



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2026 – 10:11 PM UTC

PDB ID : 9G2O / pdb\_00009g2o  
BMRB ID : 34934  
Title : Trp-cage fortified Tc5b-Exenatide chimera (Ex-4-Tc5bDR) at 299K  
Authors : Horvath, D.  
Deposited on : 2024-07-11

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

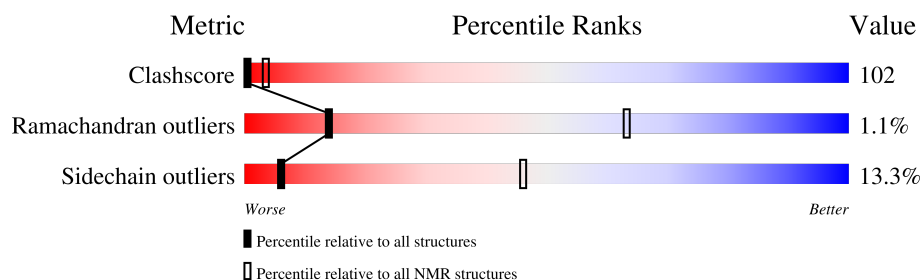
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 53%.

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     | 25     | <div> <div></div> <div>12%</div> <div>44%</div> <div>16%</div> <div>28%</div> </div> |

## 2 Ensemble composition and analysis

This entry contains 10 models. Model 5 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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

| Well-defined (core) protein residues |                          |                   |              |
|--------------------------------------|--------------------------|-------------------|--------------|
| Well-defined core                    | Residue range (total)    | Backbone RMSD (Å) | Medoid model |
| 1                                    | A:2-A:17, A:23-A:24 (18) | 0.17              | 5            |

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

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

The models can be grouped into 2 clusters and 1 single-model cluster was found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 385 atoms, of which 189 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Exendin-4.

| Mol | Chain | Residues | Atoms |     |     |    |    | Trace |
|-----|-------|----------|-------|-----|-----|----|----|-------|
| 1   | A     | 25       | Total | C   | H   | N  | O  | 0     |
|     |       |          | 385   | 123 | 189 | 34 | 39 |       |

There are 4 discrepancies between the modelled and reference sequences:

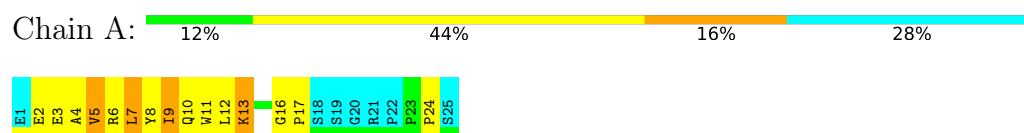
| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| A     | 8       | TYR      | PHE    | engineered mutation | UNP P26349 |
| A     | 10      | GLN      | GLU    | engineered mutation | UNP P26349 |
| A     | 14      | ASP      | ASN    | engineered mutation | UNP P26349 |
| A     | 21      | ARG      | ALA    | engineered mutation | UNP P26349 |

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

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

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

- Molecule 1: Exendin-4

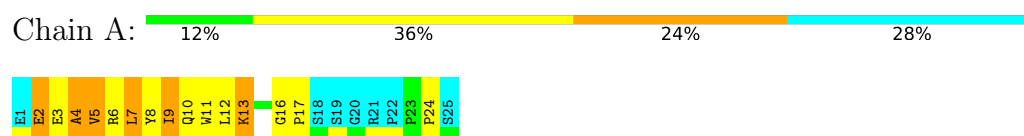


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

- Molecule 1: Exendin-4



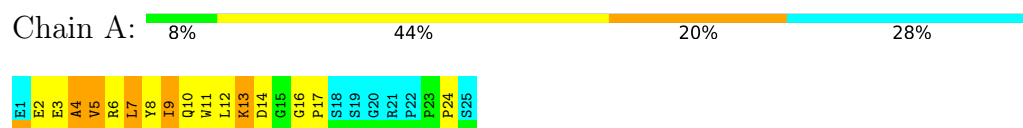
#### 4.2.2 Score per residue for model 2

