MET:HE2  | 12       | 0.12          |
| (1,582) | 1:139:A:ILE:HG23 | 1:205:A:MET:HE3  | 12       | 0.12          |
| (1,538) | 1:146:A:GLU:HG3  | 1:205:A:MET:HE1  | 18       | 0.12          |
| (1,538) | 1:146:A:GLU:HG3  | 1:205:A:MET:HE2  | 18       | 0.12          |
| (1,538) | 1:146:A:GLU:HG3  | 1:205:A:MET:HE3  | 18       | 0.12          |
| (1,527) | 1:202:A:ASP:HB2  | 1:203:A:VAL:HG11 | 5        | 0.12          |
| (1,527) | 1:202:A:ASP:HB2  | 1:203:A:VAL:HG12 | 5        | 0.12          |
| (1,527) | 1:202:A:ASP:HB2  | 1:203:A:VAL:HG13 | 5        | 0.12          |
| (1,507) | 1:211:A:GLU:HG3  | 1:214:A:CYS:HB2  | 5        | 0.12          |
| (1,472) | 1:194:A:LYS:HE2  | 1:195:A:GLY:HA3  | 17       | 0.12          |
| (1,472) | 1:194:A:LYS:HE3  | 1:195:A:GLY:HA3  | 17       | 0.12          |
| (1,448) | 1:226:A:TYR:HE1  | 1:230:A:ARG:HD2  | 14       | 0.12          |
| (1,448) | 1:226:A:TYR:HE2  | 1:230:A:ARG:HD2  | 14       | 0.12          |
| (1,445) | 1:180:A:VAL:HA   | 1:184:A:ILE:HG12 | 15       | 0.12          |
| (1,434) | 1:226:A:TYR:HD1  | 1:230:A:ARG:HD2  | 13       | 0.12          |
| (1,434) | 1:226:A:TYR:HD2  | 1:230:A:ARG:HD2  | 13       | 0.12          |
| (1,421) | 1:121:A:VAL:HG11 | 1:123:A:GLY:HA2  | 17       | 0.12          |
| (1,421) | 1:121:A:VAL:HG11 | 1:123:A:GLY:HA3  | 17       | 0.12          |
| (1,421) | 1:121:A:VAL:HG12 | 1:123:A:GLY:HA2  | 17       | 0.12          |
| (1,421) | 1:121:A:VAL:HG12 | 1:123:A:GLY:HA3  | 17       | 0.12          |
| (1,421) | 1:121:A:VAL:HG13 | 1:123:A:GLY:HA2  | 17       | 0.12          |
| (1,421) | 1:121:A:VAL:HG13 | 1:123:A:GLY:HA3  | 17       | 0.12          |
| (1,393) | 1:120:A:SER:HB2  | 1:121:A:VAL:HG11 | 1        | 0.12          |
| (1,393) | 1:120:A:SER:HB2  | 1:121:A:VAL:HG12 | 1        | 0.12          |
| (1,393) | 1:120:A:SER:HB2  | 1:121:A:VAL:HG13 | 1        | 0.12          |
| (1,393) | 1:120:A:SER:HB3  | 1:121:A:VAL:HG11 | 1        | 0.12          |
| (1,393) | 1:120:A:SER:HB3  | 1:121:A:VAL:HG12 | 1        | 0.12          |
| (1,393) | 1:120:A:SER:HB3  | 1:121:A:VAL:HG13 | 1        | 0.12          |
| (1,393) | 1:120:A:SER:HB2  | 1:121:A:VAL:HG11 | 11       | 0.12          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,393) | 1:120:A:SER:HB2  | 1:121:A:VAL:HG12 | 11       | 0.12          |
| (1,393) | 1:120:A:SER:HB2  | 1:121:A:VAL:HG13 | 11       | 0.12          |
| (1,393) | 1:120:A:SER:HB3  | 1:121:A:VAL:HG11 | 11       | 0.12          |
| (1,393) | 1:120:A:SER:HB3  | 1:121:A:VAL:HG12 | 11       | 0.12          |
| (1,393) | 1:120:A:SER:HB3  | 1:121:A:VAL:HG13 | 11       | 0.12          |
| (1,393) | 1:120:A:SER:HB2  | 1:121:A:VAL:HG11 | 13       | 0.12          |
| (1,393) | 1:120:A:SER:HB2  | 1:121:A:VAL:HG12 | 13       | 0.12          |
| (1,393) | 1:120:A:SER:HB2  | 1:121:A:VAL:HG13 | 13       | 0.12          |
| (1,393) | 1:120:A:SER:HB3  | 1:121:A:VAL:HG11 | 13       | 0.12          |
| (1,393) | 1:120:A:SER:HB3  | 1:121:A:VAL:HG12 | 13       | 0.12          |
| (1,393) | 1:120:A:SER:HB3  | 1:121:A:VAL:HG13 | 13       | 0.12          |
| (1,393) | 1:120:A:SER:HB2  | 1:121:A:VAL:HG11 | 14       | 0.12          |
| (1,393) | 1:120:A:SER:HB2  | 1:121:A:VAL:HG12 | 14       | 0.12          |
| (1,393) | 1:120:A:SER:HB2  | 1:121:A:VAL:HG13 | 14       | 0.12          |
| (1,393) | 1:120:A:SER:HB3  | 1:121:A:VAL:HG11 | 14       | 0.12          |
| (1,393) | 1:120:A:SER:HB3  | 1:121:A:VAL:HG12 | 14       | 0.12          |
| (1,393) | 1:120:A:SER:HB3  | 1:121:A:VAL:HG13 | 14       | 0.12          |
| (1,389) | 1:121:A:VAL:HA   | 1:122:A:VAL:HG11 | 8        | 0.12          |
| (1,389) | 1:121:A:VAL:HA   | 1:122:A:VAL:HG12 | 8        | 0.12          |
| (1,389) | 1:121:A:VAL:HA   | 1:122:A:VAL:HG13 | 8        | 0.12          |
| (1,362) | 1:172:A:GLN:HG3  | 1:215:A:VAL:HG21 | 11       | 0.12          |
| (1,362) | 1:172:A:GLN:HG3  | 1:215:A:VAL:HG22 | 11       | 0.12          |
| (1,362) | 1:172:A:GLN:HG3  | 1:215:A:VAL:HG23 | 11       | 0.12          |
| (1,361) | 1:121:A:VAL:HG21 | 1:122:A:VAL:H    | 15       | 0.12          |
| (1,361) | 1:121:A:VAL:HG22 | 1:122:A:VAL:H    | 15       | 0.12          |
| (1,361) | 1:121:A:VAL:HG23 | 1:122:A:VAL:H    | 15       | 0.12          |
| (1,359) | 1:122:A:VAL:HG21 | 1:182:A:ILE:HG21 | 7        | 0.12          |
| (1,359) | 1:122:A:VAL:HG21 | 1:182:A:ILE:HG22 | 7        | 0.12          |
| (1,359) | 1:122:A:VAL:HG21 | 1:182:A:ILE:HG23 | 7        | 0.12          |
| (1,359) | 1:122:A:VAL:HG22 | 1:182:A:ILE:HG21 | 7        | 0.12          |
| (1,359) | 1:122:A:VAL:HG22 | 1:182:A:ILE:HG22 | 7        | 0.12          |
| (1,359) | 1:122:A:VAL:HG22 | 1:182:A:ILE:HG23 | 7        | 0.12          |
| (1,359) | 1:122:A:VAL:HG23 | 1:182:A:ILE:HG21 | 7        | 0.12          |
| (1,359) | 1:122:A:VAL:HG23 | 1:182:A:ILE:HG22 | 7        | 0.12          |
| (1,359) | 1:122:A:VAL:HG23 | 1:182:A:ILE:HG23 | 7        | 0.12          |
| (1,350) | 1:122:A:VAL:HG21 | 1:123:A:GLY:H    | 15       | 0.12          |
| (1,350) | 1:122:A:VAL:HG22 | 1:123:A:GLY:H    | 15       | 0.12          |
| (1,350) | 1:122:A:VAL:HG23 | 1:123:A:GLY:H    | 15       | 0.12          |
| (1,348) | 1:122:A:VAL:HG21 | 1:124:A:GLY:HA2  | 3        | 0.12          |
| (1,348) | 1:122:A:VAL:HG21 | 1:124:A:GLY:HA3  | 3        | 0.12          |
| (1,348) | 1:122:A:VAL:HG22 | 1:124:A:GLY:HA2  | 3        | 0.12          |
| (1,348) | 1:122:A:VAL:HG22 | 1:124:A:GLY:HA3  | 3        | 0.12          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,348) | 1:122:A:VAL:HG23 | 1:124:A:GLY:HA2  | 3        | 0.12          |
| (1,348) | 1:122:A:VAL:HG23 | 1:124:A:GLY:HA3  | 3        | 0.12          |
| (1,348) | 1:122:A:VAL:HG21 | 1:124:A:GLY:HA2  | 5        | 0.12          |
| (1,348) | 1:122:A:VAL:HG21 | 1:124:A:GLY:HA3  | 5        | 0.12          |
| (1,348) | 1:122:A:VAL:HG22 | 1:124:A:GLY:HA2  | 5        | 0.12          |
| (1,348) | 1:122:A:VAL:HG22 | 1:124:A:GLY:HA3  | 5        | 0.12          |
| (1,348) | 1:122:A:VAL:HG23 | 1:124:A:GLY:HA2  | 5        | 0.12          |
| (1,348) | 1:122:A:VAL:HG23 | 1:124:A:GLY:HA3  | 5        | 0.12          |
| (1,348) | 1:122:A:VAL:HG21 | 1:124:A:GLY:HA2  | 17       | 0.12          |
| (1,348) | 1:122:A:VAL:HG21 | 1:124:A:GLY:HA3  | 17       | 0.12          |
| (1,348) | 1:122:A:VAL:HG22 | 1:124:A:GLY:HA2  | 17       | 0.12          |
| (1,348) | 1:122:A:VAL:HG22 | 1:124:A:GLY:HA3  | 17       | 0.12          |
| (1,348) | 1:122:A:VAL:HG23 | 1:124:A:GLY:HA2  | 17       | 0.12          |
| (1,348) | 1:122:A:VAL:HG23 | 1:124:A:GLY:HA3  | 17       | 0.12          |
| (1,348) | 1:122:A:VAL:HG21 | 1:124:A:GLY:HA2  | 20       | 0.12          |
| (1,348) | 1:122:A:VAL:HG21 | 1:124:A:GLY:HA3  | 20       | 0.12          |
| (1,348) | 1:122:A:VAL:HG22 | 1:124:A:GLY:HA2  | 20       | 0.12          |
| (1,348) | 1:122:A:VAL:HG22 | 1:124:A:GLY:HA3  | 20       | 0.12          |
| (1,348) | 1:122:A:VAL:HG23 | 1:124:A:GLY:HA2  | 20       | 0.12          |
| (1,348) | 1:122:A:VAL:HG23 | 1:124:A:GLY:HA3  | 20       | 0.12          |
| (1,341) | 1:186:A:GLN:H    | 1:189:A:VAL:HG21 | 15       | 0.12          |
| (1,341) | 1:186:A:GLN:H    | 1:189:A:VAL:HG22 | 15       | 0.12          |
| (1,341) | 1:186:A:GLN:H    | 1:189:A:VAL:HG23 | 15       | 0.12          |
| (1,332) | 1:185:A:LYS:HD2  | 1:189:A:VAL:HG11 | 17       | 0.12          |
| (1,332) | 1:185:A:LYS:HD2  | 1:189:A:VAL:HG12 | 17       | 0.12          |
| (1,332) | 1:185:A:LYS:HD2  | 1:189:A:VAL:HG13 | 17       | 0.12          |
| (1,332) | 1:185:A:LYS:HD3  | 1:189:A:VAL:HG11 | 17       | 0.12          |
| (1,332) | 1:185:A:LYS:HD3  | 1:189:A:VAL:HG12 | 17       | 0.12          |
| (1,332) | 1:185:A:LYS:HD3  | 1:189:A:VAL:HG13 | 17       | 0.12          |
| (1,329) | 1:185:A:LYS:HD2  | 1:189:A:VAL:HG21 | 11       | 0.12          |
| (1,329) | 1:185:A:LYS:HD2  | 1:189:A:VAL:HG22 | 11       | 0.12          |
| (1,329) | 1:185:A:LYS:HD2  | 1:189:A:VAL:HG23 | 11       | 0.12          |
| (1,329) | 1:185:A:LYS:HD3  | 1:189:A:VAL:HG21 | 11       | 0.12          |
| (1,329) | 1:185:A:LYS:HD3  | 1:189:A:VAL:HG22 | 11       | 0.12          |
| (1,329) | 1:185:A:LYS:HD3  | 1:189:A:VAL:HG23 | 11       | 0.12          |
| (1,312) | 1:166:A:VAL:HG21 | 1:170:A:SER:HB3  | 9        | 0.12          |
| (1,312) | 1:166:A:VAL:HG22 | 1:170:A:SER:HB3  | 9        | 0.12          |
| (1,312) | 1:166:A:VAL:HG23 | 1:170:A:SER:HB3  | 9        | 0.12          |
| (1,307) | 1:176:A:VAL:HG11 | 1:215:A:VAL:HG21 | 10       | 0.12          |
| (1,307) | 1:176:A:VAL:HG11 | 1:215:A:VAL:HG22 | 10       | 0.12          |
| (1,307) | 1:176:A:VAL:HG11 | 1:215:A:VAL:HG23 | 10       | 0.12          |
| (1,307) | 1:176:A:VAL:HG12 | 1:215:A:VAL:HG21 | 10       | 0.12          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,307) | 1:176:A:VAL:HG12 | 1:215:A:VAL:HG22 | 10       | 0.12          |
| (1,307) | 1:176:A:VAL:HG12 | 1:215:A:VAL:HG23 | 10       | 0.12          |
| (1,307) | 1:176:A:VAL:HG13 | 1:215:A:VAL:HG21 | 10       | 0.12          |
| (1,307) | 1:176:A:VAL:HG13 | 1:215:A:VAL:HG22 | 10       | 0.12          |
| (1,307) | 1:176:A:VAL:HG13 | 1:215:A:VAL:HG23 | 10       | 0.12          |
| (1,307) | 1:176:A:VAL:HG11 | 1:215:A:VAL:HG21 | 11       | 0.12          |
| (1,307) | 1:176:A:VAL:HG11 | 1:215:A:VAL:HG22 | 11       | 0.12          |
| (1,307) | 1:176:A:VAL:HG11 | 1:215:A:VAL:HG23 | 11       | 0.12          |
| (1,307) | 1:176:A:VAL:HG12 | 1:215:A:VAL:HG21 | 11       | 0.12          |
| (1,307) | 1:176:A:VAL:HG12 | 1:215:A:VAL:HG22 | 11       | 0.12          |
| (1,307) | 1:176:A:VAL:HG12 | 1:215:A:VAL:HG23 | 11       | 0.12          |
| (1,307) | 1:176:A:VAL:HG13 | 1:215:A:VAL:HG21 | 11       | 0.12          |
| (1,307) | 1:176:A:VAL:HG13 | 1:215:A:VAL:HG22 | 11       | 0.12          |
| (1,307) | 1:176:A:VAL:HG13 | 1:215:A:VAL:HG23 | 11       | 0.12          |
| (1,296) | 1:187:A:HIS:HB3  | 1:190:A:THR:HG21 | 2        | 0.12          |
| (1,296) | 1:187:A:HIS:HB3  | 1:190:A:THR:HG22 | 2        | 0.12          |
| (1,296) | 1:187:A:HIS:HB3  | 1:190:A:THR:HG23 | 2        | 0.12          |
| (1,296) | 1:187:A:HIS:HB3  | 1:190:A:THR:HG21 | 4        | 0.12          |
| (1,296) | 1:187:A:HIS:HB3  | 1:190:A:THR:HG22 | 4        | 0.12          |
| (1,296) | 1:187:A:HIS:HB3  | 1:190:A:THR:HG23 | 4        | 0.12          |
| (1,296) | 1:187:A:HIS:HB3  | 1:190:A:THR:HG21 | 6        | 0.12          |
| (1,296) | 1:187:A:HIS:HB3  | 1:190:A:THR:HG22 | 6        | 0.12          |
| (1,296) | 1:187:A:HIS:HB3  | 1:190:A:THR:HG23 | 6        | 0.12          |
| (1,296) | 1:187:A:HIS:HB3  | 1:190:A:THR:HG21 | 10       | 0.12          |
| (1,296) | 1:187:A:HIS:HB3  | 1:190:A:THR:HG22 | 10       | 0.12          |
| (1,296) | 1:187:A:HIS:HB3  | 1:190:A:THR:HG23 | 10       | 0.12          |
| (1,296) | 1:187:A:HIS:HB3  | 1:190:A:THR:HG21 | 16       | 0.12          |
| (1,296) | 1:187:A:HIS:HB3  | 1:190:A:THR:HG22 | 16       | 0.12          |
| (1,296) | 1:187:A:HIS:HB3  | 1:190:A:THR:HG23 | 16       | 0.12          |
| (1,288) | 1:192:A:THR:HG21 | 1:196:A:GLU:HB2  | 18       | 0.12          |
| (1,288) | 1:192:A:THR:HG21 | 1:196:A:GLU:HB3  | 18       | 0.12          |
| (1,288) | 1:192:A:THR:HG22 | 1:196:A:GLU:HB2  | 18       | 0.12          |
| (1,288) | 1:192:A:THR:HG22 | 1:196:A:GLU:HB3  | 18       | 0.12          |
| (1,288) | 1:192:A:THR:HG23 | 1:196:A:GLU:HB2  | 18       | 0.12          |
| (1,288) | 1:192:A:THR:HG23 | 1:196:A:GLU:HB3  | 18       | 0.12          |
| (1,288) | 1:192:A:THR:HG21 | 1:196:A:GLU:HB2  | 19       | 0.12          |
| (1,288) | 1:192:A:THR:HG21 | 1:196:A:GLU:HB3  | 19       | 0.12          |
| (1,288) | 1:192:A:THR:HG22 | 1:196:A:GLU:HB2  | 19       | 0.12          |
| (1,288) | 1:192:A:THR:HG22 | 1:196:A:GLU:HB3  | 19       | 0.12          |
| (1,288) | 1:192:A:THR:HG23 | 1:196:A:GLU:HB2  | 19       | 0.12          |
| (1,288) | 1:192:A:THR:HG23 | 1:196:A:GLU:HB3  | 19       | 0.12          |
| (1,261) | 1:185:A:LYS:HD2  | 1:188:A:THR:HG21 | 4        | 0.12          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,261) | 1:185:A:LYS:HD2  | 1:188:A:THR:HG22 | 4        | 0.12          |
| (1,261) | 1:185:A:LYS:HD2  | 1:188:A:THR:HG23 | 4        | 0.12          |
| (1,261) | 1:185:A:LYS:HD3  | 1:188:A:THR:HG21 | 4        | 0.12          |
| (1,261) | 1:185:A:LYS:HD3  | 1:188:A:THR:HG22 | 4        | 0.12          |
| (1,261) | 1:185:A:LYS:HD3  | 1:188:A:THR:HG23 | 4        | 0.12          |
| (1,261) | 1:185:A:LYS:HD2  | 1:188:A:THR:HG21 | 6        | 0.12          |
| (1,261) | 1:185:A:LYS:HD2  | 1:188:A:THR:HG22 | 6        | 0.12          |
| (1,261) | 1:185:A:LYS:HD2  | 1:188:A:THR:HG23 | 6        | 0.12          |
| (1,261) | 1:185:A:LYS:HD3  | 1:188:A:THR:HG21 | 6        | 0.12          |
| (1,261) | 1:185:A:LYS:HD3  | 1:188:A:THR:HG22 | 6        | 0.12          |
| (1,261) | 1:185:A:LYS:HD3  | 1:188:A:THR:HG23 | 6        | 0.12          |
| (1,261) | 1:185:A:LYS:HD2  | 1:188:A:THR:HG21 | 10       | 0.12          |
| (1,261) | 1:185:A:LYS:HD2  | 1:188:A:THR:HG22 | 10       | 0.12          |
| (1,261) | 1:185:A:LYS:HD2  | 1:188:A:THR:HG23 | 10       | 0.12          |
| (1,261) | 1:185:A:LYS:HD3  | 1:188:A:THR:HG21 | 10       | 0.12          |
| (1,261) | 1:185:A:LYS:HD3  | 1:188:A:THR:HG22 | 10       | 0.12          |
| (1,261) | 1:185:A:LYS:HD3  | 1:188:A:THR:HG23 | 10       | 0.12          |
| (1,261) | 1:185:A:LYS:HD2  | 1:188:A:THR:HG21 | 12       | 0.12          |
| (1,261) | 1:185:A:LYS:HD2  | 1:188:A:THR:HG22 | 12       | 0.12          |
| (1,261) | 1:185:A:LYS:HD2  | 1:188:A:THR:HG23 | 12       | 0.12          |
| (1,261) | 1:185:A:LYS:HD3  | 1:188:A:THR:HG21 | 12       | 0.12          |
| (1,261) | 1:185:A:LYS:HD3  | 1:188:A:THR:HG22 | 12       | 0.12          |
| (1,261) | 1:185:A:LYS:HD3  | 1:188:A:THR:HG23 | 12       | 0.12          |
| (1,261) | 1:185:A:LYS:HD2  | 1:188:A:THR:HG21 | 15       | 0.12          |
| (1,261) | 1:185:A:LYS:HD2  | 1:188:A:THR:HG22 | 15       | 0.12          |
| (1,261) | 1:185:A:LYS:HD2  | 1:188:A:THR:HG23 | 15       | 0.12          |
| (1,261) | 1:185:A:LYS:HD3  | 1:188:A:THR:HG21 | 15       | 0.12          |
| (1,261) | 1:185:A:LYS:HD3  | 1:188:A:THR:HG22 | 15       | 0.12          |
| (1,261) | 1:185:A:LYS:HD3  | 1:188:A:THR:HG23 | 15       | 0.12          |
| (1,261) | 1:185:A:LYS:HD2  | 1:188:A:THR:HG21 | 16       | 0.12          |
| (1,261) | 1:185:A:LYS:HD2  | 1:188:A:THR:HG22 | 16       | 0.12          |
| (1,261) | 1:185:A:LYS:HD2  | 1:188:A:THR:HG23 | 16       | 0.12          |
| (1,261) | 1:185:A:LYS:HD3  | 1:188:A:THR:HG21 | 16       | 0.12          |
| (1,261) | 1:185:A:LYS:HD3  | 1:188:A:THR:HG22 | 16       | 0.12          |
| (1,261) | 1:185:A:LYS:HD3  | 1:188:A:THR:HG23 | 16       | 0.12          |
| (1,217) | 1:193:A:THR:HG21 | 1:196:A:GLU:HB2  | 1        | 0.12          |
| (1,217) | 1:193:A:THR:HG21 | 1:196:A:GLU:HB3  | 1        | 0.12          |
| (1,217) | 1:193:A:THR:HG22 | 1:196:A:GLU:HB2  | 1        | 0.12          |
| (1,217) | 1:193:A:THR:HG22 | 1:196:A:GLU:HB3  | 1        | 0.12          |
| (1,217) | 1:193:A:THR:HG23 | 1:196:A:GLU:HB2  | 1        | 0.12          |
| (1,217) | 1:193:A:THR:HG23 | 1:196:A:GLU:HB3  | 1        | 0.12          |
| (1,217) | 1:193:A:THR:HG21 | 1:196:A:GLU:HB2  | 7        | 0.12          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,217) | 1:193:A:THR:HG21 | 1:196:A:GLU:HB3  | 7        | 0.12          |
| (1,217) | 1:193:A:THR:HG22 | 1:196:A:GLU:HB2  | 7        | 0.12          |
| (1,217) | 1:193:A:THR:HG22 | 1:196:A:GLU:HB3  | 7        | 0.12          |
| (1,217) | 1:193:A:THR:HG23 | 1:196:A:GLU:HB2  | 7        | 0.12          |
| (1,217) | 1:193:A:THR:HG23 | 1:196:A:GLU:HB3  | 7        | 0.12          |
| (1,196) | 1:161:A:VAL:HG21 | 1:216:A:THR:HG21 | 1        | 0.12          |
| (1,196) | 1:161:A:VAL:HG21 | 1:216:A:THR:HG22 | 1        | 0.12          |
| (1,196) | 1:161:A:VAL:HG21 | 1:216:A:THR:HG23 | 1        | 0.12          |
| (1,196) | 1:161:A:VAL:HG22 | 1:216:A:THR:HG21 | 1        | 0.12          |
| (1,196) | 1:161:A:VAL:HG22 | 1:216:A:THR:HG22 | 1        | 0.12          |
| (1,196) | 1:161:A:VAL:HG22 | 1:216:A:THR:HG23 | 1        | 0.12          |
| (1,196) | 1:161:A:VAL:HG23 | 1:216:A:THR:HG21 | 1        | 0.12          |
| (1,196) | 1:161:A:VAL:HG23 | 1:216:A:THR:HG22 | 1        | 0.12          |
| (1,196) | 1:161:A:VAL:HG23 | 1:216:A:THR:HG23 | 1        | 0.12          |
| (1,196) | 1:161:A:VAL:HG21 | 1:216:A:THR:HG21 | 3        | 0.12          |
| (1,196) | 1:161:A:VAL:HG21 | 1:216:A:THR:HG22 | 3        | 0.12          |
| (1,196) | 1:161:A:VAL:HG21 | 1:216:A:THR:HG23 | 3        | 0.12          |
| (1,196) | 1:161:A:VAL:HG22 | 1:216:A:THR:HG21 | 3        | 0.12          |
| (1,196) | 1:161:A:VAL:HG22 | 1:216:A:THR:HG22 | 3        | 0.12          |
| (1,196) | 1:161:A:VAL:HG22 | 1:216:A:THR:HG23 | 3        | 0.12          |
| (1,196) | 1:161:A:VAL:HG23 | 1:216:A:THR:HG21 | 3        | 0.12          |
| (1,196) | 1:161:A:VAL:HG23 | 1:216:A:THR:HG22 | 3        | 0.12          |
| (1,196) | 1:161:A:VAL:HG23 | 1:216:A:THR:HG23 | 3        | 0.12          |
| (1,196) | 1:161:A:VAL:HG21 | 1:216:A:THR:HG21 | 6        | 0.12          |
| (1,196) | 1:161:A:VAL:HG21 | 1:216:A:THR:HG22 | 6        | 0.12          |
| (1,196) | 1:161:A:VAL:HG21 | 1:216:A:THR:HG23 | 6        | 0.12          |
| (1,196) | 1:161:A:VAL:HG22 | 1:216:A:THR:HG21 | 6        | 0.12          |
| (1,196) | 1:161:A:VAL:HG22 | 1:216:A:THR:HG22 | 6        | 0.12          |
| (1,196) | 1:161:A:VAL:HG22 | 1:216:A:THR:HG23 | 6        | 0.12          |
| (1,196) | 1:161:A:VAL:HG23 | 1:216:A:THR:HG21 | 6        | 0.12          |
| (1,196) | 1:161:A:VAL:HG23 | 1:216:A:THR:HG22 | 6        | 0.12          |
| (1,196) | 1:161:A:VAL:HG23 | 1:216:A:THR:HG23 | 6        | 0.12          |
| (1,177) | 1:195:A:GLY:HA3  | 1:197:A:ASN:HD21 | 8        | 0.12          |
| (1,112) | 1:214:A:CYS:HA   | 1:215:A:VAL:HG11 | 3        | 0.12          |
| (1,112) | 1:214:A:CYS:HA   | 1:215:A:VAL:HG12 | 3        | 0.12          |
| (1,112) | 1:214:A:CYS:HA   | 1:215:A:VAL:HG13 | 3        | 0.12          |
| (1,112) | 1:214:A:CYS:HA   | 1:215:A:VAL:HG11 | 7        | 0.12          |
| (1,112) | 1:214:A:CYS:HA   | 1:215:A:VAL:HG12 | 7        | 0.12          |
| (1,112) | 1:214:A:CYS:HA   | 1:215:A:VAL:HG13 | 7        | 0.12          |
| (1,112) | 1:214:A:CYS:HA   | 1:215:A:VAL:HG11 | 16       | 0.12          |
| (1,112) | 1:214:A:CYS:HA   | 1:215:A:VAL:HG12 | 16       | 0.12          |
| (1,112) | 1:214:A:CYS:HA   | 1:215:A:VAL:HG13 | 16       | 0.12          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,112)  | 1:214:A:CYS:HA   | 1:215:A:VAL:HG11 | 18       | 0.12          |
| (1,112)  | 1:214:A:CYS:HA   | 1:215:A:VAL:HG12 | 18       | 0.12          |
| (1,112)  | 1:214:A:CYS:HA   | 1:215:A:VAL:HG13 | 18       | 0.12          |
| (1,112)  | 1:214:A:CYS:HA   | 1:215:A:VAL:HG11 | 20       | 0.12          |
| (1,112)  | 1:214:A:CYS:HA   | 1:215:A:VAL:HG12 | 20       | 0.12          |
| (1,112)  | 1:214:A:CYS:HA   | 1:215:A:VAL:HG13 | 20       | 0.12          |
| (1,92)   | 1:209:A:VAL:H    | 1:209:A:VAL:HG11 | 2        | 0.12          |
| (1,92)   | 1:209:A:VAL:H    | 1:209:A:VAL:HG12 | 2        | 0.12          |
| (1,92)   | 1:209:A:VAL:H    | 1:209:A:VAL:HG13 | 2        | 0.12          |
| (1,77)   | 1:208:A:ARG:H    | 1:209:A:VAL:HG11 | 17       | 0.12          |
| (1,77)   | 1:208:A:ARG:H    | 1:209:A:VAL:HG12 | 17       | 0.12          |
| (1,77)   | 1:208:A:ARG:H    | 1:209:A:VAL:HG13 | 17       | 0.12          |
| (1,32)   | 1:219:A:GLN:HB3  | 1:220:A:LYS:HG3  | 7        | 0.12          |
| (1,31)   | 1:219:A:GLN:HA   | 1:220:A:LYS:HG3  | 20       | 0.12          |
| (1,15)   | 1:130:A:LEU:HD21 | 1:161:A:VAL:HA   | 8        | 0.12          |
| (1,15)   | 1:130:A:LEU:HD22 | 1:161:A:VAL:HA   | 8        | 0.12          |
| (1,15)   | 1:130:A:LEU:HD23 | 1:161:A:VAL:HA   | 8        | 0.12          |
| (1,15)   | 1:130:A:LEU:HD21 | 1:161:A:VAL:HA   | 13       | 0.12          |
| (1,15)   | 1:130:A:LEU:HD22 | 1:161:A:VAL:HA   | 13       | 0.12          |
| (1,15)   | 1:130:A:LEU:HD23 | 1:161:A:VAL:HA   | 13       | 0.12          |
| (1,2843) | 1:157:A:TYR:HE1  | 1:206:A:MET:HE1  | 8        | 0.11          |
| (1,2843) | 1:157:A:TYR:HE1  | 1:206:A:MET:HE2  | 8        | 0.11          |
| (1,2843) | 1:157:A:TYR:HE1  | 1:206:A:MET:HE3  | 8        | 0.11          |
| (1,2843) | 1:157:A:TYR:HE2  | 1:206:A:MET:HE1  | 8        | 0.11          |
| (1,2843) | 1:157:A:TYR:HE2  | 1:206:A:MET:HE2  | 8        | 0.11          |
| (1,2843) | 1:157:A:TYR:HE2  | 1:206:A:MET:HE3  | 8        | 0.11          |
| (1,2841) | 1:150:A:TYR:HA   | 1:157:A:TYR:HE1  | 5        | 0.11          |
| (1,2841) | 1:150:A:TYR:HA   | 1:157:A:TYR:HE2  | 5        | 0.11          |
| (1,2834) | 1:163:A:TYR:HE1  | 1:221:A:GLU:HG2  | 1        | 0.11          |
| (1,2834) | 1:163:A:TYR:HE2  | 1:221:A:GLU:HG2  | 1        | 0.11          |
| (1,2829) | 1:166:A:VAL:HB   | 1:218:A:TYR:HE1  | 3        | 0.11          |
| (1,2829) | 1:166:A:VAL:HB   | 1:218:A:TYR:HE2  | 3        | 0.11          |
| (1,2829) | 1:166:A:VAL:HB   | 1:218:A:TYR:HE1  | 12       | 0.11          |
| (1,2829) | 1:166:A:VAL:HB   | 1:218:A:TYR:HE2  | 12       | 0.11          |
| (1,2829) | 1:166:A:VAL:HB   | 1:218:A:TYR:HE1  | 17       | 0.11          |
| (1,2829) | 1:166:A:VAL:HB   | 1:218:A:TYR:HE2  | 17       | 0.11          |
| (1,2825) | 1:176:A:VAL:HG21 | 1:218:A:TYR:HE1  | 17       | 0.11          |
| (1,2825) | 1:176:A:VAL:HG21 | 1:218:A:TYR:HE2  | 17       | 0.11          |
| (1,2825) | 1:176:A:VAL:HG22 | 1:218:A:TYR:HE1  | 17       | 0.11          |
| (1,2825) | 1:176:A:VAL:HG22 | 1:218:A:TYR:HE2  | 17       | 0.11          |
| (1,2825) | 1:176:A:VAL:HG23 | 1:218:A:TYR:HE1  | 17       | 0.11          |
| (1,2825) | 1:176:A:VAL:HG23 | 1:218:A:TYR:HE2  | 17       | 0.11          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2807) | 1:149:A:TYR:HE1  | 1:153:A:ASN:HB3 | 5        | 0.11          |
| (1,2807) | 1:149:A:TYR:HE2  | 1:153:A:ASN:HB3 | 5        | 0.11          |
| (1,2806) | 1:149:A:TYR:HE1  | 1:205:A:MET:HB2 | 5        | 0.11          |
| (1,2806) | 1:149:A:TYR:HE2  | 1:205:A:MET:HB2 | 5        | 0.11          |
| (1,2791) | 1:126:A:GLY:HA2  | 1:128:A:TYR:HE1 | 4        | 0.11          |
| (1,2791) | 1:126:A:GLY:HA2  | 1:128:A:TYR:HE2 | 4        | 0.11          |
| (1,2752) | 1:169:A:TYR:HE1  | 1:174:A:ASN:HA  | 3        | 0.11          |
| (1,2752) | 1:169:A:TYR:HE2  | 1:174:A:ASN:HA  | 3        | 0.11          |
| (1,2752) | 1:169:A:TYR:HE1  | 1:174:A:ASN:HA  | 20       | 0.11          |
| (1,2752) | 1:169:A:TYR:HE2  | 1:174:A:ASN:HA  | 20       | 0.11          |
| (1,2751) | 1:164:A:ARG:HG2  | 1:169:A:TYR:HE1 | 3        | 0.11          |
| (1,2751) | 1:164:A:ARG:HG2  | 1:169:A:TYR:HE2 | 3        | 0.11          |
| (1,2751) | 1:164:A:ARG:HG2  | 1:169:A:TYR:HE1 | 8        | 0.11          |
| (1,2751) | 1:164:A:ARG:HG2  | 1:169:A:TYR:HE2 | 8        | 0.11          |
| (1,2751) | 1:164:A:ARG:HG2  | 1:169:A:TYR:HE1 | 12       | 0.11          |
| (1,2751) | 1:164:A:ARG:HG2  | 1:169:A:TYR:HE2 | 12       | 0.11          |
| (1,2751) | 1:164:A:ARG:HG2  | 1:169:A:TYR:HE1 | 15       | 0.11          |
| (1,2751) | 1:164:A:ARG:HG2  | 1:169:A:TYR:HE2 | 15       | 0.11          |
| (1,2744) | 1:164:A:ARG:HB3  | 1:169:A:TYR:HE1 | 5        | 0.11          |
| (1,2744) | 1:164:A:ARG:HB3  | 1:169:A:TYR:HE2 | 5        | 0.11          |
| (1,2709) | 1:145:A:TRP:HZ3  | 1:205:A:MET:HE1 | 18       | 0.11          |
| (1,2709) | 1:145:A:TRP:HZ3  | 1:205:A:MET:HE2 | 18       | 0.11          |
| (1,2709) | 1:145:A:TRP:HZ3  | 1:205:A:MET:HE3 | 18       | 0.11          |
| (1,2703) | 1:143:A:ASN:HB2  | 1:145:A:TRP:HD1 | 11       | 0.11          |
| (1,2703) | 1:143:A:ASN:HB3  | 1:145:A:TRP:HD1 | 11       | 0.11          |
| (1,2696) | 1:141:A:PHE:HZ   | 1:205:A:MET:HE1 | 8        | 0.11          |
| (1,2696) | 1:141:A:PHE:HZ   | 1:205:A:MET:HE2 | 8        | 0.11          |
| (1,2696) | 1:141:A:PHE:HZ   | 1:205:A:MET:HE3 | 8        | 0.11          |
| (1,2668) | 1:158:A:PRO:HD3  | 1:198:A:PHE:HE1 | 18       | 0.11          |
| (1,2668) | 1:158:A:PRO:HD3  | 1:198:A:PHE:HE2 | 18       | 0.11          |
| (1,2667) | 1:191:A:THR:HG21 | 1:198:A:PHE:HE1 | 6        | 0.11          |
| (1,2667) | 1:191:A:THR:HG21 | 1:198:A:PHE:HE2 | 6        | 0.11          |
| (1,2667) | 1:191:A:THR:HG22 | 1:198:A:PHE:HE1 | 6        | 0.11          |
| (1,2667) | 1:191:A:THR:HG22 | 1:198:A:PHE:HE2 | 6        | 0.11          |
| (1,2667) | 1:191:A:THR:HG23 | 1:198:A:PHE:HE1 | 6        | 0.11          |
| (1,2667) | 1:191:A:THR:HG23 | 1:198:A:PHE:HE2 | 6        | 0.11          |
| (1,2667) | 1:191:A:THR:HG21 | 1:198:A:PHE:HE1 | 13       | 0.11          |
| (1,2667) | 1:191:A:THR:HG21 | 1:198:A:PHE:HE2 | 13       | 0.11          |
| (1,2667) | 1:191:A:THR:HG22 | 1:198:A:PHE:HE1 | 13       | 0.11          |
| (1,2667) | 1:191:A:THR:HG22 | 1:198:A:PHE:HE2 | 13       | 0.11          |
| (1,2667) | 1:191:A:THR:HG23 | 1:198:A:PHE:HE1 | 13       | 0.11          |
| (1,2667) | 1:191:A:THR:HG23 | 1:198:A:PHE:HE2 | 13       | 0.11          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2667) | 1:191:A:THR:HG21 | 1:198:A:PHE:HE1 | 18       | 0.11          |
| (1,2667) | 1:191:A:THR:HG21 | 1:198:A:PHE:HE2 | 18       | 0.11          |
| (1,2667) | 1:191:A:THR:HG22 | 1:198:A:PHE:HE1 | 18       | 0.11          |
| (1,2667) | 1:191:A:THR:HG22 | 1:198:A:PHE:HE2 | 18       | 0.11          |
| (1,2667) | 1:191:A:THR:HG23 | 1:198:A:PHE:HE1 | 18       | 0.11          |
| (1,2667) | 1:191:A:THR:HG23 | 1:198:A:PHE:HE2 | 18       | 0.11          |
| (1,2639) | 1:150:A:TYR:HE1  | 1:157:A:TYR:HD1 | 16       | 0.11          |
| (1,2639) | 1:150:A:TYR:HE1  | 1:157:A:TYR:HD2 | 16       | 0.11          |
| (1,2639) | 1:150:A:TYR:HE2  | 1:157:A:TYR:HD1 | 16       | 0.11          |
| (1,2639) | 1:150:A:TYR:HE2  | 1:157:A:TYR:HD2 | 16       | 0.11          |
| (1,2636) | 1:157:A:TYR:HD1  | 1:209:A:VAL:H   | 4        | 0.11          |
| (1,2636) | 1:157:A:TYR:HD2  | 1:209:A:VAL:H   | 4        | 0.11          |
| (1,2636) | 1:157:A:TYR:HD1  | 1:209:A:VAL:H   | 10       | 0.11          |
| (1,2636) | 1:157:A:TYR:HD2  | 1:209:A:VAL:H   | 10       | 0.11          |
| (1,2631) | 1:198:A:PHE:HD1  | 1:203:A:VAL:HA  | 8        | 0.11          |
| (1,2631) | 1:198:A:PHE:HD2  | 1:203:A:VAL:HA  | 8        | 0.11          |
| (1,2631) | 1:198:A:PHE:HD1  | 1:203:A:VAL:HA  | 9        | 0.11          |
| (1,2631) | 1:198:A:PHE:HD2  | 1:203:A:VAL:HA  | 9        | 0.11          |
| (1,2631) | 1:198:A:PHE:HD1  | 1:203:A:VAL:HA  | 13       | 0.11          |
| (1,2631) | 1:198:A:PHE:HD2  | 1:203:A:VAL:HA  | 13       | 0.11          |
| (1,2631) | 1:198:A:PHE:HD1  | 1:203:A:VAL:HA  | 14       | 0.11          |
| (1,2631) | 1:198:A:PHE:HD2  | 1:203:A:VAL:HA  | 14       | 0.11          |
| (1,2631) | 1:198:A:PHE:HD1  | 1:203:A:VAL:HA  | 15       | 0.11          |
| (1,2631) | 1:198:A:PHE:HD2  | 1:203:A:VAL:HA  | 15       | 0.11          |
| (1,2631) | 1:198:A:PHE:HD1  | 1:203:A:VAL:HA  | 19       | 0.11          |
| (1,2631) | 1:198:A:PHE:HD2  | 1:203:A:VAL:HA  | 19       | 0.11          |
| (1,2600) | 1:166:A:VAL:HG21 | 1:175:A:PHE:HE1 | 20       | 0.11          |
| (1,2600) | 1:166:A:VAL:HG21 | 1:175:A:PHE:HE2 | 20       | 0.11          |
| (1,2600) | 1:166:A:VAL:HG22 | 1:175:A:PHE:HE1 | 20       | 0.11          |
| (1,2600) | 1:166:A:VAL:HG22 | 1:175:A:PHE:HE2 | 20       | 0.11          |
| (1,2600) | 1:166:A:VAL:HG23 | 1:175:A:PHE:HE1 | 20       | 0.11          |
| (1,2600) | 1:166:A:VAL:HG23 | 1:175:A:PHE:HE2 | 20       | 0.11          |
| (1,2599) | 1:166:A:VAL:HB   | 1:175:A:PHE:HE1 | 12       | 0.11          |
| (1,2599) | 1:166:A:VAL:HB   | 1:175:A:PHE:HE2 | 12       | 0.11          |
| (1,2591) | 1:169:A:TYR:HE1  | 1:175:A:PHE:HE1 | 17       | 0.11          |
| (1,2591) | 1:169:A:TYR:HE1  | 1:175:A:PHE:HE2 | 17       | 0.11          |
| (1,2591) | 1:169:A:TYR:HE2  | 1:175:A:PHE:HE1 | 17       | 0.11          |
| (1,2591) | 1:169:A:TYR:HE2  | 1:175:A:PHE:HE2 | 17       | 0.11          |
| (1,2580) | 1:166:A:VAL:HB   | 1:218:A:TYR:HD1 | 12       | 0.11          |
| (1,2580) | 1:166:A:VAL:HB   | 1:218:A:TYR:HD2 | 12       | 0.11          |
| (1,2580) | 1:166:A:VAL:HB   | 1:218:A:TYR:HD1 | 17       | 0.11          |
| (1,2580) | 1:166:A:VAL:HB   | 1:218:A:TYR:HD2 | 17       | 0.11          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2575) | 1:166:A:VAL:HG21 | 1:218:A:TYR:HD1  | 14       | 0.11          |
| (1,2575) | 1:166:A:VAL:HG21 | 1:218:A:TYR:HD2  | 14       | 0.11          |
| (1,2575) | 1:166:A:VAL:HG22 | 1:218:A:TYR:HD1  | 14       | 0.11          |
| (1,2575) | 1:166:A:VAL:HG22 | 1:218:A:TYR:HD2  | 14       | 0.11          |
| (1,2575) | 1:166:A:VAL:HG23 | 1:218:A:TYR:HD1  | 14       | 0.11          |
| (1,2575) | 1:166:A:VAL:HG23 | 1:218:A:TYR:HD2  | 14       | 0.11          |
| (1,2557) | 1:128:A:TYR:HD1  | 1:164:A:ARG:HA   | 8        | 0.11          |
| (1,2557) | 1:128:A:TYR:HD2  | 1:164:A:ARG:HA   | 8        | 0.11          |
| (1,2526) | 1:155:A:TYR:HD1  | 1:156:A:ARG:HG3  | 13       | 0.11          |
| (1,2526) | 1:155:A:TYR:HD2  | 1:156:A:ARG:HG3  | 13       | 0.11          |
| (1,2520) | 1:154:A:MET:HE1  | 1:155:A:TYR:HD1  | 3        | 0.11          |
| (1,2520) | 1:154:A:MET:HE1  | 1:155:A:TYR:HD2  | 3        | 0.11          |
| (1,2520) | 1:154:A:MET:HE2  | 1:155:A:TYR:HD1  | 3        | 0.11          |
| (1,2520) | 1:154:A:MET:HE2  | 1:155:A:TYR:HD2  | 3        | 0.11          |
| (1,2520) | 1:154:A:MET:HE3  | 1:155:A:TYR:HD1  | 3        | 0.11          |
| (1,2520) | 1:154:A:MET:HE3  | 1:155:A:TYR:HD2  | 3        | 0.11          |
| (1,2520) | 1:154:A:MET:HE1  | 1:155:A:TYR:HD1  | 4        | 0.11          |
| (1,2520) | 1:154:A:MET:HE1  | 1:155:A:TYR:HD2  | 4        | 0.11          |
| (1,2520) | 1:154:A:MET:HE2  | 1:155:A:TYR:HD1  | 4        | 0.11          |
| (1,2520) | 1:154:A:MET:HE2  | 1:155:A:TYR:HD2  | 4        | 0.11          |
| (1,2520) | 1:154:A:MET:HE3  | 1:155:A:TYR:HD1  | 4        | 0.11          |
| (1,2520) | 1:154:A:MET:HE3  | 1:155:A:TYR:HD2  | 4        | 0.11          |
| (1,2520) | 1:154:A:MET:HE1  | 1:155:A:TYR:HD1  | 17       | 0.11          |
| (1,2520) | 1:154:A:MET:HE1  | 1:155:A:TYR:HD2  | 17       | 0.11          |
| (1,2520) | 1:154:A:MET:HE2  | 1:155:A:TYR:HD1  | 17       | 0.11          |
| (1,2520) | 1:154:A:MET:HE2  | 1:155:A:TYR:HD2  | 17       | 0.11          |
| (1,2520) | 1:154:A:MET:HE3  | 1:155:A:TYR:HD1  | 17       | 0.11          |
| (1,2520) | 1:154:A:MET:HE3  | 1:155:A:TYR:HD2  | 17       | 0.11          |
| (1,2511) | 1:154:A:MET:HG2  | 1:155:A:TYR:HD1  | 1        | 0.11          |
| (1,2511) | 1:154:A:MET:HG2  | 1:155:A:TYR:HD2  | 1        | 0.11          |
| (1,2510) | 1:226:A:TYR:HD1  | 1:229:A:ARG:HB2  | 16       | 0.11          |
| (1,2510) | 1:226:A:TYR:HD2  | 1:229:A:ARG:HB2  | 16       | 0.11          |
| (1,2500) | 1:149:A:TYR:HD1  | 1:201:A:THR:HG21 | 12       | 0.11          |
| (1,2500) | 1:149:A:TYR:HD1  | 1:201:A:THR:HG22 | 12       | 0.11          |
| (1,2500) | 1:149:A:TYR:HD1  | 1:201:A:THR:HG23 | 12       | 0.11          |
| (1,2500) | 1:149:A:TYR:HD2  | 1:201:A:THR:HG21 | 12       | 0.11          |