- Molecule 1: Exendin-4



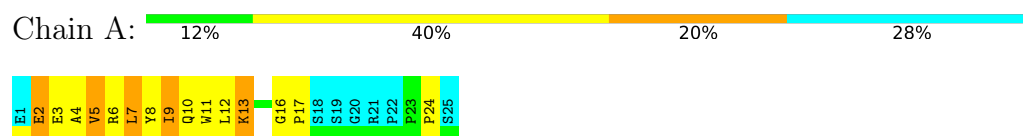
### 4.2.3 Score per residue for model 3

- Molecule 1: Exendin-4



### 4.2.4 Score per residue for model 4

- Molecule 1: Exendin-4



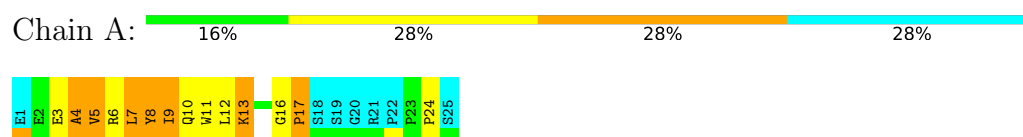
### 4.2.5 Score per residue for model 5 (medoid)

- Molecule 1: Exendin-4



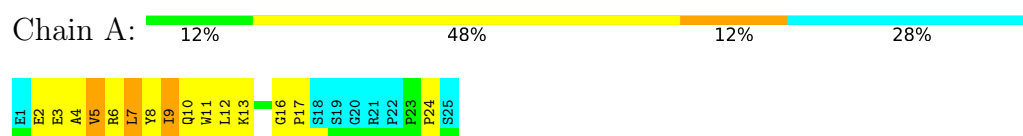
### 4.2.6 Score per residue for model 6

- Molecule 1: Exendin-4



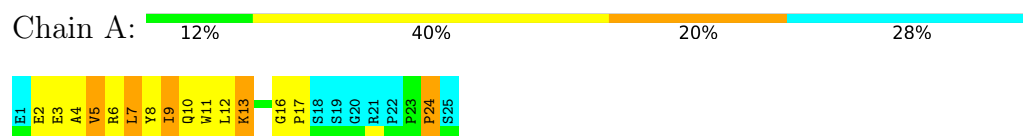
### 4.2.7 Score per residue for model 7

- Molecule 1: Exendin-4



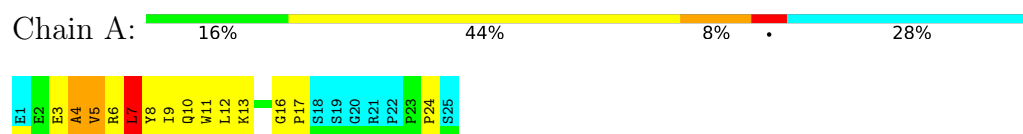
#### 4.2.8 Score per residue for model 8

- Molecule 1: Exendin-4



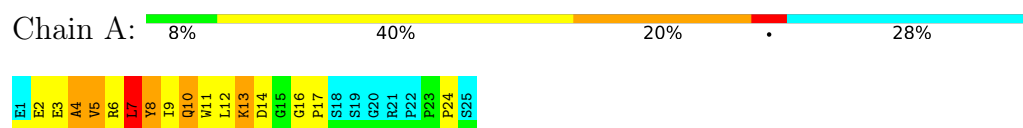
#### 4.2.9 Score per residue for model 9

- Molecule 1: Exendin-4



#### 4.2.10 Score per residue for model 10

- Molecule 1: Exendin-4



## 5 Refinement protocol and experimental data overview

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

Of the 20 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy*.

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

| Software name          | Classification        | Version |
|------------------------|-----------------------|---------|
| CcpNmr Analysis Assign | refinement            | 2.4.1.  |
| ARIA2alpha             | structure calculation | 2.3.1.  |

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                       | 168            |
| Number of shifts mapped to atoms             | 168            |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 53%            |

## 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     | 1.66±0.03    | 3±0/152 ( 2.0± 0.0%) | 1.65±0.04   | 1±0/208 ( 0.7± 0.2%) |
| All | All   | 1.66         | 30/1520 ( 2.0%)      | 1.65        | 14/2080 ( 0.7%)      |

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

| Mol | Chain | Chirality | Planarity |
|-----|-------|-----------|-----------|
| 1   | A     | 0.0±0.0   | 0.1±0.3   |
| All | All   | 0         | 1         |

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

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) | Models |       |
|-----|-------|-----|------|-------|-------|-------------|----------|--------|-------|
|     |       |     |      |       |       |             |          | Worst  | Total |
| 1   | A     | 5   | VAL  | N-CA  | -6.22 | 1.38        | 1.46     | 5      | 10    |
| 1   | A     | 9   | ILE  | N-CA  | -5.79 | 1.39        | 1.46     | 7      | 8     |
| 1   | A     | 5   | VAL  | CA-CB | -5.57 | 1.47        | 1.54     | 10     | 2     |
| 1   | A     | 7   | LEU  | C-N   | -5.49 | 1.27        | 1.33     | 2      | 10    |

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     | 4   | ALA  | N-CA-C  | -7.90 | 103.77      | 113.41   | 2      | 9     |
| 1   | A     | 7   | LEU  | CB-CA-C | -5.20 | 102.68      | 110.90   | 8      | 5     |

There are no chirality outliers.

All unique planar outliers are listed below.

| Mol | Chain | Res | Type | Group     | Models (Total) |
|-----|-------|-----|------|-----------|----------------|
| 1   | A     | 8   | 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     | 146   | 143      | 143      | 30±3    |
| All | All   | 1460  | 1430     | 1430     | 296     |

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 102.

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

| Atom-1          | Atom-2         | Clash(Å) | Distance(Å) | Models |       |
|-----------------|----------------|----------|-------------|--------|-------|
|                 |                |          |             | Worst  | Total |
| 1:A:8:TYR:CD1   | 1:A:24:PRO:HG2 | 0.86     | 2.05        | 10     | 9     |
| 1:A:5:VAL:HA    | 1:A:8:TYR:HB2  | 0.73     | 1.61        | 1      | 10    |
| 1:A:5:VAL:HA    | 1:A:8:TYR:CB   | 0.70     | 2.16        | 4      | 10    |
| 1:A:12:LEU:HD23 | 1:A:16:GLY:CA  | 0.70     | 2.17        | 6      | 1     |
| 1:A:12:LEU:HA   | 1:A:16:GLY:N   | 0.69     | 2.02        | 3      | 10    |
| 1:A:12:LEU:HD23 | 1:A:16:GLY:HA3 | 0.68     | 1.64        | 9      | 9     |
| 1:A:8:TYR:CG    | 1:A:24:PRO:HG2 | 0.67     | 2.24        | 10     | 9     |
| 1:A:9:ILE:O     | 1:A:13:LYS:HD2 | 0.67     | 1.89        | 7      | 10    |
| 1:A:8:TYR:O     | 1:A:11:TRP:HB3 | 0.65     | 1.90        | 1      | 10    |
| 1:A:12:LEU:HD23 | 1:A:16:GLY:HA2 | 0.65     | 1.66        | 6      | 1     |
| 1:A:6:ARG:HA    | 1:A:9:ILE:HD12 | 0.64     | 1.69        | 9      | 10    |
| 1:A:11:TRP:CH2  | 1:A:17:PRO:HD3 | 0.64     | 2.28        | 2      | 10    |
| 1:A:7:LEU:H     | 1:A:7:LEU:CD2  | 0.60     | 2.07        | 10     | 1     |
| 1:A:11:TRP:CD2  | 1:A:16:GLY:HA2 | 0.59     | 2.32        | 4      | 9     |
| 1:A:7:LEU:HD23  | 1:A:7:LEU:N    | 0.59     | 2.13        | 9      | 2     |
| 1:A:12:LEU:CD2  | 1:A:16:GLY:HA3 | 0.57     | 2.30        | 10     | 9     |
| 1:A:6:ARG:O     | 1:A:10:GLN:HB3 | 0.56     | 1.99        | 10     | 1     |
| 1:A:7:LEU:O     | 1:A:10:GLN:HB3 | 0.56     | 1.99        | 7      | 8     |
| 1:A:11:TRP:CE3  | 1:A:12:LEU:HG  | 0.55     | 2.35        | 6      | 10    |
| 1:A:8:TYR:CA    | 1:A:24:PRO:HG2 | 0.55     | 2.30        | 8      | 1     |
| 1:A:12:LEU:CD2  | 1:A:16:GLY:HA2 | 0.55     | 2.31        | 6      | 1     |
| 1:A:8:TYR:HA    | 1:A:24:PRO:HG2 | 0.55     | 1.79        | 8      | 1     |
| 1:A:7:LEU:CD2   | 1:A:7:LEU:H    | 0.54     | 2.10        | 9      | 1     |