| (1,2500) | 1:149:A:TYR:HD2  | 1:201:A:THR:HG22 | 12       | 0.11          |
| (1,2500) | 1:149:A:TYR:HD2  | 1:201:A:THR:HG23 | 12       | 0.11          |
| (1,2483) | 1:161:A:VAL:HG21 | 1:163:A:TYR:HD1  | 2        | 0.11          |
| (1,2483) | 1:161:A:VAL:HG21 | 1:163:A:TYR:HD2  | 2        | 0.11          |
| (1,2483) | 1:161:A:VAL:HG22 | 1:163:A:TYR:HD1  | 2        | 0.11          |
| (1,2483) | 1:161:A:VAL:HG22 | 1:163:A:TYR:HD2  | 2        | 0.11          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2483) | 1:161:A:VAL:HG23 | 1:163:A:TYR:HD1  | 2        | 0.11          |
| (1,2483) | 1:161:A:VAL:HG23 | 1:163:A:TYR:HD2  | 2        | 0.11          |
| (1,2483) | 1:161:A:VAL:HG21 | 1:163:A:TYR:HD1  | 14       | 0.11          |
| (1,2483) | 1:161:A:VAL:HG21 | 1:163:A:TYR:HD2  | 14       | 0.11          |
| (1,2483) | 1:161:A:VAL:HG22 | 1:163:A:TYR:HD1  | 14       | 0.11          |
| (1,2483) | 1:161:A:VAL:HG22 | 1:163:A:TYR:HD2  | 14       | 0.11          |
| (1,2483) | 1:161:A:VAL:HG23 | 1:163:A:TYR:HD1  | 14       | 0.11          |
| (1,2483) | 1:161:A:VAL:HG23 | 1:163:A:TYR:HD2  | 14       | 0.11          |
| (1,2483) | 1:161:A:VAL:HG21 | 1:163:A:TYR:HD1  | 20       | 0.11          |
| (1,2483) | 1:161:A:VAL:HG21 | 1:163:A:TYR:HD2  | 20       | 0.11          |
| (1,2483) | 1:161:A:VAL:HG22 | 1:163:A:TYR:HD1  | 20       | 0.11          |
| (1,2483) | 1:161:A:VAL:HG22 | 1:163:A:TYR:HD2  | 20       | 0.11          |
| (1,2483) | 1:161:A:VAL:HG23 | 1:163:A:TYR:HD1  | 20       | 0.11          |
| (1,2483) | 1:161:A:VAL:HG23 | 1:163:A:TYR:HD2  | 20       | 0.11          |
| (1,2466) | 1:169:A:TYR:HD1  | 1:174:A:ASN:HB3  | 8        | 0.11          |
| (1,2466) | 1:169:A:TYR:HD2  | 1:174:A:ASN:HB3  | 8        | 0.11          |
| (1,2397) | 1:185:A:LYS:HB2  | 1:186:A:GLN:HE22 | 6        | 0.11          |
| (1,2397) | 1:185:A:LYS:HB3  | 1:186:A:GLN:HE22 | 6        | 0.11          |
| (1,2397) | 1:185:A:LYS:HB2  | 1:186:A:GLN:HE22 | 8        | 0.11          |
| (1,2397) | 1:185:A:LYS:HB3  | 1:186:A:GLN:HE22 | 8        | 0.11          |
| (1,2397) | 1:185:A:LYS:HB2  | 1:186:A:GLN:HE22 | 11       | 0.11          |
| (1,2397) | 1:185:A:LYS:HB3  | 1:186:A:GLN:HE22 | 11       | 0.11          |
| (1,2323) | 1:133:A:ALA:HB1  | 1:160:A:GLN:HE22 | 6        | 0.11          |
| (1,2323) | 1:133:A:ALA:HB2  | 1:160:A:GLN:HE22 | 6        | 0.11          |
| (1,2323) | 1:133:A:ALA:HB3  | 1:160:A:GLN:HE22 | 6        | 0.11          |
| (1,2323) | 1:133:A:ALA:HB1  | 1:160:A:GLN:HE22 | 7        | 0.11          |
| (1,2323) | 1:133:A:ALA:HB2  | 1:160:A:GLN:HE22 | 7        | 0.11          |
| (1,2323) | 1:133:A:ALA:HB3  | 1:160:A:GLN:HE22 | 7        | 0.11          |
| (1,2323) | 1:133:A:ALA:HB1  | 1:160:A:GLN:HE22 | 10       | 0.11          |
| (1,2323) | 1:133:A:ALA:HB2  | 1:160:A:GLN:HE22 | 10       | 0.11          |
| (1,2323) | 1:133:A:ALA:HB3  | 1:160:A:GLN:HE22 | 10       | 0.11          |
| (1,2166) | 1:133:A:ALA:HB1  | 1:159:A:ASN:H    | 16       | 0.11          |
| (1,2166) | 1:133:A:ALA:HB2  | 1:159:A:ASN:H    | 16       | 0.11          |
| (1,2166) | 1:133:A:ALA:HB3  | 1:159:A:ASN:H    | 16       | 0.11          |
| (1,2022) | 1:161:A:VAL:HB   | 1:183:A:THR:H    | 10       | 0.11          |
| (1,1975) | 1:184:A:ILE:HD11 | 1:206:A:MET:H    | 15       | 0.11          |
| (1,1975) | 1:184:A:ILE:HD12 | 1:206:A:MET:H    | 15       | 0.11          |
| (1,1975) | 1:184:A:ILE:HD13 | 1:206:A:MET:H    | 15       | 0.11          |
| (1,1975) | 1:184:A:ILE:HD11 | 1:206:A:MET:H    | 17       | 0.11          |
| (1,1975) | 1:184:A:ILE:HD12 | 1:206:A:MET:H    | 17       | 0.11          |
| (1,1975) | 1:184:A:ILE:HD13 | 1:206:A:MET:H    | 17       | 0.11          |
| (1,1975) | 1:184:A:ILE:HD11 | 1:206:A:MET:H    | 19       | 0.11          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1975) | 1:184:A:ILE:HD12 | 1:206:A:MET:H    | 19       | 0.11          |
| (1,1975) | 1:184:A:ILE:HD13 | 1:206:A:MET:H    | 19       | 0.11          |
| (1,1968) | 1:205:A:MET:H    | 1:205:A:MET:HG3  | 3        | 0.11          |
| (1,1926) | 1:134:A:MET:HE1  | 1:214:A:CYS:H    | 5        | 0.11          |
| (1,1926) | 1:134:A:MET:HE2  | 1:214:A:CYS:H    | 5        | 0.11          |
| (1,1926) | 1:134:A:MET:HE3  | 1:214:A:CYS:H    | 5        | 0.11          |
| (1,1926) | 1:134:A:MET:HE1  | 1:214:A:CYS:H    | 6        | 0.11          |
| (1,1926) | 1:134:A:MET:HE2  | 1:214:A:CYS:H    | 6        | 0.11          |
| (1,1926) | 1:134:A:MET:HE3  | 1:214:A:CYS:H    | 6        | 0.11          |
| (1,1926) | 1:134:A:MET:HE1  | 1:214:A:CYS:H    | 10       | 0.11          |
| (1,1926) | 1:134:A:MET:HE2  | 1:214:A:CYS:H    | 10       | 0.11          |
| (1,1926) | 1:134:A:MET:HE3  | 1:214:A:CYS:H    | 10       | 0.11          |
| (1,1926) | 1:134:A:MET:HE1  | 1:214:A:CYS:H    | 12       | 0.11          |
| (1,1926) | 1:134:A:MET:HE2  | 1:214:A:CYS:H    | 12       | 0.11          |
| (1,1926) | 1:134:A:MET:HE3  | 1:214:A:CYS:H    | 12       | 0.11          |
| (1,1926) | 1:134:A:MET:HE1  | 1:214:A:CYS:H    | 16       | 0.11          |
| (1,1926) | 1:134:A:MET:HE2  | 1:214:A:CYS:H    | 16       | 0.11          |
| (1,1926) | 1:134:A:MET:HE3  | 1:214:A:CYS:H    | 16       | 0.11          |
| (1,1926) | 1:134:A:MET:HE1  | 1:214:A:CYS:H    | 19       | 0.11          |
| (1,1926) | 1:134:A:MET:HE2  | 1:214:A:CYS:H    | 19       | 0.11          |
| (1,1926) | 1:134:A:MET:HE3  | 1:214:A:CYS:H    | 19       | 0.11          |
| (1,1893) | 1:208:A:ARG:HB3  | 1:209:A:VAL:H    | 2        | 0.11          |
| (1,1678) | 1:125:A:LEU:H    | 1:125:A:LEU:HB2  | 13       | 0.11          |
| (1,1632) | 1:231:A:SER:HB3  | 1:232:A:SER:H    | 3        | 0.11          |
| (1,1562) | 1:228:A:GLY:HA2  | 1:229:A:ARG:HG2  | 7        | 0.11          |
| (1,1562) | 1:228:A:GLY:HA2  | 1:229:A:ARG:HG3  | 7        | 0.11          |
| (1,1562) | 1:228:A:GLY:HA3  | 1:229:A:ARG:HG2  | 7        | 0.11          |
| (1,1562) | 1:228:A:GLY:HA3  | 1:229:A:ARG:HG3  | 7        | 0.11          |
| (1,1505) | 1:137:A:PRO:HD2  | 1:209:A:VAL:HG11 | 6        | 0.11          |
| (1,1505) | 1:137:A:PRO:HD2  | 1:209:A:VAL:HG12 | 6        | 0.11          |
| (1,1505) | 1:137:A:PRO:HD2  | 1:209:A:VAL:HG13 | 6        | 0.11          |
| (1,1505) | 1:137:A:PRO:HD2  | 1:209:A:VAL:HG11 | 9        | 0.11          |
| (1,1505) | 1:137:A:PRO:HD2  | 1:209:A:VAL:HG12 | 9        | 0.11          |
| (1,1505) | 1:137:A:PRO:HD2  | 1:209:A:VAL:HG13 | 9        | 0.11          |
| (1,1495) | 1:212:A:GLN:HB2  | 1:216:A:THR:H    | 12       | 0.11          |
| (1,1479) | 1:145:A:TRP:HB2  | 1:146:A:GLU:HG2  | 17       | 0.11          |
| (1,1479) | 1:145:A:TRP:HB3  | 1:146:A:GLU:HG2  | 17       | 0.11          |
| (1,1450) | 1:182:A:ILE:HD11 | 1:185:A:LYS:HD2  | 4        | 0.11          |
| (1,1450) | 1:182:A:ILE:HD11 | 1:185:A:LYS:HD3  | 4        | 0.11          |
| (1,1450) | 1:182:A:ILE:HD12 | 1:185:A:LYS:HD2  | 4        | 0.11          |
| (1,1450) | 1:182:A:ILE:HD12 | 1:185:A:LYS:HD3  | 4        | 0.11          |
| (1,1450) | 1:182:A:ILE:HD13 | 1:185:A:LYS:HD2  | 4        | 0.11          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1450) | 1:182:A:ILE:HD13 | 1:185:A:LYS:HD3  | 4        | 0.11          |
| (1,1425) | 1:193:A:THR:HG21 | 1:194:A:LYS:HD2  | 12       | 0.11          |
| (1,1425) | 1:193:A:THR:HG21 | 1:194:A:LYS:HD3  | 12       | 0.11          |
| (1,1425) | 1:193:A:THR:HG22 | 1:194:A:LYS:HD2  | 12       | 0.11          |
| (1,1425) | 1:193:A:THR:HG22 | 1:194:A:LYS:HD3  | 12       | 0.11          |
| (1,1425) | 1:193:A:THR:HG23 | 1:194:A:LYS:HD2  | 12       | 0.11          |
| (1,1425) | 1:193:A:THR:HG23 | 1:194:A:LYS:HD3  | 12       | 0.11          |
| (1,1422) | 1:194:A:LYS:HD2  | 1:195:A:GLY:H    | 10       | 0.11          |
| (1,1422) | 1:194:A:LYS:HD3  | 1:195:A:GLY:H    | 10       | 0.11          |
| (1,1406) | 1:172:A:GLN:HB2  | 1:219:A:GLN:HE21 | 17       | 0.11          |
| (1,1406) | 1:172:A:GLN:HB3  | 1:219:A:GLN:HE21 | 17       | 0.11          |
| (1,1385) | 1:183:A:THR:HG21 | 1:187:A:HIS:HB2  | 15       | 0.11          |
| (1,1385) | 1:183:A:THR:HG22 | 1:187:A:HIS:HB2  | 15       | 0.11          |
| (1,1385) | 1:183:A:THR:HG23 | 1:187:A:HIS:HB2  | 15       | 0.11          |
| (1,1309) | 1:129:A:MET:HG2  | 1:164:A:ARG:HA   | 19       | 0.11          |
| (1,1286) | 1:201:A:THR:HA   | 1:204:A:LYS:HB2  | 8        | 0.11          |
| (1,1286) | 1:201:A:THR:HA   | 1:204:A:LYS:HB3  | 8        | 0.11          |
| (1,1282) | 1:165:A:PRO:HA   | 1:166:A:VAL:HB   | 1        | 0.11          |
| (1,1278) | 1:137:A:PRO:HB2  | 1:139:A:ILE:HG21 | 14       | 0.11          |
| (1,1278) | 1:137:A:PRO:HB2  | 1:139:A:ILE:HG22 | 14       | 0.11          |
| (1,1278) | 1:137:A:PRO:HB2  | 1:139:A:ILE:HG23 | 14       | 0.11          |
| (1,1278) | 1:137:A:PRO:HB2  | 1:139:A:ILE:HG21 | 16       | 0.11          |
| (1,1278) | 1:137:A:PRO:HB2  | 1:139:A:ILE:HG22 | 16       | 0.11          |
| (1,1278) | 1:137:A:PRO:HB2  | 1:139:A:ILE:HG23 | 16       | 0.11          |
| (1,1272) | 1:137:A:PRO:HB3  | 1:213:A:MET:HE1  | 17       | 0.11          |
| (1,1272) | 1:137:A:PRO:HB3  | 1:213:A:MET:HE2  | 17       | 0.11          |
| (1,1272) | 1:137:A:PRO:HB3  | 1:213:A:MET:HE3  | 17       | 0.11          |
| (1,1255) | 1:200:A:GLU:HB2  | 1:204:A:LYS:HB2  | 2        | 0.11          |
| (1,1255) | 1:200:A:GLU:HB2  | 1:204:A:LYS:HB3  | 2        | 0.11          |
| (1,1250) | 1:205:A:MET:HB2  | 1:206:A:MET:HG2  | 6        | 0.11          |
| (1,1246) | 1:157:A:TYR:HE1  | 1:209:A:VAL:HB   | 6        | 0.11          |
| (1,1246) | 1:157:A:TYR:HE2  | 1:209:A:VAL:HB   | 6        | 0.11          |
| (1,1234) | 1:122:A:VAL:HB   | 1:123:A:GLY:HA2  | 5        | 0.11          |
| (1,1234) | 1:122:A:VAL:HB   | 1:123:A:GLY:HA3  | 5        | 0.11          |
| (1,1234) | 1:122:A:VAL:HB   | 1:123:A:GLY:HA2  | 13       | 0.11          |
| (1,1234) | 1:122:A:VAL:HB   | 1:123:A:GLY:HA3  | 13       | 0.11          |
| (1,1227) | 1:210:A:VAL:HA   | 1:213:A:MET:HG2  | 2        | 0.11          |
| (1,1220) | 1:195:A:GLY:HA2  | 1:196:A:GLU:HA   | 6        | 0.11          |
| (1,1215) | 1:227:A:ASP:HB2  | 1:229:A:ARG:HA   | 4        | 0.11          |
| (1,1215) | 1:227:A:ASP:HB3  | 1:229:A:ARG:HA   | 4        | 0.11          |
| (1,1215) | 1:227:A:ASP:HB2  | 1:229:A:ARG:HA   | 14       | 0.11          |
| (1,1215) | 1:227:A:ASP:HB3  | 1:229:A:ARG:HA   | 14       | 0.11          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1215) | 1:227:A:ASP:HB2  | 1:229:A:ARG:HA   | 15       | 0.11          |
| (1,1215) | 1:227:A:ASP:HB3  | 1:229:A:ARG:HA   | 15       | 0.11          |
| (1,1215) | 1:227:A:ASP:HB2  | 1:229:A:ARG:HA   | 19       | 0.11          |
| (1,1215) | 1:227:A:ASP:HB3  | 1:229:A:ARG:HA   | 19       | 0.11          |
| (1,1152) | 1:205:A:MET:HA   | 1:205:A:MET:HG3  | 7        | 0.11          |
| (1,1152) | 1:205:A:MET:HA   | 1:205:A:MET:HG3  | 14       | 0.11          |
| (1,1152) | 1:205:A:MET:HA   | 1:205:A:MET:HG3  | 17       | 0.11          |
| (1,1152) | 1:205:A:MET:HA   | 1:205:A:MET:HG3  | 19       | 0.11          |
| (1,1108) | 1:178:A:ASP:HA   | 1:180:A:VAL:HG21 | 10       | 0.11          |
| (1,1108) | 1:178:A:ASP:HA   | 1:180:A:VAL:HG22 | 10       | 0.11          |
| (1,1108) | 1:178:A:ASP:HA   | 1:180:A:VAL:HG23 | 10       | 0.11          |
| (1,1007) | 1:137:A:PRO:HA   | 1:139:A:ILE:HD11 | 1        | 0.11          |
| (1,1007) | 1:137:A:PRO:HA   | 1:139:A:ILE:HD12 | 1        | 0.11          |
| (1,1007) | 1:137:A:PRO:HA   | 1:139:A:ILE:HD13 | 1        | 0.11          |
| (1,1007) | 1:137:A:PRO:HA   | 1:139:A:ILE:HD11 | 12       | 0.11          |
| (1,1007) | 1:137:A:PRO:HA   | 1:139:A:ILE:HD12 | 12       | 0.11          |
| (1,1007) | 1:137:A:PRO:HA   | 1:139:A:ILE:HD13 | 12       | 0.11          |
| (1,983)  | 1:149:A:TYR:H    | 1:152:A:GLU:HG2  | 10       | 0.11          |
| (1,963)  | 1:184:A:ILE:HD11 | 1:185:A:LYS:HA   | 11       | 0.11          |
| (1,963)  | 1:184:A:ILE:HD12 | 1:185:A:LYS:HA   | 11       | 0.11          |
| (1,963)  | 1:184:A:ILE:HD13 | 1:185:A:LYS:HA   | 11       | 0.11          |
| (1,963)  | 1:184:A:ILE:HD11 | 1:185:A:LYS:HA   | 12       | 0.11          |
| (1,963)  | 1:184:A:ILE:HD12 | 1:185:A:LYS:HA   | 12       | 0.11          |
| (1,963)  | 1:184:A:ILE:HD13 | 1:185:A:LYS:HA   | 12       | 0.11          |
| (1,963)  | 1:184:A:ILE:HD11 | 1:185:A:LYS:HA   | 14       | 0.11          |
| (1,963)  | 1:184:A:ILE:HD12 | 1:185:A:LYS:HA   | 14       | 0.11          |
| (1,963)  | 1:184:A:ILE:HD13 | 1:185:A:LYS:HA   | 14       | 0.11          |
| (1,960)  | 1:180:A:VAL:HG21 | 1:184:A:ILE:HD11 | 16       | 0.11          |
| (1,960)  | 1:180:A:VAL:HG21 | 1:184:A:ILE:HD12 | 16       | 0.11          |
| (1,960)  | 1:180:A:VAL:HG21 | 1:184:A:ILE:HD13 | 16       | 0.11          |
| (1,960)  | 1:180:A:VAL:HG22 | 1:184:A:ILE:HD11 | 16       | 0.11          |
| (1,960)  | 1:180:A:VAL:HG22 | 1:184:A:ILE:HD12 | 16       | 0.11          |
| (1,960)  | 1:180:A:VAL:HG22 | 1:184:A:ILE:HD13 | 16       | 0.11          |
| (1,960)  | 1:180:A:VAL:HG23 | 1:184:A:ILE:HD11 | 16       | 0.11          |
| (1,960)  | 1:180:A:VAL:HG23 | 1:184:A:ILE:HD12 | 16       | 0.11          |
| (1,960)  | 1:180:A:VAL:HG23 | 1:184:A:ILE:HD13 | 16       | 0.11          |
| (1,939)  | 1:169:A:TYR:HA   | 1:170:A:SER:HA   | 3        | 0.11          |
| (1,902)  | 1:147:A:ASP:HB2  | 1:148:A:ARG:HA   | 7        | 0.11          |
| (1,807)  | 1:181:A:ASN:HB3  | 1:184:A:ILE:HG21 | 1        | 0.11          |
| (1,807)  | 1:181:A:ASN:HB3  | 1:184:A:ILE:HG22 | 1        | 0.11          |
| (1,807)  | 1:181:A:ASN:HB3  | 1:184:A:ILE:HG23 | 1        | 0.11          |
| (1,807)  | 1:181:A:ASN:HB3  | 1:184:A:ILE:HG21 | 2        | 0.11          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,807) | 1:181:A:ASN:HB3  | 1:184:A:ILE:HG22 | 2        | 0.11          |
| (1,807) | 1:181:A:ASN:HB3  | 1:184:A:ILE:HG23 | 2        | 0.11          |
| (1,807) | 1:181:A:ASN:HB3  | 1:184:A:ILE:HG21 | 3        | 0.11          |
| (1,807) | 1:181:A:ASN:HB3  | 1:184:A:ILE:HG22 | 3        | 0.11          |
| (1,807) | 1:181:A:ASN:HB3  | 1:184:A:ILE:HG23 | 3        | 0.11          |
| (1,807) | 1:181:A:ASN:HB3  | 1:184:A:ILE:HG21 | 5        | 0.11          |
| (1,807) | 1:181:A:ASN:HB3  | 1:184:A:ILE:HG22 | 5        | 0.11          |
| (1,807) | 1:181:A:ASN:HB3  | 1:184:A:ILE:HG23 | 5        | 0.11          |
| (1,807) | 1:181:A:ASN:HB3  | 1:184:A:ILE:HG21 | 7        | 0.11          |
| (1,807) | 1:181:A:ASN:HB3  | 1:184:A:ILE:HG22 | 7        | 0.11          |
| (1,807) | 1:181:A:ASN:HB3  | 1:184:A:ILE:HG23 | 7        | 0.11          |
| (1,807) | 1:181:A:ASN:HB3  | 1:184:A:ILE:HG21 | 9        | 0.11          |
| (1,807) | 1:181:A:ASN:HB3  | 1:184:A:ILE:HG22 | 9        | 0.11          |
| (1,807) | 1:181:A:ASN:HB3  | 1:184:A:ILE:HG23 | 9        | 0.11          |
| (1,807) | 1:181:A:ASN:HB3  | 1:184:A:ILE:HG21 | 15       | 0.11          |
| (1,807) | 1:181:A:ASN:HB3  | 1:184:A:ILE:HG22 | 15       | 0.11          |
| (1,807) | 1:181:A:ASN:HB3  | 1:184:A:ILE:HG23 | 15       | 0.11          |
| (1,807) | 1:181:A:ASN:HB3  | 1:184:A:ILE:HG21 | 17       | 0.11          |
| (1,807) | 1:181:A:ASN:HB3  | 1:184:A:ILE:HG22 | 17       | 0.11          |
| (1,807) | 1:181:A:ASN:HB3  | 1:184:A:ILE:HG23 | 17       | 0.11          |
| (1,807) | 1:181:A:ASN:HB3  | 1:184:A:ILE:HG21 | 19       | 0.11          |
| (1,807) | 1:181:A:ASN:HB3  | 1:184:A:ILE:HG22 | 19       | 0.11          |
| (1,807) | 1:181:A:ASN:HB3  | 1:184:A:ILE:HG23 | 19       | 0.11          |
| (1,807) | 1:181:A:ASN:HB3  | 1:184:A:ILE:HG21 | 20       | 0.11          |