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| Atom-1         | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|----------------|-----------------|----------|-------------|--------|-------|
|                |                 |          |             | Worst  | Total |
| 1:A:7:LEU:H    | 1:A:7:LEU:HD23  | 0.54     | 1.61        | 10     | 1     |
| 1:A:5:VAL:HG22 | 1:A:9:ILE:CD1   | 0.54     | 2.33        | 1      | 10    |
| 1:A:9:ILE:HG22 | 1:A:13:LYS:CE   | 0.54     | 2.33        | 1      | 10    |
| 1:A:8:TYR:HA   | 1:A:24:PRO:HG3  | 0.53     | 1.80        | 6      | 8     |
| 1:A:9:ILE:HG22 | 1:A:13:LYS:HE3  | 0.53     | 1.81        | 2      | 7     |
| 1:A:3:GLU:O    | 1:A:3:GLU:HG2   | 0.53     | 2.03        | 10     | 9     |
| 1:A:3:GLU:O    | 1:A:7:LEU:HD21  | 0.53     | 2.04        | 10     | 2     |
| 1:A:7:LEU:HD23 | 1:A:7:LEU:H     | 0.51     | 1.65        | 9      | 1     |
| 1:A:7:LEU:HD12 | 1:A:24:PRO:CB   | 0.50     | 2.37        | 10     | 1     |
| 1:A:8:TYR:HA   | 1:A:24:PRO:CG   | 0.48     | 2.38        | 7      | 9     |
| 1:A:9:ILE:HG22 | 1:A:13:LYS:HE2  | 0.48     | 1.85        | 7      | 2     |
| 1:A:10:GLN:HA  | 1:A:13:LYS:CD   | 0.48     | 2.39        | 1      | 6     |
| 1:A:7:LEU:O    | 1:A:11:TRP:N    | 0.47     | 2.47        | 10     | 10    |
| 1:A:8:TYR:O    | 1:A:12:LEU:HD12 | 0.47     | 2.08        | 6      | 10    |
| 1:A:8:TYR:CE2  | 1:A:11:TRP:CZ3  | 0.47     | 3.01        | 10     | 6     |
| 1:A:4:ALA:HA   | 1:A:7:LEU:HD11  | 0.47     | 1.87        | 10     | 2     |
| 1:A:5:VAL:CA   | 1:A:8:TYR:HB2   | 0.47     | 2.38        | 10     | 4     |
| 1:A:4:ALA:HA   | 1:A:7:LEU:HD12  | 0.47     | 1.86        | 4      | 2     |
| 1:A:2:GLU:HG3  | 1:A:5:VAL:HG11  | 0.46     | 1.87        | 7      | 3     |
| 1:A:6:ARG:O    | 1:A:10:GLN:CB   | 0.46     | 2.63        | 10     | 2     |
| 1:A:6:ARG:O    | 1:A:10:GLN:HB2  | 0.46     | 2.10        | 2      | 5     |
| 1:A:3:GLU:O    | 1:A:7:LEU:HG    | 0.46     | 2.10        | 4      | 1     |
| 1:A:2:GLU:HG3  | 1:A:5:VAL:CG1   | 0.44     | 2.42        | 4      | 1     |
| 1:A:11:TRP:CZ3 | 1:A:17:PRO:HD3  | 0.44     | 2.47        | 1      | 4     |
| 1:A:5:VAL:O    | 1:A:8:TYR:HB3   | 0.44     | 2.12        | 4      | 5     |
| 1:A:9:ILE:O    | 1:A:13:LYS:N    | 0.44     | 2.50        | 9      | 5     |
| 1:A:5:VAL:O    | 1:A:9:ILE:N     | 0.44     | 2.48        | 10     | 4     |
| 1:A:3:GLU:HA   | 1:A:6:ARG:HB2   | 0.44     | 1.89        | 7      | 8     |
| 1:A:2:GLU:HG2  | 1:A:5:VAL:HG11  | 0.43     | 1.90        | 1      | 1     |
| 1:A:7:LEU:CA   | 1:A:10:GLN:HB3  | 0.43     | 2.44        | 9      | 1     |
| 1:A:10:GLN:HA  | 1:A:13:LYS:HD2  | 0.43     | 1.90        | 1      | 2     |
| 1:A:7:LEU:C    | 1:A:10:GLN:HB3  | 0.42     | 2.40        | 9      | 1     |
| 1:A:5:VAL:HG22 | 1:A:9:ILE:HD11  | 0.42     | 1.91        | 1      | 1     |
| 1:A:8:TYR:CA   | 1:A:24:PRO:HG3  | 0.42     | 2.45        | 7      | 3     |
| 1:A:4:ALA:CA   | 1:A:7:LEU:HD12  | 0.41     | 2.45        | 4      | 1     |
| 1:A:11:TRP:CZ2 | 1:A:17:PRO:HA   | 0.41     | 2.50        | 6      | 1     |
| 1:A:5:VAL:O    | 1:A:8:TYR:CB    | 0.41     | 2.68        | 10     | 1     |
| 1:A:4:ALA:C    | 1:A:7:LEU:HD12  | 0.40     | 2.40        | 6      | 1     |
| 1:A:4:ALA:O    | 1:A:7:LEU:HD12  | 0.40     | 2.17        | 3      | 1     |
| 1:A:2:GLU:C    | 1:A:4:ALA:N     | 0.40     | 2.78        | 10     | 1     |