| (1,807) | 1:181:A:ASN:HB3  | 1:184:A:ILE:HG22 | 20       | 0.11          |
| (1,807) | 1:181:A:ASN:HB3  | 1:184:A:ILE:HG23 | 20       | 0.11          |
| (1,787) | 1:206:A:MET:HE1  | 1:207:A:GLU:HA   | 13       | 0.11          |
| (1,787) | 1:206:A:MET:HE2  | 1:207:A:GLU:HA   | 13       | 0.11          |
| (1,787) | 1:206:A:MET:HE3  | 1:207:A:GLU:HA   | 13       | 0.11          |
| (1,784) | 1:166:A:VAL:HG11 | 1:218:A:TYR:HA   | 17       | 0.11          |
| (1,784) | 1:166:A:VAL:HG12 | 1:218:A:TYR:HA   | 17       | 0.11          |
| (1,784) | 1:166:A:VAL:HG13 | 1:218:A:TYR:HA   | 17       | 0.11          |
| (1,774) | 1:206:A:MET:HB2  | 1:206:A:MET:HE1  | 16       | 0.11          |
| (1,774) | 1:206:A:MET:HB2  | 1:206:A:MET:HE2  | 16       | 0.11          |
| (1,774) | 1:206:A:MET:HB2  | 1:206:A:MET:HE3  | 16       | 0.11          |
| (1,772) | 1:202:A:ASP:HB3  | 1:206:A:MET:HE1  | 2        | 0.11          |
| (1,772) | 1:202:A:ASP:HB3  | 1:206:A:MET:HE2  | 2        | 0.11          |
| (1,772) | 1:202:A:ASP:HB3  | 1:206:A:MET:HE3  | 2        | 0.11          |
| (1,768) | 1:198:A:PHE:HD1  | 1:206:A:MET:HE1  | 2        | 0.11          |
| (1,768) | 1:198:A:PHE:HD1  | 1:206:A:MET:HE2  | 2        | 0.11          |
| (1,768) | 1:198:A:PHE:HD1  | 1:206:A:MET:HE3  | 2        | 0.11          |
| (1,768) | 1:198:A:PHE:HD2  | 1:206:A:MET:HE1  | 2        | 0.11          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,768) | 1:198:A:PHE:HD2 | 1:206:A:MET:HE2 | 2        | 0.11          |
| (1,768) | 1:198:A:PHE:HD2 | 1:206:A:MET:HE3 | 2        | 0.11          |
| (1,760) | 1:184:A:ILE:HB  | 1:206:A:MET:HE1 | 5        | 0.11          |
| (1,760) | 1:184:A:ILE:HB  | 1:206:A:MET:HE2 | 5        | 0.11          |
| (1,760) | 1:184:A:ILE:HB  | 1:206:A:MET:HE3 | 5        | 0.11          |
| (1,757) | 1:138:A:MET:HE1 | 1:140:A:HIS:HB2 | 8        | 0.11          |
| (1,757) | 1:138:A:MET:HE2 | 1:140:A:HIS:HB2 | 8        | 0.11          |
| (1,757) | 1:138:A:MET:HE3 | 1:140:A:HIS:HB2 | 8        | 0.11          |
| (1,742) | 1:138:A:MET:HE1 | 1:140:A:HIS:HD2 | 12       | 0.11          |
| (1,742) | 1:138:A:MET:HE2 | 1:140:A:HIS:HD2 | 12       | 0.11          |
| (1,742) | 1:138:A:MET:HE3 | 1:140:A:HIS:HD2 | 12       | 0.11          |
| (1,694) | 1:129:A:MET:HE1 | 1:130:A:LEU:HG  | 16       | 0.11          |
| (1,694) | 1:129:A:MET:HE2 | 1:130:A:LEU:HG  | 16       | 0.11          |
| (1,694) | 1:129:A:MET:HE3 | 1:130:A:LEU:HG  | 16       | 0.11          |
| (1,667) | 1:138:A:MET:HE1 | 1:154:A:MET:HE1 | 2        | 0.11          |
| (1,667) | 1:138:A:MET:HE1 | 1:154:A:MET:HE2 | 2        | 0.11          |
| (1,667) | 1:138:A:MET:HE1 | 1:154:A:MET:HE3 | 2        | 0.11          |
| (1,667) | 1:138:A:MET:HE2 | 1:154:A:MET:HE1 | 2        | 0.11          |
| (1,667) | 1:138:A:MET:HE2 | 1:154:A:MET:HE2 | 2        | 0.11          |
| (1,667) | 1:138:A:MET:HE2 | 1:154:A:MET:HE3 | 2        | 0.11          |
| (1,667) | 1:138:A:MET:HE3 | 1:154:A:MET:HE1 | 2        | 0.11          |
| (1,667) | 1:138:A:MET:HE3 | 1:154:A:MET:HE2 | 2        | 0.11          |
| (1,667) | 1:138:A:MET:HE3 | 1:154:A:MET:HE3 | 2        | 0.11          |
| (1,667) | 1:138:A:MET:HE1 | 1:154:A:MET:HE1 | 6        | 0.11          |
| (1,667) | 1:138:A:MET:HE1 | 1:154:A:MET:HE2 | 6        | 0.11          |
| (1,667) | 1:138:A:MET:HE1 | 1:154:A:MET:HE3 | 6        | 0.11          |
| (1,667) | 1:138:A:MET:HE2 | 1:154:A:MET:HE1 | 6        | 0.11          |
| (1,667) | 1:138:A:MET:HE2 | 1:154:A:MET:HE2 | 6        | 0.11          |
| (1,667) | 1:138:A:MET:HE2 | 1:154:A:MET:HE3 | 6        | 0.11          |
| (1,667) | 1:138:A:MET:HE3 | 1:154:A:MET:HE1 | 6        | 0.11          |
| (1,667) | 1:138:A:MET:HE3 | 1:154:A:MET:HE2 | 6        | 0.11          |
| (1,667) | 1:138:A:MET:HE3 | 1:154:A:MET:HE3 | 6        | 0.11          |
| (1,667) | 1:138:A:MET:HE1 | 1:154:A:MET:HE1 | 11       | 0.11          |
| (1,667) | 1:138:A:MET:HE1 | 1:154:A:MET:HE2 | 11       | 0.11          |
| (1,667) | 1:138:A:MET:HE1 | 1:154:A:MET:HE3 | 11       | 0.11          |
| (1,667) | 1:138:A:MET:HE2 | 1:154:A:MET:HE1 | 11       | 0.11          |
| (1,667) | 1:138:A:MET:HE2 | 1:154:A:MET:HE2 | 11       | 0.11          |
| (1,667) | 1:138:A:MET:HE2 | 1:154:A:MET:HE3 | 11       | 0.11          |
| (1,667) | 1:138:A:MET:HE3 | 1:154:A:MET:HE1 | 11       | 0.11          |
| (1,667) | 1:138:A:MET:HE3 | 1:154:A:MET:HE2 | 11       | 0.11          |
| (1,667) | 1:138:A:MET:HE3 | 1:154:A:MET:HE3 | 11       | 0.11          |
| (1,660) | 1:154:A:MET:HB2 | 1:154:A:MET:HE1 | 1        | 0.11          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,660) | 1:154:A:MET:HB2 | 1:154:A:MET:HE2 | 1        | 0.11          |
| (1,660) | 1:154:A:MET:HB2 | 1:154:A:MET:HE3 | 1        | 0.11          |
| (1,659) | 1:136:A:ARG:HG2 | 1:154:A:MET:HE1 | 2        | 0.11          |
| (1,659) | 1:136:A:ARG:HG2 | 1:154:A:MET:HE2 | 2        | 0.11          |
| (1,659) | 1:136:A:ARG:HG2 | 1:154:A:MET:HE3 | 2        | 0.11          |
| (1,659) | 1:136:A:ARG:HG3 | 1:154:A:MET:HE1 | 2        | 0.11          |
| (1,659) | 1:136:A:ARG:HG3 | 1:154:A:MET:HE2 | 2        | 0.11          |
| (1,659) | 1:136:A:ARG:HG3 | 1:154:A:MET:HE3 | 2        | 0.11          |
| (1,659) | 1:136:A:ARG:HG2 | 1:154:A:MET:HE1 | 10       | 0.11          |
| (1,659) | 1:136:A:ARG:HG2 | 1:154:A:MET:HE2 | 10       | 0.11          |
| (1,659) | 1:136:A:ARG:HG2 | 1:154:A:MET:HE3 | 10       | 0.11          |
| (1,659) | 1:136:A:ARG:HG3 | 1:154:A:MET:HE1 | 10       | 0.11          |
| (1,659) | 1:136:A:ARG:HG3 | 1:154:A:MET:HE2 | 10       | 0.11          |
| (1,659) | 1:136:A:ARG:HG3 | 1:154:A:MET:HE3 | 10       | 0.11          |
| (1,656) | 1:138:A:MET:HG3 | 1:154:A:MET:HE1 | 10       | 0.11          |
| (1,656) | 1:138:A:MET:HG3 | 1:154:A:MET:HE2 | 10       | 0.11          |
| (1,656) | 1:138:A:MET:HG3 | 1:154:A:MET:HE3 | 10       | 0.11          |
| (1,656) | 1:138:A:MET:HG3 | 1:154:A:MET:HE1 | 19       | 0.11          |
| (1,656) | 1:138:A:MET:HG3 | 1:154:A:MET:HE2 | 19       | 0.11          |
| (1,656) | 1:138:A:MET:HG3 | 1:154:A:MET:HE3 | 19       | 0.11          |
| (1,653) | 1:139:A:ILE:H   | 1:154:A:MET:HE1 | 20       | 0.11          |
| (1,653) | 1:139:A:ILE:H   | 1:154:A:MET:HE2 | 20       | 0.11          |
| (1,653) | 1:139:A:ILE:H   | 1:154:A:MET:HE3 | 20       | 0.11          |
| (1,617) | 1:134:A:MET:HE1 | 1:220:A:LYS:HE2 | 12       | 0.11          |
| (1,617) | 1:134:A:MET:HE1 | 1:220:A:LYS:HE3 | 12       | 0.11          |
| (1,617) | 1:134:A:MET:HE2 | 1:220:A:LYS:HE2 | 12       | 0.11          |
| (1,617) | 1:134:A:MET:HE2 | 1:220:A:LYS:HE3 | 12       | 0.11          |
| (1,617) | 1:134:A:MET:HE3 | 1:220:A:LYS:HE2 | 12       | 0.11          |
| (1,617) | 1:134:A:MET:HE3 | 1:220:A:LYS:HE3 | 12       | 0.11          |
| (1,612) | 1:134:A:MET:HE1 | 1:213:A:MET:H   | 1        | 0.11          |
| (1,612) | 1:134:A:MET:HE2 | 1:213:A:MET:H   | 1        | 0.11          |
| (1,612) | 1:134:A:MET:HE3 | 1:213:A:MET:H   | 1        | 0.11          |
| (1,612) | 1:134:A:MET:HE1 | 1:213:A:MET:H   | 7        | 0.11          |
| (1,612) | 1:134:A:MET:HE2 | 1:213:A:MET:H   | 7        | 0.11          |
| (1,612) | 1:134:A:MET:HE3 | 1:213:A:MET:H   | 7        | 0.11          |
| (1,612) | 1:134:A:MET:HE1 | 1:213:A:MET:H   | 8        | 0.11          |
| (1,612) | 1:134:A:MET:HE2 | 1:213:A:MET:H   | 8        | 0.11          |
| (1,612) | 1:134:A:MET:HE3 | 1:213:A:MET:H   | 8        | 0.11          |
| (1,612) | 1:134:A:MET:HE1 | 1:213:A:MET:H   | 17       | 0.11          |
| (1,612) | 1:134:A:MET:HE2 | 1:213:A:MET:H   | 17       | 0.11          |
| (1,612) | 1:134:A:MET:HE3 | 1:213:A:MET:H   | 17       | 0.11          |
| (1,612) | 1:134:A:MET:HE1 | 1:213:A:MET:H   | 19       | 0.11          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,612) | 1:134:A:MET:HE2  | 1:213:A:MET:H   | 19       | 0.11          |
| (1,612) | 1:134:A:MET:HE3  | 1:213:A:MET:H   | 19       | 0.11          |
| (1,611) | 1:134:A:MET:HE1  | 1:218:A:TYR:H   | 5        | 0.11          |
| (1,611) | 1:134:A:MET:HE2  | 1:218:A:TYR:H   | 5        | 0.11          |
| (1,611) | 1:134:A:MET:HE3  | 1:218:A:TYR:H   | 5        | 0.11          |
| (1,611) | 1:134:A:MET:HE1  | 1:218:A:TYR:H   | 11       | 0.11          |
| (1,611) | 1:134:A:MET:HE2  | 1:218:A:TYR:H   | 11       | 0.11          |
| (1,611) | 1:134:A:MET:HE3  | 1:218:A:TYR:H   | 11       | 0.11          |
| (1,611) | 1:134:A:MET:HE1  | 1:218:A:TYR:H   | 12       | 0.11          |
| (1,611) | 1:134:A:MET:HE2  | 1:218:A:TYR:H   | 12       | 0.11          |
| (1,611) | 1:134:A:MET:HE3  | 1:218:A:TYR:H   | 12       | 0.11          |
| (1,611) | 1:134:A:MET:HE1  | 1:218:A:TYR:H   | 18       | 0.11          |
| (1,611) | 1:134:A:MET:HE2  | 1:218:A:TYR:H   | 18       | 0.11          |
| (1,611) | 1:134:A:MET:HE3  | 1:218:A:TYR:H   | 18       | 0.11          |
| (1,605) | 1:128:A:TYR:HE1  | 1:178:A:ASP:HB3 | 6        | 0.11          |
| (1,605) | 1:128:A:TYR:HE2  | 1:178:A:ASP:HB3 | 6        | 0.11          |
| (1,591) | 1:139:A:ILE:HD11 | 1:205:A:MET:HE1 | 7        | 0.11          |
| (1,591) | 1:139:A:ILE:HD11 | 1:205:A:MET:HE2 | 7        | 0.11          |
| (1,591) | 1:139:A:ILE:HD11 | 1:205:A:MET:HE3 | 7        | 0.11          |
| (1,591) | 1:139:A:ILE:HD12 | 1:205:A:MET:HE1 | 7        | 0.11          |
| (1,591) | 1:139:A:ILE:HD12 | 1:205:A:MET:HE2 | 7        | 0.11          |
| (1,591) | 1:139:A:ILE:HD12 | 1:205:A:MET:HE3 | 7        | 0.11          |
| (1,591) | 1:139:A:ILE:HD13 | 1:205:A:MET:HE1 | 7        | 0.11          |
| (1,591) | 1:139:A:ILE:HD13 | 1:205:A:MET:HE2 | 7        | 0.11          |
| (1,591) | 1:139:A:ILE:HD13 | 1:205:A:MET:HE3 | 7        | 0.11          |
| (1,582) | 1:139:A:ILE:HG21 | 1:205:A:MET:HE1 | 3        | 0.11          |
| (1,582) | 1:139:A:ILE:HG21 | 1:205:A:MET:HE2 | 3        | 0.11          |
| (1,582) | 1:139:A:ILE:HG21 | 1:205:A:MET:HE3 | 3        | 0.11          |
| (1,582) | 1:139:A:ILE:HG22 | 1:205:A:MET:HE1 | 3        | 0.11          |
| (1,582) | 1:139:A:ILE:HG22 | 1:205:A:MET:HE2 | 3        | 0.11          |
| (1,582) | 1:139:A:ILE:HG22 | 1:205:A:MET:HE3 | 3        | 0.11          |
| (1,582) | 1:139:A:ILE:HG23 | 1:205:A:MET:HE1 | 3        | 0.11          |
| (1,582) | 1:139:A:ILE:HG23 | 1:205:A:MET:HE2 | 3        | 0.11          |
| (1,582) | 1:139:A:ILE:HG23 | 1:205:A:MET:HE3 | 3        | 0.11          |
| (1,582) | 1:139:A:ILE:HG21 | 1:205:A:MET:HE1 | 13       | 0.11          |
| (1,582) | 1:139:A:ILE:HG21 | 1:205:A:MET:HE2 | 13       | 0.11          |
| (1,582) | 1:139:A:ILE:HG21 | 1:205:A:MET:HE3 | 13       | 0.11          |
| (1,582) | 1:139:A:ILE:HG22 | 1:205:A:MET:HE1 | 13       | 0.11          |
| (1,582) | 1:139:A:ILE:HG22 | 1:205:A:MET:HE2 | 13       | 0.11          |
| (1,582) | 1:139:A:ILE:HG22 | 1:205:A:MET:HE3 | 13       | 0.11          |
| (1,582) | 1:139:A:ILE:HG23 | 1:205:A:MET:HE1 | 13       | 0.11          |
| (1,582) | 1:139:A:ILE:HG23 | 1:205:A:MET:HE2 | 13       | 0.11          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,582) | 1:139:A:ILE:HG23 | 1:205:A:MET:HE3 | 13       | 0.11          |
| (1,582) | 1:139:A:ILE:HG21 | 1:205:A:MET:HE1 | 18       | 0.11          |
| (1,582) | 1:139:A:ILE:HG21 | 1:205:A:MET:HE2 | 18       | 0.11          |
| (1,582) | 1:139:A:ILE:HG21 | 1:205:A:MET:HE3 | 18       | 0.11          |
| (1,582) | 1:139:A:ILE:HG22 | 1:205:A:MET:HE1 | 18       | 0.11          |
| (1,582) | 1:139:A:ILE:HG22 | 1:205:A:MET:HE2 | 18       | 0.11          |
| (1,582) | 1:139:A:ILE:HG22 | 1:205:A:MET:HE3 | 18       | 0.11          |
| (1,582) | 1:139:A:ILE:HG23 | 1:205:A:MET:HE1 | 18       | 0.11          |
| (1,582) | 1:139:A:ILE:HG23 | 1:205:A:MET:HE2 | 18       | 0.11          |
| (1,582) | 1:139:A:ILE:HG23 | 1:205:A:MET:HE3 | 18       | 0.11          |
| (1,574) | 1:153:A:ASN:HB2  | 1:155:A:TYR:HE1 | 11       | 0.11          |
| (1,574) | 1:153:A:ASN:HB2  | 1:155:A:TYR:HE2 | 11       | 0.11          |
| (1,569) | 1:128:A:TYR:HE1  | 1:179:A:CYS:HB3 | 15       | 0.11          |
| (1,569) | 1:128:A:TYR:HE2  | 1:179:A:CYS:HB3 | 15       | 0.11          |
| (1,501) | 1:161:A:VAL:HA   | 1:162:A:TYR:HB3 | 8        | 0.11          |
| (1,497) | 1:128:A:TYR:HB2  | 1:162:A:TYR:HB2 | 19       | 0.11          |
| (1,494) | 1:185:A:LYS:HE2  | 1:188:A:THR:H   | 15       | 0.11          |
| (1,494) | 1:185:A:LYS:HE3  | 1:188:A:THR:H   | 15       | 0.11          |
| (1,473) | 1:193:A:THR:HG21 | 1:194:A:LYS:HE2 | 6        | 0.11          |
| (1,473) | 1:193:A:THR:HG21 | 1:194:A:LYS:HE3 | 6        | 0.11          |
| (1,473) | 1:193:A:THR:HG22 | 1:194:A:LYS:HE2 | 6        | 0.11          |
| (1,473) | 1:193:A:THR:HG22 | 1:194:A:LYS:HE3 | 6        | 0.11          |
| (1,473) | 1:193:A:THR:HG23 | 1:194:A:LYS:HE2 | 6        | 0.11          |
| (1,473) | 1:193:A:THR:HG23 | 1:194:A:LYS:HE3 | 6        | 0.11          |
| (1,472) | 1:194:A:LYS:HE2  | 1:195:A:GLY:HA3 | 4        | 0.11          |
| (1,472) | 1:194:A:LYS:HE3  | 1:195:A:GLY:HA3 | 4        | 0.11          |
| (1,421) | 1:121:A:VAL:HG11 | 1:123:A:GLY:HA2 | 2        | 0.11          |
| (1,421) | 1:121:A:VAL:HG11 | 1:123:A:GLY:HA3 | 2        | 0.11          |
| (1,421) | 1:121:A:VAL:HG12 | 1:123:A:GLY:HA2 | 2        | 0.11          |
| (1,421) | 1:121:A:VAL:HG12 | 1:123:A:GLY:HA3 | 2        | 0.11          |
| (1,421) | 1:121:A:VAL:HG13 | 1:123:A:GLY:HA2 | 2        | 0.11          |
| (1,421) | 1:121:A:VAL:HG13 | 1:123:A:GLY:HA3 | 2        | 0.11          |
| (1,421) | 1:121:A:VAL:HG11 | 1:123:A:GLY:HA2 | 9        | 0.11          |
| (1,421) | 1:121:A:VAL:HG11 | 1:123:A:GLY:HA3 | 9        | 0.11          |
| (1,421) | 1:121:A:VAL:HG12 | 1:123:A:GLY:HA2 | 9        | 0.11          |
| (1,421) | 1:121:A:VAL:HG12 | 1:123:A:GLY:HA3 | 9        | 0.11          |
| (1,421) | 1:121:A:VAL:HG13 | 1:123:A:GLY:HA2 | 9        | 0.11          |
| (1,421) | 1:121:A:VAL:HG13 | 1:123:A:GLY:HA3 | 9        | 0.11          |
| (1,421) | 1:121:A:VAL:HG11 | 1:123:A:GLY:HA2 | 10       | 0.11          |
| (1,421) | 1:121:A:VAL:HG11 | 1:123:A:GLY:HA3 | 10       | 0.11          |
| (1,421) | 1:121:A:VAL:HG12 | 1:123:A:GLY:HA2 | 10       | 0.11          |
| (1,421) | 1:121:A:VAL:HG12 | 1:123:A:GLY:HA3 | 10       | 0.11          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,421) | 1:121:A:VAL:HG13 | 1:123:A:GLY:HA2  | 10       | 0.11          |
| (1,421) | 1:121:A:VAL:HG13 | 1:123:A:GLY:HA3  | 10       | 0.11          |
| (1,421) | 1:121:A:VAL:HG11 | 1:123:A:GLY:HA2  | 14       | 0.11          |
| (1,421) | 1:121:A:VAL:HG11 | 1:123:A:GLY:HA3  | 14       | 0.11          |
| (1,421) | 1:121:A:VAL:HG12 | 1:123:A:GLY:HA2  | 14       | 0.11          |
| (1,421) | 1:121:A:VAL:HG12 | 1:123:A:GLY:HA3  | 14       | 0.11          |
| (1,421) | 1:121:A:VAL:HG13 | 1:123:A:GLY:HA2  | 14       | 0.11          |
| (1,421) | 1:121:A:VAL:HG13 | 1:123:A:GLY:HA3  | 14       | 0.11          |
| (1,421) | 1:121:A:VAL:HG11 | 1:123:A:GLY:HA2  | 19       | 0.11          |
| (1,421) | 1:121:A:VAL:HG11 | 1:123:A:GLY:HA3  | 19       | 0.11          |
| (1,421) | 1:121:A:VAL:HG12 | 1:123:A:GLY:HA2  | 19       | 0.11          |
| (1,421) | 1:121:A:VAL:HG12 | 1:123:A:GLY:HA3  | 19       | 0.11          |
| (1,421) | 1:121:A:VAL:HG13 | 1:123:A:GLY:HA2  | 19       | 0.11          |
| (1,421) | 1:121:A:VAL:HG13 | 1:123:A:GLY:HA3  | 19       | 0.11          |
| (1,418) | 1:164:A:ARG:HB2  | 1:164:A:ARG:HD2  | 6        | 0.11          |
| (1,393) | 1:120:A:SER:HB2  | 1:121:A:VAL:HG11 | 15       | 0.11          |
| (1,393) | 1:120:A:SER:HB2  | 1:121:A:VAL:HG12 | 15       | 0.11          |