## 6.3 Torsion angles [i](#)

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

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

| Mol | Chain | Analysed      | Favoured     | Allowed     | Outliers   | Percentiles |    |
|-----|-------|---------------|--------------|-------------|------------|-------------|----|
| 1   | A     | 18/25 (72%)   | 15±1 (83±8%) | 3±1 (16±7%) | 0±0 (1±2%) | 14          | 63 |
| All | All   | 180/250 (72%) | 150 (83%)    | 28 (16%)    | 2 (1%)     | 14          | 63 |

All 2 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     | 17  | PRO  | 1              |
| 1   | A     | 24  | PRO  | 1              |

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

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

| Mol | Chain | Analysed      | Rotameric    | Outliers    | Percentiles |    |
|-----|-------|---------------|--------------|-------------|-------------|----|
| 1   | A     | 15/21 (71%)   | 13±1 (87±9%) | 2±1 (13±9%) | 6           | 46 |
| All | All   | 150/210 (71%) | 130 (87%)    | 20 (13%)    | 6           | 46 |

All 6 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     | 13  | LYS  | 8              |
| 1   | A     | 2   | GLU  | 4              |
| 1   | A     | 14  | ASP  | 4              |
| 1   | A     | 7   | LEU  | 2              |
| 1   | A     | 8   | TYR  | 1              |
| 1   | A     | 10  | GLN  | 1              |

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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

There are no ligands in this entry.

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

There are no such molecules in this entry.

### 6.8 Polymer linkage issues [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 53% for the well-defined parts and 51% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

Chemical shift list name: *nef\_chemical\_shift\_list\_ShiftList\_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                  | 168 |
| Number of shifts mapped to atoms        | 168 |
| Number of unparsed shifts               | 0   |
| Number of shifts with mapping errors    | 0   |
| Number of shifts with mapping warnings  | 0   |
| Number of shift outliers (ShiftChecker) | 2   |

#### 7.1.2 Chemical shift referencing

No chemical shift referencing corrections were calculated (not enough data).

#### 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 53%, i.e. 133 atoms were assigned a chemical shift out of a possible 252. 0 out of 3 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total         | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|-----------|---------------|----------------|-----------------|-----------------|
| Backbone  | 34/86 (40%)   | 34/35 (97%)    | 0/36 (0%)       | 0/15 (0%)       |
| Sidechain | 89/145 (61%)  | 89/94 (95%)    | 0/46 (0%)       | 0/5 (0%)        |
| Aromatic  | 10/21 (48%)   | 10/10 (100%)   | 0/10 (0%)       | 0/1 (0%)        |
| Overall   | 133/252 (53%) | 133/139 (96%)  | 0/92 (0%)       | 0/21 (0%)       |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 51%, i.e. 168 atoms were assigned a chemical shift out of a possible 329. 0 out of 3 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total         | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|-----------|---------------|----------------|-----------------|-----------------|
| Backbone  | 47/120 (39%)  | 47/49 (96%)    | 0/50 (0%)       | 0/21 (0%)       |
| Sidechain | 111/188 (59%) | 111/121 (92%)  | 0/59 (0%)       | 0/8 (0%)        |
| Aromatic  | 10/21 (48%)   | 10/10 (100%)   | 0/10 (0%)       | 0/1 (0%)        |
| Overall   | 168/329 (51%) | 168/180 (93%)  | 0/119 (0%)      | 0/30 (0%)       |

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

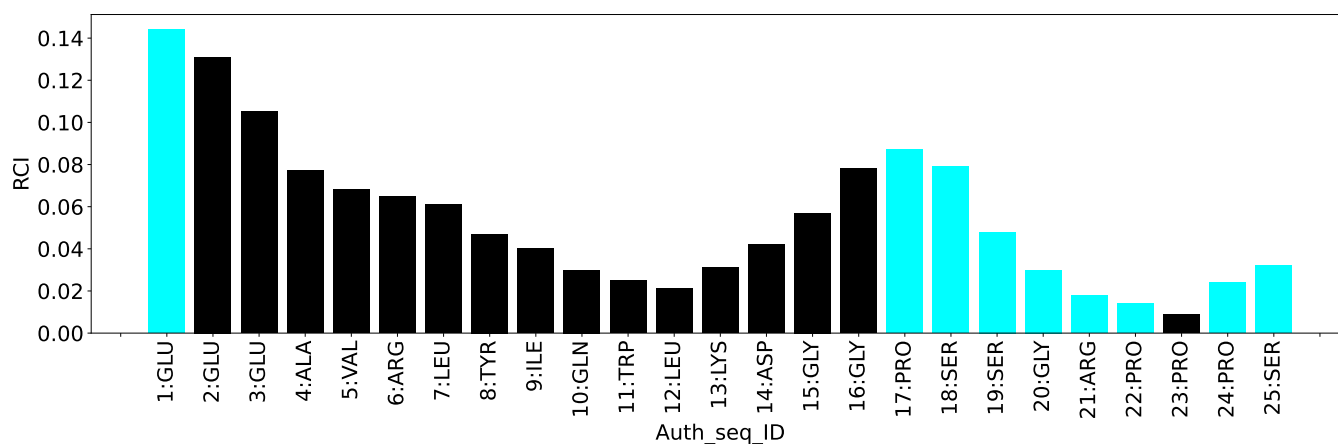
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