| (1,393) | 1:120:A:SER:HB2  | 1:121:A:VAL:HG13 | 15       | 0.11          |
| (1,393) | 1:120:A:SER:HB3  | 1:121:A:VAL:HG11 | 15       | 0.11          |
| (1,393) | 1:120:A:SER:HB3  | 1:121:A:VAL:HG12 | 15       | 0.11          |
| (1,393) | 1:120:A:SER:HB3  | 1:121:A:VAL:HG13 | 15       | 0.11          |
| (1,393) | 1:120:A:SER:HB2  | 1:121:A:VAL:HG11 | 16       | 0.11          |
| (1,393) | 1:120:A:SER:HB2  | 1:121:A:VAL:HG12 | 16       | 0.11          |
| (1,393) | 1:120:A:SER:HB2  | 1:121:A:VAL:HG13 | 16       | 0.11          |
| (1,393) | 1:120:A:SER:HB3  | 1:121:A:VAL:HG11 | 16       | 0.11          |
| (1,393) | 1:120:A:SER:HB3  | 1:121:A:VAL:HG12 | 16       | 0.11          |
| (1,393) | 1:120:A:SER:HB3  | 1:121:A:VAL:HG13 | 16       | 0.11          |
| (1,393) | 1:120:A:SER:HB2  | 1:121:A:VAL:HG11 | 20       | 0.11          |
| (1,393) | 1:120:A:SER:HB2  | 1:121:A:VAL:HG12 | 20       | 0.11          |
| (1,393) | 1:120:A:SER:HB2  | 1:121:A:VAL:HG13 | 20       | 0.11          |
| (1,393) | 1:120:A:SER:HB3  | 1:121:A:VAL:HG11 | 20       | 0.11          |
| (1,393) | 1:120:A:SER:HB3  | 1:121:A:VAL:HG12 | 20       | 0.11          |
| (1,393) | 1:120:A:SER:HB3  | 1:121:A:VAL:HG13 | 20       | 0.11          |
| (1,380) | 1:122:A:VAL:HG21 | 1:123:A:GLY:HA2  | 7        | 0.11          |
| (1,380) | 1:122:A:VAL:HG21 | 1:123:A:GLY:HA3  | 7        | 0.11          |
| (1,380) | 1:122:A:VAL:HG22 | 1:123:A:GLY:HA2  | 7        | 0.11          |
| (1,380) | 1:122:A:VAL:HG22 | 1:123:A:GLY:HA3  | 7        | 0.11          |
| (1,380) | 1:122:A:VAL:HG23 | 1:123:A:GLY:HA2  | 7        | 0.11          |
| (1,380) | 1:122:A:VAL:HG23 | 1:123:A:GLY:HA3  | 7        | 0.11          |
| (1,370) | 1:158:A:PRO:HG2  | 1:209:A:VAL:HG21 | 15       | 0.11          |
| (1,370) | 1:158:A:PRO:HG2  | 1:209:A:VAL:HG22 | 15       | 0.11          |
| (1,370) | 1:158:A:PRO:HG2  | 1:209:A:VAL:HG23 | 15       | 0.11          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,357) | 1:122:A:VAL:HG21 | 1:125:A:LEU:HG   | 11       | 0.11          |
| (1,357) | 1:122:A:VAL:HG22 | 1:125:A:LEU:HG   | 11       | 0.11          |
| (1,357) | 1:122:A:VAL:HG23 | 1:125:A:LEU:HG   | 11       | 0.11          |
| (1,350) | 1:122:A:VAL:HG21 | 1:123:A:GLY:H    | 3        | 0.11          |
| (1,350) | 1:122:A:VAL:HG22 | 1:123:A:GLY:H    | 3        | 0.11          |
| (1,350) | 1:122:A:VAL:HG23 | 1:123:A:GLY:H    | 3        | 0.11          |
| (1,349) | 1:122:A:VAL:HG21 | 1:186:A:GLN:HE21 | 5        | 0.11          |
| (1,349) | 1:122:A:VAL:HG22 | 1:186:A:GLN:HE21 | 5        | 0.11          |
| (1,349) | 1:122:A:VAL:HG23 | 1:186:A:GLN:HE21 | 5        | 0.11          |
| (1,348) | 1:122:A:VAL:HG21 | 1:124:A:GLY:HA2  | 14       | 0.11          |
| (1,348) | 1:122:A:VAL:HG21 | 1:124:A:GLY:HA3  | 14       | 0.11          |
| (1,348) | 1:122:A:VAL:HG22 | 1:124:A:GLY:HA2  | 14       | 0.11          |
| (1,348) | 1:122:A:VAL:HG22 | 1:124:A:GLY:HA3  | 14       | 0.11          |
| (1,348) | 1:122:A:VAL:HG23 | 1:124:A:GLY:HA2  | 14       | 0.11          |
| (1,348) | 1:122:A:VAL:HG23 | 1:124:A:GLY:HA3  | 14       | 0.11          |
| (1,324) | 1:191:A:THR:HG21 | 1:198:A:PHE:HD1  | 4        | 0.11          |
| (1,324) | 1:191:A:THR:HG21 | 1:198:A:PHE:HD2  | 4        | 0.11          |
| (1,324) | 1:191:A:THR:HG22 | 1:198:A:PHE:HD1  | 4        | 0.11          |
| (1,324) | 1:191:A:THR:HG22 | 1:198:A:PHE:HD2  | 4        | 0.11          |
| (1,324) | 1:191:A:THR:HG23 | 1:198:A:PHE:HD1  | 4        | 0.11          |
| (1,324) | 1:191:A:THR:HG23 | 1:198:A:PHE:HD2  | 4        | 0.11          |
| (1,297) | 1:188:A:THR:HG21 | 1:198:A:PHE:HB3  | 14       | 0.11          |
| (1,297) | 1:188:A:THR:HG22 | 1:198:A:PHE:HB3  | 14       | 0.11          |
| (1,297) | 1:188:A:THR:HG23 | 1:198:A:PHE:HB3  | 14       | 0.11          |
| (1,296) | 1:187:A:HIS:HB3  | 1:190:A:THR:HG21 | 3        | 0.11          |
| (1,296) | 1:187:A:HIS:HB3  | 1:190:A:THR:HG22 | 3        | 0.11          |
| (1,296) | 1:187:A:HIS:HB3  | 1:190:A:THR:HG23 | 3        | 0.11          |
| (1,296) | 1:187:A:HIS:HB3  | 1:190:A:THR:HG21 | 9        | 0.11          |
| (1,296) | 1:187:A:HIS:HB3  | 1:190:A:THR:HG22 | 9        | 0.11          |
| (1,296) | 1:187:A:HIS:HB3  | 1:190:A:THR:HG23 | 9        | 0.11          |
| (1,296) | 1:187:A:HIS:HB3  | 1:190:A:THR:HG21 | 13       | 0.11          |
| (1,296) | 1:187:A:HIS:HB3  | 1:190:A:THR:HG22 | 13       | 0.11          |
| (1,296) | 1:187:A:HIS:HB3  | 1:190:A:THR:HG23 | 13       | 0.11          |
| (1,296) | 1:187:A:HIS:HB3  | 1:190:A:THR:HG21 | 17       | 0.11          |
| (1,296) | 1:187:A:HIS:HB3  | 1:190:A:THR:HG22 | 17       | 0.11          |
| (1,296) | 1:187:A:HIS:HB3  | 1:190:A:THR:HG23 | 17       | 0.11          |
| (1,289) | 1:189:A:VAL:HG21 | 1:192:A:THR:HG21 | 9        | 0.11          |
| (1,289) | 1:189:A:VAL:HG21 | 1:192:A:THR:HG22 | 9        | 0.11          |
| (1,289) | 1:189:A:VAL:HG21 | 1:192:A:THR:HG23 | 9        | 0.11          |
| (1,289) | 1:189:A:VAL:HG22 | 1:192:A:THR:HG21 | 9        | 0.11          |
| (1,289) | 1:189:A:VAL:HG22 | 1:192:A:THR:HG22 | 9        | 0.11          |
| (1,289) | 1:189:A:VAL:HG22 | 1:192:A:THR:HG23 | 9        | 0.11          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,289) | 1:189:A:VAL:HG23 | 1:192:A:THR:HG21 | 9        | 0.11          |
| (1,289) | 1:189:A:VAL:HG23 | 1:192:A:THR:HG22 | 9        | 0.11          |
| (1,289) | 1:189:A:VAL:HG23 | 1:192:A:THR:HG23 | 9        | 0.11          |
| (1,288) | 1:192:A:THR:HG21 | 1:196:A:GLU:HB2  | 8        | 0.11          |
| (1,288) | 1:192:A:THR:HG21 | 1:196:A:GLU:HB3  | 8        | 0.11          |
| (1,288) | 1:192:A:THR:HG22 | 1:196:A:GLU:HB2  | 8        | 0.11          |
| (1,288) | 1:192:A:THR:HG22 | 1:196:A:GLU:HB3  | 8        | 0.11          |
| (1,288) | 1:192:A:THR:HG23 | 1:196:A:GLU:HB2  | 8        | 0.11          |
| (1,288) | 1:192:A:THR:HG23 | 1:196:A:GLU:HB3  | 8        | 0.11          |
| (1,261) | 1:185:A:LYS:HD2  | 1:188:A:THR:HG21 | 1        | 0.11          |
| (1,261) | 1:185:A:LYS:HD2  | 1:188:A:THR:HG22 | 1        | 0.11          |
| (1,261) | 1:185:A:LYS:HD2  | 1:188:A:THR:HG23 | 1        | 0.11          |
| (1,261) | 1:185:A:LYS:HD3  | 1:188:A:THR:HG21 | 1        | 0.11          |
| (1,261) | 1:185:A:LYS:HD3  | 1:188:A:THR:HG22 | 1        | 0.11          |
| (1,261) | 1:185:A:LYS:HD3  | 1:188:A:THR:HG23 | 1        | 0.11          |
| (1,261) | 1:185:A:LYS:HD2  | 1:188:A:THR:HG21 | 2        | 0.11          |
| (1,261) | 1:185:A:LYS:HD2  | 1:188:A:THR:HG22 | 2        | 0.11          |
| (1,261) | 1:185:A:LYS:HD2  | 1:188:A:THR:HG23 | 2        | 0.11          |
| (1,261) | 1:185:A:LYS:HD3  | 1:188:A:THR:HG21 | 2        | 0.11          |
| (1,261) | 1:185:A:LYS:HD3  | 1:188:A:THR:HG22 | 2        | 0.11          |
| (1,261) | 1:185:A:LYS:HD3  | 1:188:A:THR:HG23 | 2        | 0.11          |
| (1,261) | 1:185:A:LYS:HD2  | 1:188:A:THR:HG21 | 3        | 0.11          |
| (1,261) | 1:185:A:LYS:HD2  | 1:188:A:THR:HG22 | 3        | 0.11          |
| (1,261) | 1:185:A:LYS:HD2  | 1:188:A:THR:HG23 | 3        | 0.11          |
| (1,261) | 1:185:A:LYS:HD3  | 1:188:A:THR:HG21 | 3        | 0.11          |
| (1,261) | 1:185:A:LYS:HD3  | 1:188:A:THR:HG22 | 3        | 0.11          |
| (1,261) | 1:185:A:LYS:HD3  | 1:188:A:THR:HG23 | 3        | 0.11          |
| (1,261) | 1:185:A:LYS:HD2  | 1:188:A:THR:HG21 | 7        | 0.11          |
| (1,261) | 1:185:A:LYS:HD2  | 1:188:A:THR:HG22 | 7        | 0.11          |
| (1,261) | 1:185:A:LYS:HD2  | 1:188:A:THR:HG23 | 7        | 0.11          |
| (1,261) | 1:185:A:LYS:HD3  | 1:188:A:THR:HG21 | 7        | 0.11          |
| (1,261) | 1:185:A:LYS:HD3  | 1:188:A:THR:HG22 | 7        | 0.11          |
| (1,261) | 1:185:A:LYS:HD3  | 1:188:A:THR:HG23 | 7        | 0.11          |
| (1,261) | 1:185:A:LYS:HD2  | 1:188:A:THR:HG21 | 8        | 0.11          |
| (1,261) | 1:185:A:LYS:HD2  | 1:188:A:THR:HG22 | 8        | 0.11          |
| (1,261) | 1:185:A:LYS:HD2  | 1:188:A:THR:HG23 | 8        | 0.11          |
| (1,261) | 1:185:A:LYS:HD3  | 1:188:A:THR:HG21 | 8        | 0.11          |
| (1,261) | 1:185:A:LYS:HD3  | 1:188:A:THR:HG22 | 8        | 0.11          |
| (1,261) | 1:185:A:LYS:HD3  | 1:188:A:THR:HG23 | 8        | 0.11          |
| (1,261) | 1:185:A:LYS:HD2  | 1:188:A:THR:HG21 | 11       | 0.11          |
| (1,261) | 1:185:A:LYS:HD2  | 1:188:A:THR:HG22 | 11       | 0.11          |
| (1,261) | 1:185:A:LYS:HD2  | 1:188:A:THR:HG23 | 11       | 0.11          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,261) | 1:185:A:LYS:HD3  | 1:188:A:THR:HG21 | 11       | 0.11          |
| (1,261) | 1:185:A:LYS:HD3  | 1:188:A:THR:HG22 | 11       | 0.11          |
| (1,261) | 1:185:A:LYS:HD3  | 1:188:A:THR:HG23 | 11       | 0.11          |
| (1,260) | 1:186:A:GLN:HB2  | 1:190:A:THR:HG21 | 10       | 0.11          |
| (1,260) | 1:186:A:GLN:HB2  | 1:190:A:THR:HG22 | 10       | 0.11          |
| (1,260) | 1:186:A:GLN:HB2  | 1:190:A:THR:HG23 | 10       | 0.11          |
| (1,217) | 1:193:A:THR:HG21 | 1:196:A:GLU:HB2  | 16       | 0.11          |
| (1,217) | 1:193:A:THR:HG21 | 1:196:A:GLU:HB3  | 16       | 0.11          |
| (1,217) | 1:193:A:THR:HG22 | 1:196:A:GLU:HB2  | 16       | 0.11          |
| (1,217) | 1:193:A:THR:HG22 | 1:196:A:GLU:HB3  | 16       | 0.11          |
| (1,217) | 1:193:A:THR:HG23 | 1:196:A:GLU:HB2  | 16       | 0.11          |
| (1,217) | 1:193:A:THR:HG23 | 1:196:A:GLU:HB3  | 16       | 0.11          |
| (1,217) | 1:193:A:THR:HG21 | 1:196:A:GLU:HB2  | 18       | 0.11          |
| (1,217) | 1:193:A:THR:HG21 | 1:196:A:GLU:HB3  | 18       | 0.11          |
| (1,217) | 1:193:A:THR:HG22 | 1:196:A:GLU:HB2  | 18       | 0.11          |
| (1,217) | 1:193:A:THR:HG22 | 1:196:A:GLU:HB3  | 18       | 0.11          |
| (1,217) | 1:193:A:THR:HG23 | 1:196:A:GLU:HB2  | 18       | 0.11          |
| (1,217) | 1:193:A:THR:HG23 | 1:196:A:GLU:HB3  | 18       | 0.11          |
| (1,216) | 1:216:A:THR:HG21 | 1:220:A:LYS:HG3  | 12       | 0.11          |
| (1,216) | 1:216:A:THR:HG22 | 1:220:A:LYS:HG3  | 12       | 0.11          |
| (1,216) | 1:216:A:THR:HG23 | 1:220:A:LYS:HG3  | 12       | 0.11          |
| (1,208) | 1:180:A:VAL:HG21 | 1:183:A:THR:HG21 | 10       | 0.11          |
| (1,208) | 1:180:A:VAL:HG21 | 1:183:A:THR:HG22 | 10       | 0.11          |
| (1,208) | 1:180:A:VAL:HG21 | 1:183:A:THR:HG23 | 10       | 0.11          |
| (1,208) | 1:180:A:VAL:HG22 | 1:183:A:THR:HG21 | 10       | 0.11          |
| (1,208) | 1:180:A:VAL:HG22 | 1:183:A:THR:HG22 | 10       | 0.11          |
| (1,208) | 1:180:A:VAL:HG22 | 1:183:A:THR:HG23 | 10       | 0.11          |
| (1,208) | 1:180:A:VAL:HG23 | 1:183:A:THR:HG21 | 10       | 0.11          |
| (1,208) | 1:180:A:VAL:HG23 | 1:183:A:THR:HG22 | 10       | 0.11          |
| (1,208) | 1:180:A:VAL:HG23 | 1:183:A:THR:HG23 | 10       | 0.11          |
| (1,196) | 1:161:A:VAL:HG21 | 1:216:A:THR:HG21 | 4        | 0.11          |
| (1,196) | 1:161:A:VAL:HG21 | 1:216:A:THR:HG22 | 4        | 0.11          |
| (1,196) | 1:161:A:VAL:HG21 | 1:216:A:THR:HG23 | 4        | 0.11          |
| (1,196) | 1:161:A:VAL:HG22 | 1:216:A:THR:HG21 | 4        | 0.11          |
| (1,196) | 1:161:A:VAL:HG22 | 1:216:A:THR:HG22 | 4        | 0.11          |
| (1,196) | 1:161:A:VAL:HG22 | 1:216:A:THR:HG23 | 4        | 0.11          |
| (1,196) | 1:161:A:VAL:HG23 | 1:216:A:THR:HG21 | 4        | 0.11          |
| (1,196) | 1:161:A:VAL:HG23 | 1:216:A:THR:HG22 | 4        | 0.11          |
| (1,196) | 1:161:A:VAL:HG23 | 1:216:A:THR:HG23 | 4        | 0.11          |
| (1,196) | 1:161:A:VAL:HG21 | 1:216:A:THR:HG21 | 17       | 0.11          |
| (1,196) | 1:161:A:VAL:HG21 | 1:216:A:THR:HG22 | 17       | 0.11          |
| (1,196) | 1:161:A:VAL:HG21 | 1:216:A:THR:HG23 | 17       | 0.11          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,196) | 1:161:A:VAL:HG22 | 1:216:A:THR:HG21 | 17       | 0.11          |
| (1,196) | 1:161:A:VAL:HG22 | 1:216:A:THR:HG22 | 17       | 0.11          |
| (1,196) | 1:161:A:VAL:HG22 | 1:216:A:THR:HG23 | 17       | 0.11          |
| (1,196) | 1:161:A:VAL:HG23 | 1:216:A:THR:HG21 | 17       | 0.11          |
| (1,196) | 1:161:A:VAL:HG23 | 1:216:A:THR:HG22 | 17       | 0.11          |
| (1,196) | 1:161:A:VAL:HG23 | 1:216:A:THR:HG23 | 17       | 0.11          |
| (1,189) | 1:123:A:GLY:HA2  | 1:125:A:LEU:HD21 | 5        | 0.11          |
| (1,189) | 1:123:A:GLY:HA2  | 1:125:A:LEU:HD22 | 5        | 0.11          |
| (1,189) | 1:123:A:GLY:HA2  | 1:125:A:LEU:HD23 | 5        | 0.11          |
| (1,189) | 1:123:A:GLY:HA3  | 1:125:A:LEU:HD21 | 5        | 0.11          |
| (1,189) | 1:123:A:GLY:HA3  | 1:125:A:LEU:HD22 | 5        | 0.11          |
| (1,189) | 1:123:A:GLY:HA3  | 1:125:A:LEU:HD23 | 5        | 0.11          |
| (1,189) | 1:123:A:GLY:HA2  | 1:125:A:LEU:HD21 | 18       | 0.11          |
| (1,189) | 1:123:A:GLY:HA2  | 1:125:A:LEU:HD22 | 18       | 0.11          |
| (1,189) | 1:123:A:GLY:HA2  | 1:125:A:LEU:HD23 | 18       | 0.11          |
| (1,189) | 1:123:A:GLY:HA3  | 1:125:A:LEU:HD21 | 18       | 0.11          |
| (1,189) | 1:123:A:GLY:HA3  | 1:125:A:LEU:HD22 | 18       | 0.11          |
| (1,189) | 1:123:A:GLY:HA3  | 1:125:A:LEU:HD23 | 18       | 0.11          |
| (1,185) | 1:194:A:LYS:HE2  | 1:195:A:GLY:HA2  | 4        | 0.11          |
| (1,185) | 1:194:A:LYS:HE3  | 1:195:A:GLY:HA2  | 4        | 0.11          |
| (1,185) | 1:194:A:LYS:HE2  | 1:195:A:GLY:HA2  | 17       | 0.11          |
| (1,185) | 1:194:A:LYS:HE3  | 1:195:A:GLY:HA2  | 17       | 0.11          |
| (1,150) | 1:126:A:GLY:HA3  | 1:127:A:GLY:H    | 17       | 0.11          |
| (1,132) | 1:125:A:LEU:HD21 | 1:128:A:TYR:HB3  | 11       | 0.11          |
| (1,132) | 1:125:A:LEU:HD22 | 1:128:A:TYR:HB3  | 11       | 0.11          |
| (1,132) | 1:125:A:LEU:HD23 | 1:128:A:TYR:HB3  | 11       | 0.11          |
| (1,112) | 1:214:A:CYS:HA   | 1:215:A:VAL:HG11 | 1        | 0.11          |
| (1,112) | 1:214:A:CYS:HA   | 1:215:A:VAL:HG12 | 1        | 0.11          |
| (1,112) | 1:214:A:CYS:HA   | 1:215:A:VAL:HG13 | 1        | 0.11          |
| (1,112) | 1:214:A:CYS:HA   | 1:215:A:VAL:HG11 | 9        | 0.11          |
| (1,112) | 1:214:A:CYS:HA   | 1:215:A:VAL:HG12 | 9        | 0.11          |
| (1,112) | 1:214:A:CYS:HA   | 1:215:A:VAL:HG13 | 9        | 0.11          |
| (1,112) | 1:214:A:CYS:HA   | 1:215:A:VAL:HG11 | 11       | 0.11          |
| (1,112) | 1:214:A:CYS:HA   | 1:215:A:VAL:HG12 | 11       | 0.11          |
| (1,112) | 1:214:A:CYS:HA   | 1:215:A:VAL:HG13 | 11       | 0.11          |
| (1,112) | 1:214:A:CYS:HA   | 1:215:A:VAL:HG11 | 15       | 0.11          |
| (1,112) | 1:214:A:CYS:HA   | 1:215:A:VAL:HG12 | 15       | 0.11          |
| (1,112) | 1:214:A:CYS:HA   | 1:215:A:VAL:HG13 | 15       | 0.11          |
| (1,111) | 1:215:A:VAL:HG11 | 1:216:A:THR:HB   | 17       | 0.11          |
| (1,111) | 1:215:A:VAL:HG12 | 1:216:A:THR:HB   | 17       | 0.11          |
| (1,111) | 1:215:A:VAL:HG13 | 1:216:A:THR:HB   | 17       | 0.11          |
| (1,77)  | 1:208:A:ARG:H    | 1:209:A:VAL:HG11 | 16       | 0.11          |

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| Key    | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|--------|------------------|------------------|----------|---------------|
| (1,77) | 1:208:A:ARG:H    | 1:209:A:VAL:HG12 | 16       | 0.11          |
| (1,77) | 1:208:A:ARG:H    | 1:209:A:VAL:HG13 | 16       | 0.11          |
| (1,52) | 1:176:A:VAL:HG21 | 1:217:A:GLN:HB3  | 7        | 0.11          |
| (1,52) | 1:176:A:VAL:HG22 | 1:217:A:GLN:HB3  | 7        | 0.11          |
| (1,52) | 1:176:A:VAL:HG23 | 1:217:A:GLN:HB3  | 7        | 0.11          |
| (1,34) | 1:219:A:GLN:HG3  | 1:220:A:LYS:HG2  | 17       | 0.11          |