| List Id | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|---------|-------|-----|------|------|------------|---------------------|---------|
| 1       | A     | 16  | GLY  | HA2  | 0.89       | 2.15 – 5.77         | -8.5    |
| 1       | A     | 23  | PRO  | HA   | 2.61       | 2.78 – 6.00         | -5.5    |

### 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                                | 1202  |
| Intra-residue ( $ i-j =0$ )                              | 592   |
| Sequential ( $ i-j =1$ )                                 | 242   |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 230   |
| Long range ( $ i-j \geq 5$ )                             | 138   |
| 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                         | 48.1  |
| Number of long range restraints per residue <sup>1</sup> | 5.5   |

<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)  | 59.0                                   | 0.2     |
| 0.2-0.5 (Medium) | 83.0                                   | 0.5     |
| >0.5 (Large)     | 113.8                                  | 3.25    |

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

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

## 9 Distance violation analysis ⓘ

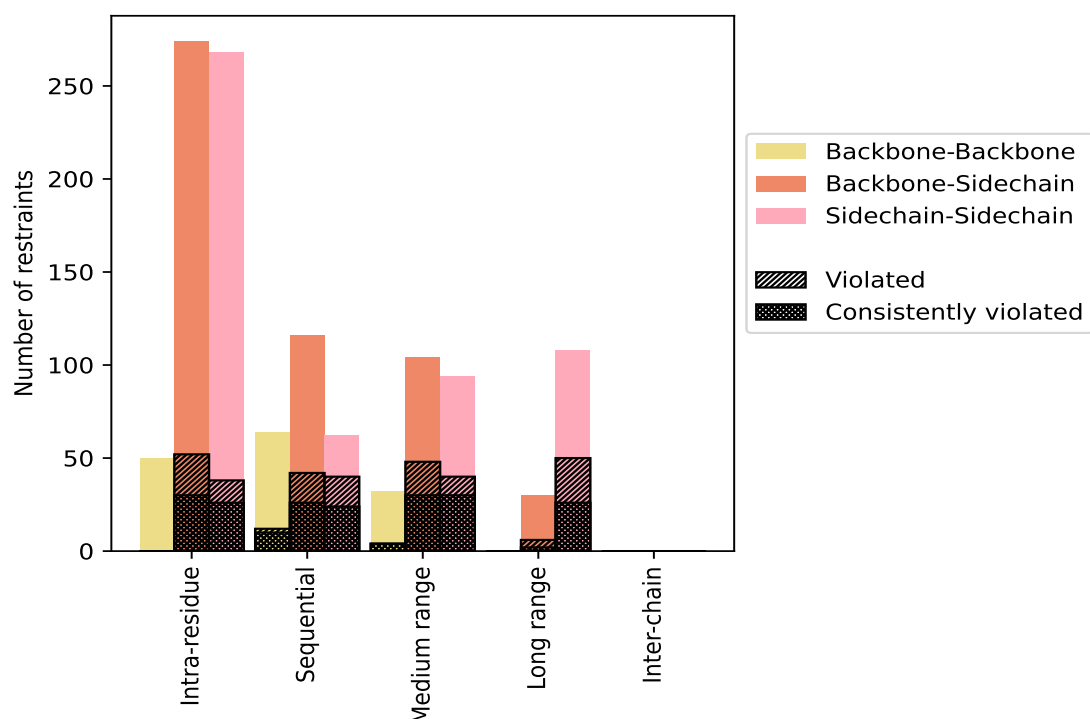
### 9.1 Summary of distance violations ⓘ