| (1,32) | 1:219:A:GLN:HB3  | 1:220:A:LYS:HG3  | 1        | 0.11          |
| (1,32) | 1:219:A:GLN:HB3  | 1:220:A:LYS:HG3  | 3        | 0.11          |
| (1,32) | 1:219:A:GLN:HB3  | 1:220:A:LYS:HG3  | 17       | 0.11          |
| (1,31) | 1:219:A:GLN:HA   | 1:220:A:LYS:HG3  | 7        | 0.11          |
| (1,15) | 1:130:A:LEU:HD21 | 1:161:A:VAL:HA   | 2        | 0.11          |
| (1,15) | 1:130:A:LEU:HD22 | 1:161:A:VAL:HA   | 2        | 0.11          |
| (1,15) | 1:130:A:LEU:HD23 | 1:161:A:VAL:HA   | 2        | 0.11          |
| (1,15) | 1:130:A:LEU:HD21 | 1:161:A:VAL:HA   | 4        | 0.11          |
| (1,15) | 1:130:A:LEU:HD22 | 1:161:A:VAL:HA   | 4        | 0.11          |
| (1,15) | 1:130:A:LEU:HD23 | 1:161:A:VAL:HA   | 4        | 0.11          |
| (1,15) | 1:130:A:LEU:HD21 | 1:161:A:VAL:HA   | 5        | 0.11          |
| (1,15) | 1:130:A:LEU:HD22 | 1:161:A:VAL:HA   | 5        | 0.11          |
| (1,15) | 1:130:A:LEU:HD23 | 1:161:A:VAL:HA   | 5        | 0.11          |
| (1,15) | 1:130:A:LEU:HD21 | 1:161:A:VAL:HA   | 9        | 0.11          |
| (1,15) | 1:130:A:LEU:HD22 | 1:161:A:VAL:HA   | 9        | 0.11          |
| (1,15) | 1:130:A:LEU:HD23 | 1:161:A:VAL:HA   | 9        | 0.11          |
| (1,15) | 1:130:A:LEU:HD21 | 1:161:A:VAL:HA   | 11       | 0.11          |
| (1,15) | 1:130:A:LEU:HD22 | 1:161:A:VAL:HA   | 11       | 0.11          |
| (1,15) | 1:130:A:LEU:HD23 | 1:161:A:VAL:HA   | 11       | 0.11          |
| (1,15) | 1:130:A:LEU:HD21 | 1:161:A:VAL:HA   | 12       | 0.11          |
| (1,15) | 1:130:A:LEU:HD22 | 1:161:A:VAL:HA   | 12       | 0.11          |
| (1,15) | 1:130:A:LEU:HD23 | 1:161:A:VAL:HA   | 12       | 0.11          |
| (1,15) | 1:130:A:LEU:HD21 | 1:161:A:VAL:HA   | 14       | 0.11          |
| (1,15) | 1:130:A:LEU:HD22 | 1:161:A:VAL:HA   | 14       | 0.11          |
| (1,15) | 1:130:A:LEU:HD23 | 1:161:A:VAL:HA   | 14       | 0.11          |
| (1,15) | 1:130:A:LEU:HD21 | 1:161:A:VAL:HA   | 16       | 0.11          |
| (1,15) | 1:130:A:LEU:HD22 | 1:161:A:VAL:HA   | 16       | 0.11          |
| (1,15) | 1:130:A:LEU:HD23 | 1:161:A:VAL:HA   | 16       | 0.11          |
| (1,15) | 1:130:A:LEU:HD21 | 1:161:A:VAL:HA   | 17       | 0.11          |
| (1,15) | 1:130:A:LEU:HD22 | 1:161:A:VAL:HA   | 17       | 0.11          |
| (1,15) | 1:130:A:LEU:HD23 | 1:161:A:VAL:HA   | 17       | 0.11          |
| (1,15) | 1:130:A:LEU:HD21 | 1:161:A:VAL:HA   | 18       | 0.11          |
| (1,15) | 1:130:A:LEU:HD22 | 1:161:A:VAL:HA   | 18       | 0.11          |
| (1,15) | 1:130:A:LEU:HD23 | 1:161:A:VAL:HA   | 18       | 0.11          |
| (1,15) | 1:130:A:LEU:HD21 | 1:161:A:VAL:HA   | 19       | 0.11          |
| (1,15) | 1:130:A:LEU:HD22 | 1:161:A:VAL:HA   | 19       | 0.11          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,15)   | 1:130:A:LEU:HD23 | 1:161:A:VAL:HA   | 19       | 0.11          |
| (1,15)   | 1:130:A:LEU:HD21 | 1:161:A:VAL:HA   | 20       | 0.11          |
| (1,15)   | 1:130:A:LEU:HD22 | 1:161:A:VAL:HA   | 20       | 0.11          |
| (1,15)   | 1:130:A:LEU:HD23 | 1:161:A:VAL:HA   | 20       | 0.11          |
| (1,2843) | 1:157:A:TYR:HE1  | 1:206:A:MET:HE1  | 10       | 0.1           |
| (1,2843) | 1:157:A:TYR:HE1  | 1:206:A:MET:HE2  | 10       | 0.1           |
| (1,2843) | 1:157:A:TYR:HE1  | 1:206:A:MET:HE3  | 10       | 0.1           |
| (1,2843) | 1:157:A:TYR:HE2  | 1:206:A:MET:HE1  | 10       | 0.1           |
| (1,2843) | 1:157:A:TYR:HE2  | 1:206:A:MET:HE2  | 10       | 0.1           |
| (1,2843) | 1:157:A:TYR:HE2  | 1:206:A:MET:HE3  | 10       | 0.1           |
| (1,2834) | 1:163:A:TYR:HE1  | 1:221:A:GLU:HG2  | 11       | 0.1           |
| (1,2834) | 1:163:A:TYR:HE2  | 1:221:A:GLU:HG2  | 11       | 0.1           |
| (1,2806) | 1:149:A:TYR:HE1  | 1:205:A:MET:HB2  | 18       | 0.1           |
| (1,2806) | 1:149:A:TYR:HE2  | 1:205:A:MET:HB2  | 18       | 0.1           |
| (1,2787) | 1:128:A:TYR:HA   | 1:128:A:TYR:HE1  | 7        | 0.1           |
| (1,2787) | 1:128:A:TYR:HA   | 1:128:A:TYR:HE2  | 7        | 0.1           |
| (1,2776) | 1:150:A:TYR:HE1  | 1:209:A:VAL:H    | 18       | 0.1           |
| (1,2776) | 1:150:A:TYR:HE2  | 1:209:A:VAL:H    | 18       | 0.1           |
| (1,2776) | 1:150:A:TYR:HE1  | 1:209:A:VAL:H    | 20       | 0.1           |
| (1,2776) | 1:150:A:TYR:HE2  | 1:209:A:VAL:H    | 20       | 0.1           |
| (1,2766) | 1:162:A:TYR:HE1  | 1:182:A:ILE:HG21 | 15       | 0.1           |
| (1,2766) | 1:162:A:TYR:HE1  | 1:182:A:ILE:HG22 | 15       | 0.1           |
| (1,2766) | 1:162:A:TYR:HE1  | 1:182:A:ILE:HG23 | 15       | 0.1           |
| (1,2766) | 1:162:A:TYR:HE2  | 1:182:A:ILE:HG21 | 15       | 0.1           |
| (1,2766) | 1:162:A:TYR:HE2  | 1:182:A:ILE:HG22 | 15       | 0.1           |
| (1,2766) | 1:162:A:TYR:HE2  | 1:182:A:ILE:HG23 | 15       | 0.1           |
| (1,2765) | 1:162:A:TYR:HE1  | 1:186:A:GLN:H    | 11       | 0.1           |
| (1,2765) | 1:162:A:TYR:HE2  | 1:186:A:GLN:H    | 11       | 0.1           |
| (1,2752) | 1:169:A:TYR:HE1  | 1:174:A:ASN:HA   | 11       | 0.1           |
| (1,2752) | 1:169:A:TYR:HE2  | 1:174:A:ASN:HA   | 11       | 0.1           |
| (1,2748) | 1:164:A:ARG:H    | 1:169:A:TYR:HE1  | 12       | 0.1           |
| (1,2748) | 1:164:A:ARG:H    | 1:169:A:TYR:HE2  | 12       | 0.1           |
| (1,2719) | 1:173:A:LYS:HD2  | 1:177:A:HIS:HD2  | 5        | 0.1           |
| (1,2719) | 1:173:A:LYS:HD3  | 1:177:A:HIS:HD2  | 5        | 0.1           |
| (1,2719) | 1:173:A:LYS:HD2  | 1:177:A:HIS:HD2  | 6        | 0.1           |
| (1,2719) | 1:173:A:LYS:HD3  | 1:177:A:HIS:HD2  | 6        | 0.1           |
| (1,2719) | 1:173:A:LYS:HD2  | 1:177:A:HIS:HD2  | 15       | 0.1           |
| (1,2719) | 1:173:A:LYS:HD3  | 1:177:A:HIS:HD2  | 15       | 0.1           |
| (1,2709) | 1:145:A:TRP:HZ3  | 1:205:A:MET:HE1  | 7        | 0.1           |
| (1,2709) | 1:145:A:TRP:HZ3  | 1:205:A:MET:HE2  | 7        | 0.1           |
| (1,2709) | 1:145:A:TRP:HZ3  | 1:205:A:MET:HE3  | 7        | 0.1           |
| (1,2703) | 1:143:A:ASN:HB2  | 1:145:A:TRP:HD1  | 2        | 0.1           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2703) | 1:143:A:ASN:HB3 | 1:145:A:TRP:HD1 | 2        | 0.1           |
| (1,2703) | 1:143:A:ASN:HB2 | 1:145:A:TRP:HD1 | 4        | 0.1           |
| (1,2703) | 1:143:A:ASN:HB3 | 1:145:A:TRP:HD1 | 4        | 0.1           |
| (1,2703) | 1:143:A:ASN:HB2 | 1:145:A:TRP:HD1 | 8        | 0.1           |
| (1,2703) | 1:143:A:ASN:HB3 | 1:145:A:TRP:HD1 | 8        | 0.1           |
| (1,2703) | 1:143:A:ASN:HB2 | 1:145:A:TRP:HD1 | 9        | 0.1           |
| (1,2703) | 1:143:A:ASN:HB3 | 1:145:A:TRP:HD1 | 9        | 0.1           |
| (1,2703) | 1:143:A:ASN:HB2 | 1:145:A:TRP:HD1 | 10       | 0.1           |
| (1,2703) | 1:143:A:ASN:HB3 | 1:145:A:TRP:HD1 | 10       | 0.1           |
| (1,2703) | 1:143:A:ASN:HB2 | 1:145:A:TRP:HD1 | 13       | 0.1           |
| (1,2703) | 1:143:A:ASN:HB3 | 1:145:A:TRP:HD1 | 13       | 0.1           |
| (1,2703) | 1:143:A:ASN:HB2 | 1:145:A:TRP:HD1 | 19       | 0.1           |
| (1,2703) | 1:143:A:ASN:HB3 | 1:145:A:TRP:HD1 | 19       | 0.1           |
| (1,2703) | 1:143:A:ASN:HB2 | 1:145:A:TRP:HD1 | 20       | 0.1           |
| (1,2703) | 1:143:A:ASN:HB3 | 1:145:A:TRP:HD1 | 20       | 0.1           |
| (1,2666) | 1:156:A:ARG:HG2 | 1:198:A:PHE:HE1 | 13       | 0.1           |
| (1,2666) | 1:156:A:ARG:HG2 | 1:198:A:PHE:HE2 | 13       | 0.1           |
| (1,2666) | 1:156:A:ARG:HG2 | 1:198:A:PHE:HE1 | 16       | 0.1           |
| (1,2666) | 1:156:A:ARG:HG2 | 1:198:A:PHE:HE2 | 16       | 0.1           |
| (1,2636) | 1:157:A:TYR:HD1 | 1:209:A:VAL:H   | 2        | 0.1           |
| (1,2636) | 1:157:A:TYR:HD2 | 1:209:A:VAL:H   | 2        | 0.1           |
| (1,2636) | 1:157:A:TYR:HD1 | 1:209:A:VAL:H   | 8        | 0.1           |
| (1,2636) | 1:157:A:TYR:HD2 | 1:209:A:VAL:H   | 8        | 0.1           |
| (1,2635) | 1:196:A:GLU:HB2 | 1:198:A:PHE:HD1 | 6        | 0.1           |
| (1,2635) | 1:196:A:GLU:HB2 | 1:198:A:PHE:HD2 | 6        | 0.1           |
| (1,2635) | 1:196:A:GLU:HB3 | 1:198:A:PHE:HD1 | 6        | 0.1           |
| (1,2635) | 1:196:A:GLU:HB3 | 1:198:A:PHE:HD2 | 6        | 0.1           |
| (1,2631) | 1:198:A:PHE:HD1 | 1:203:A:VAL:HA  | 4        | 0.1           |
| (1,2631) | 1:198:A:PHE:HD2 | 1:203:A:VAL:HA  | 4        | 0.1           |
| (1,2631) | 1:198:A:PHE:HD1 | 1:203:A:VAL:HA  | 10       | 0.1           |
| (1,2631) | 1:198:A:PHE:HD2 | 1:203:A:VAL:HA  | 10       | 0.1           |
| (1,2631) | 1:198:A:PHE:HD1 | 1:203:A:VAL:HA  | 17       | 0.1           |
| (1,2631) | 1:198:A:PHE:HD2 | 1:203:A:VAL:HA  | 17       | 0.1           |
| (1,2629) | 1:192:A:THR:HB  | 1:198:A:PHE:HD1 | 10       | 0.1           |
| (1,2629) | 1:192:A:THR:HB  | 1:198:A:PHE:HD2 | 10       | 0.1           |
| (1,2628) | 1:157:A:TYR:HE1 | 1:198:A:PHE:HD1 | 16       | 0.1           |
| (1,2628) | 1:157:A:TYR:HE1 | 1:198:A:PHE:HD2 | 16       | 0.1           |
| (1,2628) | 1:157:A:TYR:HE2 | 1:198:A:PHE:HD1 | 16       | 0.1           |
| (1,2628) | 1:157:A:TYR:HE2 | 1:198:A:PHE:HD2 | 16       | 0.1           |
| (1,2627) | 1:157:A:TYR:HD1 | 1:198:A:PHE:HD1 | 16       | 0.1           |
| (1,2627) | 1:157:A:TYR:HD1 | 1:198:A:PHE:HD2 | 16       | 0.1           |
| (1,2627) | 1:157:A:TYR:HD2 | 1:198:A:PHE:HD1 | 16       | 0.1           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2627) | 1:157:A:TYR:HD2  | 1:198:A:PHE:HD2  | 16       | 0.1           |
| (1,2600) | 1:166:A:VAL:HG21 | 1:175:A:PHE:HE1  | 10       | 0.1           |
| (1,2600) | 1:166:A:VAL:HG21 | 1:175:A:PHE:HE2  | 10       | 0.1           |
| (1,2600) | 1:166:A:VAL:HG22 | 1:175:A:PHE:HE1  | 10       | 0.1           |
| (1,2600) | 1:166:A:VAL:HG22 | 1:175:A:PHE:HE2  | 10       | 0.1           |
| (1,2600) | 1:166:A:VAL:HG23 | 1:175:A:PHE:HE1  | 10       | 0.1           |
| (1,2600) | 1:166:A:VAL:HG23 | 1:175:A:PHE:HE2  | 10       | 0.1           |
| (1,2600) | 1:166:A:VAL:HG21 | 1:175:A:PHE:HE1  | 11       | 0.1           |
| (1,2600) | 1:166:A:VAL:HG21 | 1:175:A:PHE:HE2  | 11       | 0.1           |
| (1,2600) | 1:166:A:VAL:HG22 | 1:175:A:PHE:HE1  | 11       | 0.1           |
| (1,2600) | 1:166:A:VAL:HG22 | 1:175:A:PHE:HE2  | 11       | 0.1           |
| (1,2600) | 1:166:A:VAL:HG23 | 1:175:A:PHE:HE1  | 11       | 0.1           |
| (1,2600) | 1:166:A:VAL:HG23 | 1:175:A:PHE:HE2  | 11       | 0.1           |
| (1,2600) | 1:166:A:VAL:HG21 | 1:175:A:PHE:HE1  | 16       | 0.1           |
| (1,2600) | 1:166:A:VAL:HG21 | 1:175:A:PHE:HE2  | 16       | 0.1           |
| (1,2600) | 1:166:A:VAL:HG22 | 1:175:A:PHE:HE1  | 16       | 0.1           |
| (1,2600) | 1:166:A:VAL:HG22 | 1:175:A:PHE:HE2  | 16       | 0.1           |
| (1,2600) | 1:166:A:VAL:HG23 | 1:175:A:PHE:HE1  | 16       | 0.1           |
| (1,2600) | 1:166:A:VAL:HG23 | 1:175:A:PHE:HE2  | 16       | 0.1           |
| (1,2593) | 1:175:A:PHE:HE1  | 1:221:A:GLU:HG2  | 19       | 0.1           |
| (1,2593) | 1:175:A:PHE:HE2  | 1:221:A:GLU:HG2  | 19       | 0.1           |
| (1,2562) | 1:125:A:LEU:HD21 | 1:128:A:TYR:HD1  | 19       | 0.1           |
| (1,2562) | 1:125:A:LEU:HD21 | 1:128:A:TYR:HD2  | 19       | 0.1           |
| (1,2562) | 1:125:A:LEU:HD22 | 1:128:A:TYR:HD1  | 19       | 0.1           |
| (1,2562) | 1:125:A:LEU:HD22 | 1:128:A:TYR:HD2  | 19       | 0.1           |
| (1,2562) | 1:125:A:LEU:HD23 | 1:128:A:TYR:HD1  | 19       | 0.1           |
| (1,2562) | 1:125:A:LEU:HD23 | 1:128:A:TYR:HD2  | 19       | 0.1           |
| (1,2557) | 1:128:A:TYR:HD1  | 1:164:A:ARG:HA   | 1        | 0.1           |
| (1,2557) | 1:128:A:TYR:HD2  | 1:164:A:ARG:HA   | 1        | 0.1           |
| (1,2557) | 1:128:A:TYR:HD1  | 1:164:A:ARG:HA   | 4        | 0.1           |
| (1,2557) | 1:128:A:TYR:HD2  | 1:164:A:ARG:HA   | 4        | 0.1           |
| (1,2526) | 1:155:A:TYR:HD1  | 1:156:A:ARG:HG3  | 14       | 0.1           |
| (1,2526) | 1:155:A:TYR:HD2  | 1:156:A:ARG:HG3  | 14       | 0.1           |
| (1,2508) | 1:150:A:TYR:HD1  | 1:206:A:MET:H    | 18       | 0.1           |
| (1,2508) | 1:150:A:TYR:HD2  | 1:206:A:MET:H    | 18       | 0.1           |
| (1,2500) | 1:149:A:TYR:HD1  | 1:201:A:THR:HG21 | 9        | 0.1           |
| (1,2500) | 1:149:A:TYR:HD1  | 1:201:A:THR:HG22 | 9        | 0.1           |
| (1,2500) | 1:149:A:TYR:HD1  | 1:201:A:THR:HG23 | 9        | 0.1           |
| (1,2500) | 1:149:A:TYR:HD2  | 1:201:A:THR:HG21 | 9        | 0.1           |
| (1,2500) | 1:149:A:TYR:HD2  | 1:201:A:THR:HG22 | 9        | 0.1           |
| (1,2500) | 1:149:A:TYR:HD2  | 1:201:A:THR:HG23 | 9        | 0.1           |
| (1,2496) | 1:149:A:TYR:HD1  | 1:152:A:GLU:HB2  | 13       | 0.1           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2496) | 1:149:A:TYR:HD1  | 1:152:A:GLU:HB3  | 13       | 0.1           |
| (1,2496) | 1:149:A:TYR:HD2  | 1:152:A:GLU:HB2  | 13       | 0.1           |
| (1,2496) | 1:149:A:TYR:HD2  | 1:152:A:GLU:HB3  | 13       | 0.1           |
| (1,2496) | 1:149:A:TYR:HD1  | 1:152:A:GLU:HB2  | 15       | 0.1           |
| (1,2496) | 1:149:A:TYR:HD1  | 1:152:A:GLU:HB3  | 15       | 0.1           |
| (1,2496) | 1:149:A:TYR:HD2  | 1:152:A:GLU:HB2  | 15       | 0.1           |
| (1,2496) | 1:149:A:TYR:HD2  | 1:152:A:GLU:HB3  | 15       | 0.1           |
| (1,2488) | 1:149:A:TYR:HD1  | 1:153:A:ASN:HB3  | 12       | 0.1           |
| (1,2488) | 1:149:A:TYR:HD2  | 1:153:A:ASN:HB3  | 12       | 0.1           |
| (1,2475) | 1:166:A:VAL:HB   | 1:169:A:TYR:HD1  | 3        | 0.1           |
| (1,2475) | 1:166:A:VAL:HB   | 1:169:A:TYR:HD2  | 3        | 0.1           |
| (1,2466) | 1:169:A:TYR:HD1  | 1:174:A:ASN:HB3  | 4        | 0.1           |
| (1,2466) | 1:169:A:TYR:HD2  | 1:174:A:ASN:HB3  | 4        | 0.1           |
| (1,2466) | 1:169:A:TYR:HD1  | 1:174:A:ASN:HB3  | 7        | 0.1           |
| (1,2466) | 1:169:A:TYR:HD2  | 1:174:A:ASN:HB3  | 7        | 0.1           |
| (1,2437) | 1:155:A:TYR:HD1  | 1:156:A:ARG:HE   | 4        | 0.1           |
| (1,2437) | 1:155:A:TYR:HD2  | 1:156:A:ARG:HE   | 4        | 0.1           |
| (1,2393) | 1:186:A:GLN:HE21 | 1:190:A:THR:HG21 | 11       | 0.1           |
| (1,2393) | 1:186:A:GLN:HE21 | 1:190:A:THR:HG22 | 11       | 0.1           |
| (1,2393) | 1:186:A:GLN:HE21 | 1:190:A:THR:HG23 | 11       | 0.1           |
| (1,2351) | 1:181:A:ASN:HD22 | 1:185:A:LYS:HE2  | 4        | 0.1           |
| (1,2351) | 1:181:A:ASN:HD22 | 1:185:A:LYS:HE3  | 4        | 0.1           |
| (1,2338) | 1:212:A:GLN:HE21 | 1:215:A:VAL:HG11 | 11       | 0.1           |
| (1,2338) | 1:212:A:GLN:HE21 | 1:215:A:VAL:HG12 | 11       | 0.1           |
| (1,2338) | 1:212:A:GLN:HE21 | 1:215:A:VAL:HG13 | 11       | 0.1           |
| (1,2323) | 1:133:A:ALA:HB1  | 1:160:A:GLN:HE22 | 2        | 0.1           |
| (1,2323) | 1:133:A:ALA:HB2  | 1:160:A:GLN:HE22 | 2        | 0.1           |
| (1,2323) | 1:133:A:ALA:HB3  | 1:160:A:GLN:HE22 | 2        | 0.1           |
| (1,2323) | 1:133:A:ALA:HB1  | 1:160:A:GLN:HE22 | 15       | 0.1           |
| (1,2323) | 1:133:A:ALA:HB2  | 1:160:A:GLN:HE22 | 15       | 0.1           |
| (1,2323) | 1:133:A:ALA:HB3  | 1:160:A:GLN:HE22 | 15       | 0.1           |
| (1,2322) | 1:130:A:LEU:HG   | 1:160:A:GLN:HE22 | 16       | 0.1           |
| (1,2317) | 1:133:A:ALA:HB1  | 1:160:A:GLN:HE21 | 20       | 0.1           |
| (1,2317) | 1:133:A:ALA:HB2  | 1:160:A:GLN:HE21 | 20       | 0.1           |
| (1,2317) | 1:133:A:ALA:HB3  | 1:160:A:GLN:HE21 | 20       | 0.1           |
| (1,2271) | 1:132:A:SER:H    | 1:134:A:MET:HE1  | 20       | 0.1           |
| (1,2271) | 1:132:A:SER:H    | 1:134:A:MET:HE2  | 20       | 0.1           |
| (1,2271) | 1:132:A:SER:H    | 1:134:A:MET:HE3  | 20       | 0.1           |