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

| Restraints type                                            | Count                | % <sup>1</sup>        | Violated <sup>3</sup> |                      |                      | Consistently Violated <sup>4</sup> |                      |                      |
|------------------------------------------------------------|----------------------|-----------------------|-----------------------|----------------------|----------------------|------------------------------------|----------------------|----------------------|
|                                                            |                      |                       | Count                 | % <sup>2</sup>       | % <sup>1</sup>       | Count                              | % <sup>2</sup>       | % <sup>1</sup>       |
| <a href="#">Intra-residue ( i-j =0)</a>                    | <a href="#">592</a>  | <a href="#">49.3</a>  | <a href="#">90</a>    | <a href="#">15.2</a> | <a href="#">7.5</a>  | <a href="#">56</a>                 | <a href="#">9.5</a>  | <a href="#">4.7</a>  |
| Backbone-Backbone                                          | 50                   | 4.2                   | 0                     | 0.0                  | 0.0                  | 0                                  | 0.0                  | 0.0                  |
| Backbone-Sidechain                                         | 274                  | 22.8                  | 52                    | 19.0                 | 4.3                  | 30                                 | 10.9                 | 2.5                  |
| Sidechain-Sidechain                                        | 268                  | 22.3                  | 38                    | 14.2                 | 3.2                  | 26                                 | 9.7                  | 2.2                  |
| <a href="#">Sequential ( i-j =1)</a>                       | <a href="#">242</a>  | <a href="#">20.1</a>  | <a href="#">94</a>    | <a href="#">38.8</a> | <a href="#">7.8</a>  | <a href="#">60</a>                 | <a href="#">24.8</a> | <a href="#">5.0</a>  |
| Backbone-Backbone                                          | 64                   | 5.3                   | 12                    | 18.8                 | 1.0                  | 10                                 | 15.6                 | 0.8                  |
| Backbone-Sidechain                                         | 116                  | 9.7                   | 42                    | 36.2                 | 3.5                  | 26                                 | 22.4                 | 2.2                  |
| Sidechain-Sidechain                                        | 62                   | 5.2                   | 40                    | 64.5                 | 3.3                  | 24                                 | 38.7                 | 2.0                  |
| <a href="#">Medium range ( i-j &gt;1 &amp;  i-j &lt;5)</a> | <a href="#">230</a>  | <a href="#">19.1</a>  | <a href="#">92</a>    | <a href="#">40.0</a> | <a href="#">7.7</a>  | <a href="#">64</a>                 | <a href="#">27.8</a> | <a href="#">5.3</a>  |
| Backbone-Backbone                                          | 32                   | 2.7                   | 4                     | 12.5                 | 0.3                  | 4                                  | 12.5                 | 0.3                  |
| Backbone-Sidechain                                         | 104                  | 8.7                   | 48                    | 46.2                 | 4.0                  | 30                                 | 28.8                 | 2.5                  |
| Sidechain-Sidechain                                        | 94                   | 7.8                   | 40                    | 42.6                 | 3.3                  | 30                                 | 31.9                 | 2.5                  |
| <a href="#">Long range ( i-j ≥5)</a>                       | <a href="#">138</a>  | <a href="#">11.5</a>  | <a href="#">56</a>    | <a href="#">40.6</a> | <a href="#">4.7</a>  | <a href="#">28</a>                 | <a href="#">20.3</a> | <a href="#">2.3</a>  |
| Backbone-Backbone                                          | 0                    | 0.0                   | 0                     | 0.0                  | 0.0                  | 0                                  | 0.0                  | 0.0                  |
| Backbone-Sidechain                                         | 30                   | 2.5                   | 6                     | 20.0                 | 0.5                  | 2                                  | 6.7                  | 0.2                  |
| Sidechain-Sidechain                                        | 108                  | 9.0                   | 50                    | 46.3                 | 4.2                  | 26                                 | 24.1                 | 2.2                  |
| <a href="#">Inter-chain</a>                                | <a href="#">0</a>    | <a href="#">0.0</a>   | <a href="#">0</a>     | <a href="#">0.0</a>  | <a href="#">0.0</a>  | <a href="#">0</a>                  | <a href="#">0.0</a>  | <a href="#">0.0</a>  |
| Backbone-Backbone                                          | 0                    | 0.0                   | 0                     | 0.0                  | 0.0                  | 0                                  | 0.0                  | 0.0                  |
| Backbone-Sidechain                                         | 0                    | 0.0                   | 0                     | 0.0                  | 0.0                  | 0                                  | 0.0                  | 0.0                  |
| Sidechain-Sidechain                                        | 0                    | 0.0                   | 0                     | 0.0                  | 0.0                  | 0                                  | 0.0                  | 0.0                  |
| <a href="#">Hydrogen bond</a>                              | <a href="#">0</a>    | <a href="#">0.0</a>   | <a href="#">0</a>     | <a href="#">0.0</a>  | <a href="#">0.0</a>  | <a href="#">0</a>                  | <a href="#">0.0</a>  | <a href="#">0.0</a>  |
| <a href="#">Disulfide bond</a>                             | <a href="#">0</a>    | <a href="#">0.0</a>   | <a href="#">0</a>     | <a href="#">0.0</a>  | <a href="#">0.0</a>  | <a href="#">0</a>                  | <a href="#">0.0</a>  | <a href="#">0.0</a>  |
| <a href="#">Total</a>                                      | <a href="#">1202</a> | <a href="#">100.0</a> | <a href="#">332</a>   | <a href="#">27.6</a> | <a href="#">27.6</a> | <a href="#">208</a>                | <a href="#">17.3</a> | <a href="#">17.3</a> |
| Backbone-Backbone                                          | 146                  | 12.1                  | 16                    | 11.0                 | 1.3                  | 14                                 | 9.6                  | 1.2                  |
| Backbone-Sidechain                                         | 524                  | 43.6                  | 148                   | 28.2                 | 12.3                 | 88                                 | 16.8                 | 7.3                  |
| Sidechain-Sidechain                                        | 532                  | 44.3                  | 168                   | 31.6                 | 14.0                 | 106                                | 19.9                 | 8.8                  |