| (1,2166) | 1:133:A:ALA:HB1  | 1:159:A:ASN:H    | 19       | 0.1           |
| (1,2166) | 1:133:A:ALA:HB2  | 1:159:A:ASN:H    | 19       | 0.1           |
| (1,2166) | 1:133:A:ALA:HB3  | 1:159:A:ASN:H    | 19       | 0.1           |
| (1,2152) | 1:134:A:MET:HB3  | 1:135:A:SER:H    | 16       | 0.1           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2043) | 1:231:A:SER:H    | 1:231:A:SER:HB3  | 3        | 0.1           |
| (1,1975) | 1:184:A:ILE:HD11 | 1:206:A:MET:H    | 2        | 0.1           |
| (1,1975) | 1:184:A:ILE:HD12 | 1:206:A:MET:H    | 2        | 0.1           |
| (1,1975) | 1:184:A:ILE:HD13 | 1:206:A:MET:H    | 2        | 0.1           |
| (1,1975) | 1:184:A:ILE:HD11 | 1:206:A:MET:H    | 3        | 0.1           |
| (1,1975) | 1:184:A:ILE:HD12 | 1:206:A:MET:H    | 3        | 0.1           |
| (1,1975) | 1:184:A:ILE:HD13 | 1:206:A:MET:H    | 3        | 0.1           |
| (1,1975) | 1:184:A:ILE:HD11 | 1:206:A:MET:H    | 12       | 0.1           |
| (1,1975) | 1:184:A:ILE:HD12 | 1:206:A:MET:H    | 12       | 0.1           |
| (1,1975) | 1:184:A:ILE:HD13 | 1:206:A:MET:H    | 12       | 0.1           |
| (1,1969) | 1:204:A:LYS:HB2  | 1:205:A:MET:H    | 7        | 0.1           |
| (1,1969) | 1:204:A:LYS:HB3  | 1:205:A:MET:H    | 7        | 0.1           |
| (1,1968) | 1:205:A:MET:H    | 1:205:A:MET:HG3  | 17       | 0.1           |
| (1,1926) | 1:134:A:MET:HE1  | 1:214:A:CYS:H    | 8        | 0.1           |
| (1,1926) | 1:134:A:MET:HE2  | 1:214:A:CYS:H    | 8        | 0.1           |
| (1,1926) | 1:134:A:MET:HE3  | 1:214:A:CYS:H    | 8        | 0.1           |
| (1,1926) | 1:134:A:MET:HE1  | 1:214:A:CYS:H    | 14       | 0.1           |
| (1,1926) | 1:134:A:MET:HE2  | 1:214:A:CYS:H    | 14       | 0.1           |
| (1,1926) | 1:134:A:MET:HE3  | 1:214:A:CYS:H    | 14       | 0.1           |
| (1,1926) | 1:134:A:MET:HE1  | 1:214:A:CYS:H    | 17       | 0.1           |
| (1,1926) | 1:134:A:MET:HE2  | 1:214:A:CYS:H    | 17       | 0.1           |
| (1,1926) | 1:134:A:MET:HE3  | 1:214:A:CYS:H    | 17       | 0.1           |
| (1,1707) | 1:161:A:VAL:HB   | 1:162:A:TYR:H    | 10       | 0.1           |
| (1,1671) | 1:189:A:VAL:H    | 1:189:A:VAL:HB   | 11       | 0.1           |
| (1,1562) | 1:228:A:GLY:HA2  | 1:229:A:ARG:HG2  | 15       | 0.1           |
| (1,1562) | 1:228:A:GLY:HA2  | 1:229:A:ARG:HG3  | 15       | 0.1           |
| (1,1562) | 1:228:A:GLY:HA3  | 1:229:A:ARG:HG2  | 15       | 0.1           |
| (1,1562) | 1:228:A:GLY:HA3  | 1:229:A:ARG:HG3  | 15       | 0.1           |
| (1,1562) | 1:228:A:GLY:HA2  | 1:229:A:ARG:HG2  | 18       | 0.1           |
| (1,1562) | 1:228:A:GLY:HA2  | 1:229:A:ARG:HG3  | 18       | 0.1           |
| (1,1562) | 1:228:A:GLY:HA3  | 1:229:A:ARG:HG2  | 18       | 0.1           |
| (1,1562) | 1:228:A:GLY:HA3  | 1:229:A:ARG:HG3  | 18       | 0.1           |
| (1,1505) | 1:137:A:PRO:HD2  | 1:209:A:VAL:HG11 | 3        | 0.1           |
| (1,1505) | 1:137:A:PRO:HD2  | 1:209:A:VAL:HG12 | 3        | 0.1           |
| (1,1505) | 1:137:A:PRO:HD2  | 1:209:A:VAL:HG13 | 3        | 0.1           |
| (1,1505) | 1:137:A:PRO:HD2  | 1:209:A:VAL:HG11 | 5        | 0.1           |
| (1,1505) | 1:137:A:PRO:HD2  | 1:209:A:VAL:HG12 | 5        | 0.1           |
| (1,1505) | 1:137:A:PRO:HD2  | 1:209:A:VAL:HG13 | 5        | 0.1           |
| (1,1436) | 1:194:A:LYS:HD2  | 1:196:A:GLU:HG2  | 11       | 0.1           |
| (1,1436) | 1:194:A:LYS:HD2  | 1:196:A:GLU:HG3  | 11       | 0.1           |
| (1,1436) | 1:194:A:LYS:HD3  | 1:196:A:GLU:HG2  | 11       | 0.1           |
| (1,1436) | 1:194:A:LYS:HD3  | 1:196:A:GLU:HG3  | 11       | 0.1           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1425) | 1:193:A:THR:HG21 | 1:194:A:LYS:HD2  | 9        | 0.1           |
| (1,1425) | 1:193:A:THR:HG21 | 1:194:A:LYS:HD3  | 9        | 0.1           |
| (1,1425) | 1:193:A:THR:HG22 | 1:194:A:LYS:HD2  | 9        | 0.1           |
| (1,1425) | 1:193:A:THR:HG22 | 1:194:A:LYS:HD3  | 9        | 0.1           |
| (1,1425) | 1:193:A:THR:HG23 | 1:194:A:LYS:HD2  | 9        | 0.1           |
| (1,1425) | 1:193:A:THR:HG23 | 1:194:A:LYS:HD3  | 9        | 0.1           |
| (1,1422) | 1:194:A:LYS:HD2  | 1:195:A:GLY:H    | 1        | 0.1           |
| (1,1422) | 1:194:A:LYS:HD3  | 1:195:A:GLY:H    | 1        | 0.1           |
| (1,1422) | 1:194:A:LYS:HD2  | 1:195:A:GLY:H    | 6        | 0.1           |
| (1,1422) | 1:194:A:LYS:HD3  | 1:195:A:GLY:H    | 6        | 0.1           |
| (1,1422) | 1:194:A:LYS:HD2  | 1:195:A:GLY:H    | 14       | 0.1           |
| (1,1422) | 1:194:A:LYS:HD3  | 1:195:A:GLY:H    | 14       | 0.1           |
| (1,1422) | 1:194:A:LYS:HD2  | 1:195:A:GLY:H    | 15       | 0.1           |
| (1,1422) | 1:194:A:LYS:HD3  | 1:195:A:GLY:H    | 15       | 0.1           |
| (1,1385) | 1:183:A:THR:HG21 | 1:187:A:HIS:HB2  | 5        | 0.1           |
| (1,1385) | 1:183:A:THR:HG22 | 1:187:A:HIS:HB2  | 5        | 0.1           |
| (1,1385) | 1:183:A:THR:HG23 | 1:187:A:HIS:HB2  | 5        | 0.1           |
| (1,1385) | 1:183:A:THR:HG21 | 1:187:A:HIS:HB2  | 11       | 0.1           |
| (1,1385) | 1:183:A:THR:HG22 | 1:187:A:HIS:HB2  | 11       | 0.1           |
| (1,1385) | 1:183:A:THR:HG23 | 1:187:A:HIS:HB2  | 11       | 0.1           |
| (1,1385) | 1:183:A:THR:HG21 | 1:187:A:HIS:HB2  | 13       | 0.1           |
| (1,1385) | 1:183:A:THR:HG22 | 1:187:A:HIS:HB2  | 13       | 0.1           |
| (1,1385) | 1:183:A:THR:HG23 | 1:187:A:HIS:HB2  | 13       | 0.1           |
| (1,1378) | 1:157:A:TYR:HA   | 1:206:A:MET:HE1  | 19       | 0.1           |
| (1,1378) | 1:157:A:TYR:HA   | 1:206:A:MET:HE2  | 19       | 0.1           |
| (1,1378) | 1:157:A:TYR:HA   | 1:206:A:MET:HE3  | 19       | 0.1           |
| (1,1322) | 1:133:A:ALA:HB1  | 1:134:A:MET:HG2  | 8        | 0.1           |
| (1,1322) | 1:133:A:ALA:HB2  | 1:134:A:MET:HG2  | 8        | 0.1           |
| (1,1322) | 1:133:A:ALA:HB3  | 1:134:A:MET:HG2  | 8        | 0.1           |
| (1,1322) | 1:133:A:ALA:HB1  | 1:134:A:MET:HG2  | 17       | 0.1           |
| (1,1322) | 1:133:A:ALA:HB2  | 1:134:A:MET:HG2  | 17       | 0.1           |
| (1,1322) | 1:133:A:ALA:HB3  | 1:134:A:MET:HG2  | 17       | 0.1           |
| (1,1278) | 1:137:A:PRO:HB2  | 1:139:A:ILE:HG21 | 13       | 0.1           |
| (1,1278) | 1:137:A:PRO:HB2  | 1:139:A:ILE:HG22 | 13       | 0.1           |
| (1,1278) | 1:137:A:PRO:HB2  | 1:139:A:ILE:HG23 | 13       | 0.1           |
| (1,1275) | 1:187:A:HIS:HE1  | 1:206:A:MET:HG3  | 12       | 0.1           |
| (1,1272) | 1:137:A:PRO:HB3  | 1:213:A:MET:HE1  | 2        | 0.1           |
| (1,1272) | 1:137:A:PRO:HB3  | 1:213:A:MET:HE2  | 2        | 0.1           |
| (1,1272) | 1:137:A:PRO:HB3  | 1:213:A:MET:HE3  | 2        | 0.1           |
| (1,1257) | 1:206:A:MET:HG3  | 1:210:A:VAL:HG21 | 14       | 0.1           |
| (1,1257) | 1:206:A:MET:HG3  | 1:210:A:VAL:HG22 | 14       | 0.1           |
| (1,1257) | 1:206:A:MET:HG3  | 1:210:A:VAL:HG23 | 14       | 0.1           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1253) | 1:203:A:VAL:HA   | 1:204:A:LYS:HB2  | 5        | 0.1           |
| (1,1253) | 1:203:A:VAL:HA   | 1:204:A:LYS:HB3  | 5        | 0.1           |
| (1,1253) | 1:203:A:VAL:HA   | 1:204:A:LYS:HB2  | 10       | 0.1           |
| (1,1253) | 1:203:A:VAL:HA   | 1:204:A:LYS:HB3  | 10       | 0.1           |
| (1,1253) | 1:203:A:VAL:HA   | 1:204:A:LYS:HB2  | 12       | 0.1           |
| (1,1253) | 1:203:A:VAL:HA   | 1:204:A:LYS:HB3  | 12       | 0.1           |
| (1,1244) | 1:158:A:PRO:HB3  | 1:210:A:VAL:HG21 | 19       | 0.1           |
| (1,1244) | 1:158:A:PRO:HB3  | 1:210:A:VAL:HG22 | 19       | 0.1           |
| (1,1244) | 1:158:A:PRO:HB3  | 1:210:A:VAL:HG23 | 19       | 0.1           |
| (1,1230) | 1:137:A:PRO:HD2  | 1:213:A:MET:HG3  | 4        | 0.1           |
| (1,1215) | 1:227:A:ASP:HB2  | 1:229:A:ARG:HA   | 8        | 0.1           |
| (1,1215) | 1:227:A:ASP:HB3  | 1:229:A:ARG:HA   | 8        | 0.1           |
| (1,1215) | 1:227:A:ASP:HB2  | 1:229:A:ARG:HA   | 16       | 0.1           |
| (1,1215) | 1:227:A:ASP:HB3  | 1:229:A:ARG:HA   | 16       | 0.1           |
| (1,1212) | 1:184:A:ILE:HD11 | 1:206:A:MET:HB3  | 5        | 0.1           |
| (1,1212) | 1:184:A:ILE:HD12 | 1:206:A:MET:HB3  | 5        | 0.1           |
| (1,1212) | 1:184:A:ILE:HD13 | 1:206:A:MET:HB3  | 5        | 0.1           |
| (1,1155) | 1:130:A:LEU:HB3  | 1:162:A:TYR:HA   | 17       | 0.1           |
| (1,1113) | 1:161:A:VAL:HB   | 1:163:A:TYR:HD1  | 10       | 0.1           |
| (1,1113) | 1:161:A:VAL:HB   | 1:163:A:TYR:HD2  | 10       | 0.1           |
| (1,1095) | 1:165:A:PRO:HA   | 1:168:A:GLN:HG2  | 13       | 0.1           |
| (1,1069) | 1:223:A:GLN:HA   | 1:223:A:GLN:HG2  | 7        | 0.1           |
| (1,1065) | 1:223:A:GLN:HA   | 1:225:A:TYR:HD1  | 14       | 0.1           |
| (1,1065) | 1:223:A:GLN:HA   | 1:225:A:TYR:HD2  | 14       | 0.1           |
| (1,1055) | 1:203:A:VAL:HG21 | 1:207:A:GLU:HG2  | 1        | 0.1           |
| (1,1055) | 1:203:A:VAL:HG22 | 1:207:A:GLU:HG2  | 1        | 0.1           |
| (1,1055) | 1:203:A:VAL:HG23 | 1:207:A:GLU:HG2  | 1        | 0.1           |
| (1,1048) | 1:125:A:LEU:HB3  | 1:128:A:TYR:HA   | 3        | 0.1           |
| (1,1011) | 1:208:A:ARG:HA   | 1:208:A:ARG:HG3  | 19       | 0.1           |
| (1,1007) | 1:137:A:PRO:HA   | 1:139:A:ILE:HD11 | 10       | 0.1           |
| (1,1007) | 1:137:A:PRO:HA   | 1:139:A:ILE:HD12 | 10       | 0.1           |
| (1,1007) | 1:137:A:PRO:HA   | 1:139:A:ILE:HD13 | 10       | 0.1           |
| (1,970)  | 1:161:A:VAL:HG21 | 1:217:A:GLN:HA   | 3        | 0.1           |
| (1,970)  | 1:161:A:VAL:HG22 | 1:217:A:GLN:HA   | 3        | 0.1           |
| (1,970)  | 1:161:A:VAL:HG23 | 1:217:A:GLN:HA   | 3        | 0.1           |
| (1,960)  | 1:180:A:VAL:HG21 | 1:184:A:ILE:HD11 | 8        | 0.1           |
| (1,960)  | 1:180:A:VAL:HG21 | 1:184:A:ILE:HD12 | 8        | 0.1           |
| (1,960)  | 1:180:A:VAL:HG21 | 1:184:A:ILE:HD13 | 8        | 0.1           |
| (1,960)  | 1:180:A:VAL:HG22 | 1:184:A:ILE:HD11 | 8        | 0.1           |
| (1,960)  | 1:180:A:VAL:HG22 | 1:184:A:ILE:HD12 | 8        | 0.1           |
| (1,960)  | 1:180:A:VAL:HG22 | 1:184:A:ILE:HD13 | 8        | 0.1           |
| (1,960)  | 1:180:A:VAL:HG23 | 1:184:A:ILE:HD11 | 8        | 0.1           |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,960) | 1:180:A:VAL:HG23 | 1:184:A:ILE:HD12 | 8        | 0.1           |
| (1,960) | 1:180:A:VAL:HG23 | 1:184:A:ILE:HD13 | 8        | 0.1           |
| (1,944) | 1:171:A:ASN:HB3  | 1:172:A:GLN:HA   | 6        | 0.1           |
| (1,938) | 1:184:A:ILE:HD11 | 1:185:A:LYS:HE2  | 11       | 0.1           |
| (1,938) | 1:184:A:ILE:HD11 | 1:185:A:LYS:HE3  | 11       | 0.1           |
| (1,938) | 1:184:A:ILE:HD12 | 1:185:A:LYS:HE2  | 11       | 0.1           |
| (1,938) | 1:184:A:ILE:HD12 | 1:185:A:LYS:HE3  | 11       | 0.1           |
| (1,938) | 1:184:A:ILE:HD13 | 1:185:A:LYS:HE2  | 11       | 0.1           |
| (1,938) | 1:184:A:ILE:HD13 | 1:185:A:LYS:HE3  | 11       | 0.1           |
| (1,902) | 1:147:A:ASP:HB2  | 1:148:A:ARG:HA   | 1        | 0.1           |
| (1,825) | 1:133:A:ALA:HB1  | 1:159:A:ASN:HB3  | 8        | 0.1           |
| (1,825) | 1:133:A:ALA:HB2  | 1:159:A:ASN:HB3  | 8        | 0.1           |
| (1,825) | 1:133:A:ALA:HB3  | 1:159:A:ASN:HB3  | 8        | 0.1           |
| (1,825) | 1:133:A:ALA:HB1  | 1:159:A:ASN:HB3  | 14       | 0.1           |
| (1,825) | 1:133:A:ALA:HB2  | 1:159:A:ASN:HB3  | 14       | 0.1           |
| (1,825) | 1:133:A:ALA:HB3  | 1:159:A:ASN:HB3  | 14       | 0.1           |
| (1,807) | 1:181:A:ASN:HB3  | 1:184:A:ILE:HG21 | 12       | 0.1           |
| (1,807) | 1:181:A:ASN:HB3  | 1:184:A:ILE:HG22 | 12       | 0.1           |
| (1,807) | 1:181:A:ASN:HB3  | 1:184:A:ILE:HG23 | 12       | 0.1           |
| (1,792) | 1:145:A:TRP:HA   | 1:148:A:ARG:HB2  | 12       | 0.1           |
| (1,792) | 1:145:A:TRP:HA   | 1:148:A:ARG:HB3  | 12       | 0.1           |
| (1,764) | 1:120:A:SER:HB2  | 1:121:A:VAL:HA   | 9        | 0.1           |
| (1,764) | 1:120:A:SER:HB3  | 1:121:A:VAL:HA   | 9        | 0.1           |
| (1,760) | 1:184:A:ILE:HB   | 1:206:A:MET:HE1  | 8        | 0.1           |
| (1,760) | 1:184:A:ILE:HB   | 1:206:A:MET:HE2  | 8        | 0.1           |
| (1,760) | 1:184:A:ILE:HB   | 1:206:A:MET:HE3  | 8        | 0.1           |
| (1,745) | 1:122:A:VAL:HA   | 1:190:A:THR:HG21 | 16       | 0.1           |
| (1,745) | 1:122:A:VAL:HA   | 1:190:A:THR:HG22 | 16       | 0.1           |
| (1,745) | 1:122:A:VAL:HA   | 1:190:A:THR:HG23 | 16       | 0.1           |
| (1,739) | 1:166:A:VAL:HG11 | 1:222:A:SER:HB3  | 15       | 0.1           |
| (1,739) | 1:166:A:VAL:HG12 | 1:222:A:SER:HB3  | 15       | 0.1           |
| (1,739) | 1:166:A:VAL:HG13 | 1:222:A:SER:HB3  | 15       | 0.1           |
| (1,706) | 1:136:A:ARG:HE   | 1:154:A:MET:HE1  | 3        | 0.1           |
| (1,706) | 1:136:A:ARG:HE   | 1:154:A:MET:HE2  | 3        | 0.1           |
| (1,706) | 1:136:A:ARG:HE   | 1:154:A:MET:HE3  | 3        | 0.1           |
| (1,667) | 1:138:A:MET:HE1  | 1:154:A:MET:HE1  | 4        | 0.1           |
| (1,667) | 1:138:A:MET:HE1  | 1:154:A:MET:HE2  | 4        | 0.1           |
| (1,667) | 1:138:A:MET:HE1  | 1:154:A:MET:HE3  | 4        | 0.1           |
| (1,667) | 1:138:A:MET:HE2  | 1:154:A:MET:HE1  | 4        | 0.1           |
| (1,667) | 1:138:A:MET:HE2  | 1:154:A:MET:HE2  | 4        | 0.1           |
| (1,667) | 1:138:A:MET:HE2  | 1:154:A:MET:HE3  | 4        | 0.1           |
| (1,667) | 1:138:A:MET:HE3  | 1:154:A:MET:HE1  | 4        | 0.1           |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,667) | 1:138:A:MET:HE3 | 1:154:A:MET:HE2 | 4        | 0.1           |
| (1,667) | 1:138:A:MET:HE3 | 1:154:A:MET:HE3 | 4        | 0.1           |
| (1,667) | 1:138:A:MET:HE1 | 1:154:A:MET:HE1 | 5        | 0.1           |
| (1,667) | 1:138:A:MET:HE1 | 1:154:A:MET:HE2 | 5        | 0.1           |
| (1,667) | 1:138:A:MET:HE1 | 1:154:A:MET:HE3 | 5        | 0.1           |
| (1,667) | 1:138:A:MET:HE2 | 1:154:A:MET:HE1 | 5        | 0.1           |
| (1,667) | 1:138:A:MET:HE2 | 1:154:A:MET:HE2 | 5        | 0.1           |
| (1,667) | 1:138:A:MET:HE2 | 1:154:A:MET:HE3 | 5        | 0.1           |
| (1,667) | 1:138:A:MET:HE3 | 1:154:A:MET:HE1 | 5        | 0.1           |
| (1,667) | 1:138:A:MET:HE3 | 1:154:A:MET:HE2 | 5        | 0.1           |
| (1,667) | 1:138:A:MET:HE3 | 1:154:A:MET:HE3 | 5        | 0.1           |
| (1,667) | 1:138:A:MET:HE1 | 1:154:A:MET:HE1 | 8        | 0.1           |
| (1,667) | 1:138:A:MET:HE1 | 1:154:A:MET:HE2 | 8        | 0.1           |
| (1,667) | 1:138:A:MET:HE1 | 1:154:A:MET:HE3 | 8        | 0.1           |
| (1,667) | 1:138:A:MET:HE2 | 1:154:A:MET:HE1 | 8        | 0.1           |
| (1,667) | 1:138:A:MET:HE2 | 1:154:A:MET:HE2 | 8        | 0.1           |
| (1,667) | 1:138:A:MET:HE2 | 1:154:A:MET:HE3 | 8        | 0.1           |
| (1,667) | 1:138:A:MET:HE3 | 1:154:A:MET:HE1 | 8        | 0.1           |
| (1,667) | 1:138:A:MET:HE3 | 1:154:A:MET:HE2 | 8        | 0.1           |
| (1,667) | 1:138:A:MET:HE3 | 1:154:A:MET:HE3 | 8        | 0.1           |
| (1,667) | 1:138:A:MET:HE1 | 1:154:A:MET:HE1 | 14       | 0.1           |
| (1,667) | 1:138:A:MET:HE1 | 1:154:A:MET:HE2 | 14       | 0.1           |
| (1,667) | 1:138:A:MET:HE1 | 1:154:A:MET:HE3 | 14       | 0.1           |
| (1,667) | 1:138:A:MET:HE2 | 1:154:A:MET:HE1 | 14       | 0.1           |
| (1,667) | 1:138:A:MET:HE2 | 1:154:A:MET:HE2 | 14       | 0.1           |
| (1,667) | 1:138:A:MET:HE2 | 1:154:A:MET:HE3 | 14       | 0.1           |
| (1,667) | 1:138:A:MET:HE3 | 1:154:A:MET:HE1 | 14       | 0.1           |
| (1,667) | 1:138:A:MET:HE3 | 1:154:A:MET:HE2 | 14       | 0.1           |
| (1,667) | 1:138:A:MET:HE3 | 1:154:A:MET:HE3 | 14       | 0.1           |
| (1,667) | 1:138:A:MET:HE1 | 1:154:A:MET:HE1 | 20       | 0.1           |
| (1,667) | 1:138:A:MET:HE1 | 1:154:A:MET:HE2 | 20       | 0.1           |
| (1,667) | 1:138:A:MET:HE1 | 1:154:A:MET:HE3 | 20       | 0.1           |
| (1,667) | 1:138:A:MET:HE2 | 1:154:A:MET:HE1 | 20       | 0.1           |
| (1,667) | 1:138:A:MET:HE2 | 1:154:A:MET:HE2 | 20       | 0.1           |
| (1,667) | 1:138:A:MET:HE2 | 1:154:A:MET:HE3 | 20       | 0.1           |
| (1,667) | 1:138:A:MET:HE3 | 1:154:A:MET:HE1 | 20       | 0.1           |
| (1,667) | 1:138:A:MET:HE3 | 1:154:A:MET:HE2 | 20       | 0.1           |
| (1,667) | 1:138:A:MET:HE3 | 1:154:A:MET:HE3 | 20       | 0.1           |
| (1,660) | 1:154:A:MET:HB2 | 1:154:A:MET:HE1 | 10       | 0.1           |
| (1,660) | 1:154:A:MET:HB2 | 1:154:A:MET:HE2 | 10       | 0.1           |
| (1,660) | 1:154:A:MET:HB2 | 1:154:A:MET:HE3 | 10       | 0.1           |
| (1,660) | 1:154:A:MET:HB2 | 1:154:A:MET:HE1 | 13       | 0.1           |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,660) | 1:154:A:MET:HB2  | 1:154:A:MET:HE2 | 13       | 0.1           |
| (1,660) | 1:154:A:MET:HB2  | 1:154:A:MET:HE3 | 13       | 0.1           |
| (1,645) | 1:191:A:THR:HA   | 1:196:A:GLU:HG2 | 13       | 0.1           |
| (1,645) | 1:191:A:THR:HA   | 1:196:A:GLU:HG3 | 13       | 0.1           |
| (1,639) | 1:191:A:THR:HA   | 1:194:A:LYS:HE2 | 5        | 0.1           |
| (1,639) | 1:191:A:THR:HA   | 1:194:A:LYS:HE3 | 5        | 0.1           |
| (1,612) | 1:134:A:MET:HE1  | 1:213:A:MET:H   | 10       | 0.1           |
| (1,612) | 1:134:A:MET:HE2  | 1:213:A:MET:H   | 10       | 0.1           |
| (1,612) | 1:134:A:MET:HE3  | 1:213:A:MET:H   | 10       | 0.1           |
| (1,612) | 1:134:A:MET:HE1  | 1:213:A:MET:H   | 14       | 0.1           |
| (1,612) | 1:134:A:MET:HE2  | 1:213:A:MET:H   | 14       | 0.1           |
| (1,612) | 1:134:A:MET:HE3  | 1:213:A:MET:H   | 14       | 0.1           |
| (1,601) | 1:166:A:VAL:HG21 | 1:170:A:SER:HB2 | 2        | 0.1           |
| (1,601) | 1:166:A:VAL:HG22 | 1:170:A:SER:HB2 | 2        | 0.1           |
| (1,601) | 1:166:A:VAL:HG23 | 1:170:A:SER:HB2 | 2        | 0.1           |
| (1,591) | 1:139:A:ILE:HD11 | 1:205:A:MET:HE1 | 16       | 0.1           |
| (1,591) | 1:139:A:ILE:HD11 | 1:205:A:MET:HE2 | 16       | 0.1           |
| (1,591) | 1:139:A:ILE:HD11 | 1:205:A:MET:HE3 | 16       | 0.1           |
| (1,591) | 1:139:A:ILE:HD12 | 1:205:A:MET:HE1 | 16       | 0.1           |
| (1,591) | 1:139:A:ILE:HD12 | 1:205:A:MET:HE2 | 16       | 0.1           |
| (1,591) | 1:139:A:ILE:HD12 | 1:205:A:MET:HE3 | 16       | 0.1           |
| (1,591) | 1:139:A:ILE:HD13 | 1:205:A:MET:HE1 | 16       | 0.1           |
| (1,591) | 1:139:A:ILE:HD13 | 1:205:A:MET:HE2 | 16       | 0.1           |
| (1,591) | 1:139:A:ILE:HD13 | 1:205:A:MET:HE3 | 16       | 0.1           |
| (1,591) | 1:139:A:ILE:HD11 | 1:205:A:MET:HE1 | 18       | 0.1           |
| (1,591) | 1:139:A:ILE:HD11 | 1:205:A:MET:HE2 | 18       | 0.1           |
| (1,591) | 1:139:A:ILE:HD11 | 1:205:A:MET:HE3 | 18       | 0.1           |
| (1,591) | 1:139:A:ILE:HD12 | 1:205:A:MET:HE1 | 18       | 0.1           |
| (1,591) | 1:139:A:ILE:HD12 | 1:205:A:MET:HE2 | 18       | 0.1           |
| (1,591) | 1:139:A:ILE:HD12 | 1:205:A:MET:HE3 | 18       | 0.1           |
| (1,591) | 1:139:A:ILE:HD13 | 1:205:A:MET:HE1 | 18       | 0.1           |
| (1,591) | 1:139:A:ILE:HD13 | 1:205:A:MET:HE2 | 18       | 0.1           |
| (1,591) | 1:139:A:ILE:HD13 | 1:205:A:MET:HE3 | 18       | 0.1           |
| (1,501) | 1:161:A:VAL:HA   | 1:162:A:TYR:HB3 | 5        | 0.1           |
| (1,501) | 1:161:A:VAL:HA   | 1:162:A:TYR:HB3 | 19       | 0.1           |
| (1,468) | 1:124:A:GLY:HA2  | 1:125:A:LEU:HB3 | 18       | 0.1           |
| (1,468) | 1:124:A:GLY:HA3  | 1:125:A:LEU:HB3 | 18       | 0.1           |
| (1,421) | 1:121:A:VAL:HG11 | 1:123:A:GLY:HA2 | 3        | 0.1           |
| (1,421) | 1:121:A:VAL:HG11 | 1:123:A:GLY:HA3 | 3        | 0.1           |
| (1,421) | 1:121:A:VAL:HG12 | 1:123:A:GLY:HA2 | 3        | 0.1           |
| (1,421) | 1:121:A:VAL:HG12 | 1:123:A:GLY:HA3 | 3        | 0.1           |
| (1,421) | 1:121:A:VAL:HG13 | 1:123:A:GLY:HA2 | 3        | 0.1           |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,421) | 1:121:A:VAL:HG13 | 1:123:A:GLY:HA3  | 3        | 0.1           |
| (1,421) | 1:121:A:VAL:HG11 | 1:123:A:GLY:HA2  | 11       | 0.1           |
| (1,421) | 1:121:A:VAL:HG11 | 1:123:A:GLY:HA3  | 11       | 0.1           |
| (1,421) | 1:121:A:VAL:HG12 | 1:123:A:GLY:HA2  | 11       | 0.1           |
| (1,421) | 1:121:A:VAL:HG12 | 1:123:A:GLY:HA3  | 11       | 0.1           |
| (1,421) | 1:121:A:VAL:HG13 | 1:123:A:GLY:HA2  | 11       | 0.1           |
| (1,421) | 1:121:A:VAL:HG13 | 1:123:A:GLY:HA3  | 11       | 0.1           |
| (1,421) | 1:121:A:VAL:HG11 | 1:123:A:GLY:HA2  | 12       | 0.1           |
| (1,421) | 1:121:A:VAL:HG11 | 1:123:A:GLY:HA3  | 12       | 0.1           |
| (1,421) | 1:121:A:VAL:HG12 | 1:123:A:GLY:HA2  | 12       | 0.1           |
| (1,421) | 1:121:A:VAL:HG12 | 1:123:A:GLY:HA3  | 12       | 0.1           |
| (1,421) | 1:121:A:VAL:HG13 | 1:123:A:GLY:HA2  | 12       | 0.1           |
| (1,421) | 1:121:A:VAL:HG13 | 1:123:A:GLY:HA3  | 12       | 0.1           |
| (1,421) | 1:121:A:VAL:HG11 | 1:123:A:GLY:HA2  | 20       | 0.1           |
| (1,421) | 1:121:A:VAL:HG11 | 1:123:A:GLY:HA3  | 20       | 0.1           |
| (1,421) | 1:121:A:VAL:HG12 | 1:123:A:GLY:HA2  | 20       | 0.1           |
| (1,421) | 1:121:A:VAL:HG12 | 1:123:A:GLY:HA3  | 20       | 0.1           |
| (1,421) | 1:121:A:VAL:HG13 | 1:123:A:GLY:HA2  | 20       | 0.1           |
| (1,421) | 1:121:A:VAL:HG13 | 1:123:A:GLY:HA3  | 20       | 0.1           |
| (1,415) | 1:164:A:ARG:HB2  | 1:164:A:ARG:HD3  | 1        | 0.1           |
| (1,394) | 1:216:A:THR:HA   | 1:220:A:LYS:HE2  | 2        | 0.1           |
| (1,394) | 1:216:A:THR:HA   | 1:220:A:LYS:HE3  | 2        | 0.1           |
| (1,394) | 1:216:A:THR:HA   | 1:220:A:LYS:HE2  | 6        | 0.1           |
| (1,394) | 1:216:A:THR:HA   | 1:220:A:LYS:HE3  | 6        | 0.1           |
| (1,394) | 1:216:A:THR:HA   | 1:220:A:LYS:HE2  | 13       | 0.1           |
| (1,394) | 1:216:A:THR:HA   | 1:220:A:LYS:HE3  | 13       | 0.1           |
| (1,393) | 1:120:A:SER:HB2  | 1:121:A:VAL:HG11 | 4        | 0.1           |
| (1,393) | 1:120:A:SER:HB2  | 1:121:A:VAL:HG12 | 4        | 0.1           |
| (1,393) | 1:120:A:SER:HB2  | 1:121:A:VAL:HG13 | 4        | 0.1           |
| (1,393) | 1:120:A:SER:HB3  | 1:121:A:VAL:HG11 | 4        | 0.1           |
| (1,393) | 1:120:A:SER:HB3  | 1:121:A:VAL:HG12 | 4        | 0.1           |
| (1,393) | 1:120:A:SER:HB3  | 1:121:A:VAL:HG13 | 4        | 0.1           |
| (1,393) | 1:120:A:SER:HB2  | 1:121:A:VAL:HG11 | 8        | 0.1           |
| (1,393) | 1:120:A:SER:HB2  | 1:121:A:VAL:HG12 | 8        | 0.1           |
| (1,393) | 1:120:A:SER:HB2  | 1:121:A:VAL:HG13 | 8        | 0.1           |
| (1,393) | 1:120:A:SER:HB3  | 1:121:A:VAL:HG11 | 8        | 0.1           |
| (1,393) | 1:120:A:SER:HB3  | 1:121:A:VAL:HG12 | 8        | 0.1           |
| (1,393) | 1:120:A:SER:HB3  | 1:121:A:VAL:HG13 | 8        | 0.1           |
| (1,377) | 1:209:A:VAL:HG21 | 1:213:A:MET:HG2  | 15       | 0.1           |
| (1,377) | 1:209:A:VAL:HG22 | 1:213:A:MET:HG2  | 15       | 0.1           |
| (1,377) | 1:209:A:VAL:HG23 | 1:213:A:MET:HG2  | 15       | 0.1           |
| (1,350) | 1:122:A:VAL:HG21 | 1:123:A:GLY:H    | 4        | 0.1           |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,350) | 1:122:A:VAL:HG22 | 1:123:A:GLY:H    | 4        | 0.1           |
| (1,350) | 1:122:A:VAL:HG23 | 1:123:A:GLY:H    | 4        | 0.1           |
| (1,350) | 1:122:A:VAL:HG21 | 1:123:A:GLY:H    | 10       | 0.1           |
| (1,350) | 1:122:A:VAL:HG22 | 1:123:A:GLY:H    | 10       | 0.1           |
| (1,350) | 1:122:A:VAL:HG23 | 1:123:A:GLY:H    | 10       | 0.1           |
| (1,344) | 1:189:A:VAL:H    | 1:189:A:VAL:HG11 | 19       | 0.1           |
| (1,344) | 1:189:A:VAL:H    | 1:189:A:VAL:HG12 | 19       | 0.1           |
| (1,344) | 1:189:A:VAL:H    | 1:189:A:VAL:HG13 | 19       | 0.1           |
| (1,344) | 1:189:A:VAL:H    | 1:189:A:VAL:HG11 | 20       | 0.1           |
| (1,344) | 1:189:A:VAL:H    | 1:189:A:VAL:HG12 | 20       | 0.1           |
| (1,344) | 1:189:A:VAL:H    | 1:189:A:VAL:HG13 | 20       | 0.1           |
| (1,333) | 1:172:A:GLN:HE22 | 1:215:A:VAL:HG21 | 6        | 0.1           |
| (1,333) | 1:172:A:GLN:HE22 | 1:215:A:VAL:HG22 | 6        | 0.1           |
| (1,333) | 1:172:A:GLN:HE22 | 1:215:A:VAL:HG23 | 6        | 0.1           |
| (1,332) | 1:185:A:LYS:HD2  | 1:189:A:VAL:HG11 | 2        | 0.1           |
| (1,332) | 1:185:A:LYS:HD2  | 1:189:A:VAL:HG12 | 2        | 0.1           |
| (1,332) | 1:185:A:LYS:HD2  | 1:189:A:VAL:HG13 | 2        | 0.1           |
| (1,332) | 1:185:A:LYS:HD3  | 1:189:A:VAL:HG11 | 2        | 0.1           |
| (1,332) | 1:185:A:LYS:HD3  | 1:189:A:VAL:HG12 | 2        | 0.1           |
| (1,332) | 1:185:A:LYS:HD3  | 1:189:A:VAL:HG13 | 2        | 0.1           |
| (1,332) | 1:185:A:LYS:HD2  | 1:189:A:VAL:HG11 | 5        | 0.1           |
| (1,332) | 1:185:A:LYS:HD2  | 1:189:A:VAL:HG12 | 5        | 0.1           |
| (1,332) | 1:185:A:LYS:HD2  | 1:189:A:VAL:HG13 | 5        | 0.1           |
| (1,332) | 1:185:A:LYS:HD3  | 1:189:A:VAL:HG11 | 5        | 0.1           |
| (1,332) | 1:185:A:LYS:HD3  | 1:189:A:VAL:HG12 | 5        | 0.1           |
| (1,332) | 1:185:A:LYS:HD3  | 1:189:A:VAL:HG13 | 5        | 0.1           |
| (1,309) | 1:186:A:GLN:HE21 | 1:189:A:VAL:HG11 | 6        | 0.1           |
| (1,309) | 1:186:A:GLN:HE21 | 1:189:A:VAL:HG12 | 6        | 0.1           |
| (1,309) | 1:186:A:GLN:HE21 | 1:189:A:VAL:HG13 | 6        | 0.1           |
| (1,309) | 1:186:A:GLN:HE21 | 1:189:A:VAL:HG11 | 8        | 0.1           |
| (1,309) | 1:186:A:GLN:HE21 | 1:189:A:VAL:HG12 | 8        | 0.1           |
| (1,309) | 1:186:A:GLN:HE21 | 1:189:A:VAL:HG13 | 8        | 0.1           |
| (1,309) | 1:186:A:GLN:HE21 | 1:189:A:VAL:HG11 | 9        | 0.1           |
| (1,309) | 1:186:A:GLN:HE21 | 1:189:A:VAL:HG12 | 9        | 0.1           |
| (1,309) | 1:186:A:GLN:HE21 | 1:189:A:VAL:HG13 | 9        | 0.1           |
| (1,309) | 1:186:A:GLN:HE21 | 1:189:A:VAL:HG11 | 19       | 0.1           |
| (1,309) | 1:186:A:GLN:HE21 | 1:189:A:VAL:HG12 | 19       | 0.1           |
| (1,309) | 1:186:A:GLN:HE21 | 1:189:A:VAL:HG13 | 19       | 0.1           |
| (1,307) | 1:176:A:VAL:HG11 | 1:215:A:VAL:HG21 | 7        | 0.1           |
| (1,307) | 1:176:A:VAL:HG11 | 1:215:A:VAL:HG22 | 7        | 0.1           |
| (1,307) | 1:176:A:VAL:HG11 | 1:215:A:VAL:HG23 | 7        | 0.1           |
| (1,307) | 1:176:A:VAL:HG12 | 1:215:A:VAL:HG21 | 7        | 0.1           |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,307) | 1:176:A:VAL:HG12 | 1:215:A:VAL:HG22 | 7        | 0.1           |
| (1,307) | 1:176:A:VAL:HG12 | 1:215:A:VAL:HG23 | 7        | 0.1           |
| (1,307) | 1:176:A:VAL:HG13 | 1:215:A:VAL:HG21 | 7        | 0.1           |
| (1,307) | 1:176:A:VAL:HG13 | 1:215:A:VAL:HG22 | 7        | 0.1           |
| (1,307) | 1:176:A:VAL:HG13 | 1:215:A:VAL:HG23 | 7        | 0.1           |
| (1,298) | 1:184:A:ILE:HB   | 1:188:A:THR:HG21 | 9        | 0.1           |
| (1,298) | 1:184:A:ILE:HB   | 1:188:A:THR:HG22 | 9        | 0.1           |
| (1,298) | 1:184:A:ILE:HB   | 1:188:A:THR:HG23 | 9        | 0.1           |
| (1,298) | 1:184:A:ILE:HB   | 1:188:A:THR:HG21 | 20       | 0.1           |
| (1,298) | 1:184:A:ILE:HB   | 1:188:A:THR:HG22 | 20       | 0.1           |
| (1,298) | 1:184:A:ILE:HB   | 1:188:A:THR:HG23 | 20       | 0.1           |
| (1,296) | 1:187:A:HIS:HB3  | 1:190:A:THR:HG21 | 1        | 0.1           |
| (1,296) | 1:187:A:HIS:HB3  | 1:190:A:THR:HG22 | 1        | 0.1           |
| (1,296) | 1:187:A:HIS:HB3  | 1:190:A:THR:HG23 | 1        | 0.1           |
| (1,296) | 1:187:A:HIS:HB3  | 1:190:A:THR:HG21 | 19       | 0.1           |
| (1,296) | 1:187:A:HIS:HB3  | 1:190:A:THR:HG22 | 19       | 0.1           |
| (1,296) | 1:187:A:HIS:HB3  | 1:190:A:THR:HG23 | 19       | 0.1           |
| (1,288) | 1:192:A:THR:HG21 | 1:196:A:GLU:HB2  | 17       | 0.1           |
| (1,288) | 1:192:A:THR:HG21 | 1:196:A:GLU:HB3  | 17       | 0.1           |
| (1,288) | 1:192:A:THR:HG22 | 1:196:A:GLU:HB2  | 17       | 0.1           |
| (1,288) | 1:192:A:THR:HG22 | 1:196:A:GLU:HB3  | 17       | 0.1           |
| (1,288) | 1:192:A:THR:HG23 | 1:196:A:GLU:HB2  | 17       | 0.1           |
| (1,288) | 1:192:A:THR:HG23 | 1:196:A:GLU:HB3  | 17       | 0.1           |
| (1,220) | 1:127:A:GLY:HA2  | 1:164:A:ARG:HE   | 12       | 0.1           |
| (1,216) | 1:216:A:THR:HG21 | 1:220:A:LYS:HG3  | 2        | 0.1           |
| (1,216) | 1:216:A:THR:HG22 | 1:220:A:LYS:HG3  | 2        | 0.1           |
| (1,216) | 1:216:A:THR:HG23 | 1:220:A:LYS:HG3  | 2        | 0.1           |
| (1,189) | 1:123:A:GLY:HA2  | 1:125:A:LEU:HD21 | 7        | 0.1           |
| (1,189) | 1:123:A:GLY:HA2  | 1:125:A:LEU:HD22 | 7        | 0.1           |
| (1,189) | 1:123:A:GLY:HA2  | 1:125:A:LEU:HD23 | 7        | 0.1           |
| (1,189) | 1:123:A:GLY:HA3  | 1:125:A:LEU:HD21 | 7        | 0.1           |
| (1,189) | 1:123:A:GLY:HA3  | 1:125:A:LEU:HD22 | 7        | 0.1           |
| (1,189) | 1:123:A:GLY:HA3  | 1:125:A:LEU:HD23 | 7        | 0.1           |
| (1,159) | 1:228:A:GLY:HA2  | 1:230:A:ARG:HD2  | 2        | 0.1           |
| (1,159) | 1:228:A:GLY:HA3  | 1:230:A:ARG:HD2  | 2        | 0.1           |
| (1,159) | 1:228:A:GLY:HA2  | 1:230:A:ARG:HD2  | 7        | 0.1           |
| (1,159) | 1:228:A:GLY:HA3  | 1:230:A:ARG:HD2  | 7        | 0.1           |
| (1,157) | 1:228:A:GLY:HA2  | 1:232:A:SER:HA   | 15       | 0.1           |
| (1,157) | 1:228:A:GLY:HA3  | 1:232:A:SER:HA   | 15       | 0.1           |
| (1,107) | 1:211:A:GLU:HG3  | 1:215:A:VAL:HG11 | 16       | 0.1           |
| (1,107) | 1:211:A:GLU:HG3  | 1:215:A:VAL:HG12 | 16       | 0.1           |
| (1,107) | 1:211:A:GLU:HG3  | 1:215:A:VAL:HG13 | 16       | 0.1           |

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| Key    | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|--------|------------------|-----------------|----------|---------------|
| (1,81) | 1:210:A:VAL:HG21 | 1:214:A:CYS:H   | 15       | 0.1           |
| (1,81) | 1:210:A:VAL:HG22 | 1:214:A:CYS:H   | 15       | 0.1           |
| (1,81) | 1:210:A:VAL:HG23 | 1:214:A:CYS:H   | 15       | 0.1           |
| (1,52) | 1:176:A:VAL:HG21 | 1:217:A:GLN:HB3 | 3        | 0.1           |
| (1,52) | 1:176:A:VAL:HG22 | 1:217:A:GLN:HB3 | 3        | 0.1           |
| (1,52) | 1:176:A:VAL:HG23 | 1:217:A:GLN:HB3 | 3        | 0.1           |
| (1,39) | 1:201:A:THR:HG21 | 1:204:A:LYS:HG3 | 10       | 0.1           |
| (1,39) | 1:201:A:THR:HG22 | 1:204:A:LYS:HG3 | 10       | 0.1           |
| (1,39) | 1:201:A:THR:HG23 | 1:204:A:LYS:HG3 | 10       | 0.1           |
| (1,39) | 1:201:A:THR:HG21 | 1:204:A:LYS:HG3 | 12       | 0.1           |
| (1,39) | 1:201:A:THR:HG22 | 1:204:A:LYS:HG3 | 12       | 0.1           |
| (1,39) | 1:201:A:THR:HG23 | 1:204:A:LYS:HG3 | 12       | 0.1           |
| (1,31) | 1:219:A:GLN:HA   | 1:220:A:LYS:HG3 | 11       | 0.1           |
| (1,15) | 1:130:A:LEU:HD21 | 1:161:A:VAL:HA  | 7        | 0.1           |
| (1,15) | 1:130:A:LEU:HD22 | 1:161:A:VAL:HA  | 7        | 0.1           |
| (1,15) | 1:130:A:LEU:HD23 | 1:161:A:VAL:HA  | 7        | 0.1           |

## 10 Dihedral-angle violation analysis

No dihedral-angle restraints found