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

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



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

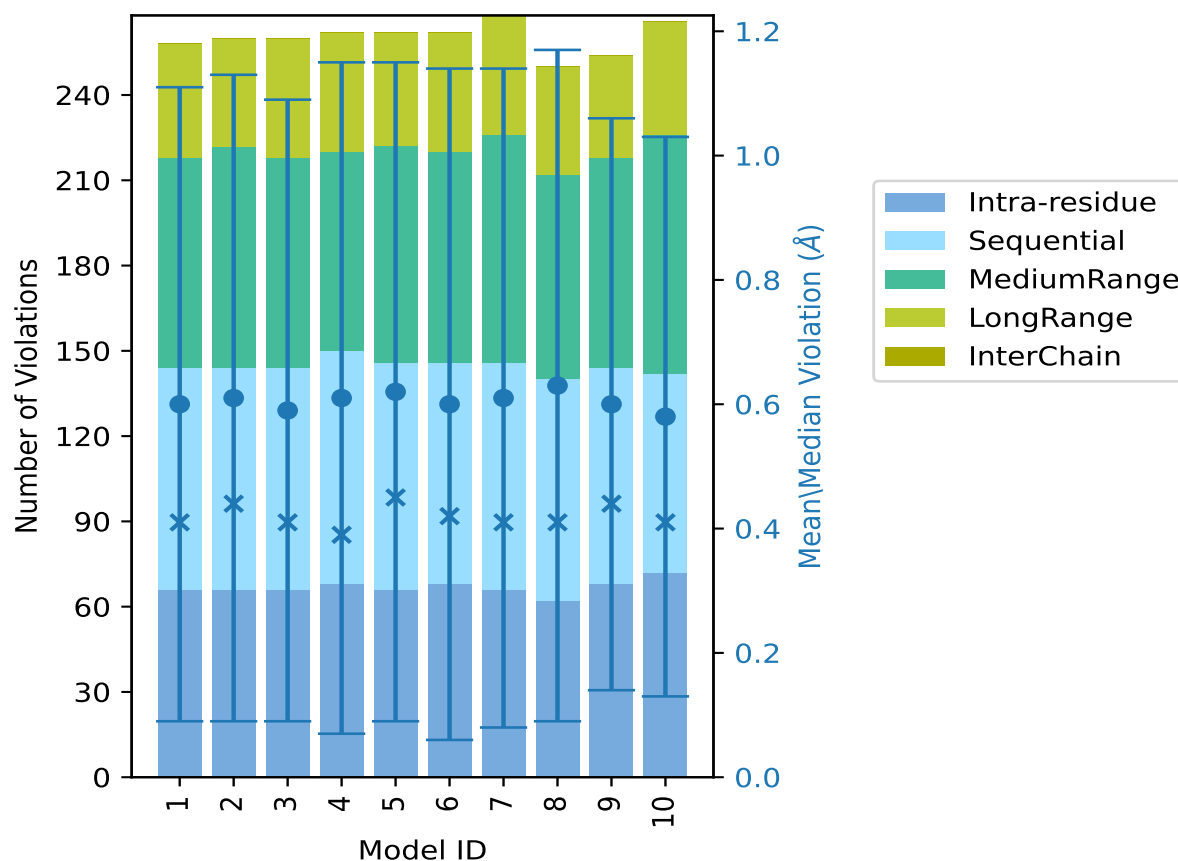
## 9.2 Distance violation statistics for each model [i](#)

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

| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 1        | 66                   | 78              | 74              | 40              | 0               | 258   | 0.6      | 2.9     | 0.51                | 0.41       |
| 2        | 66                   | 78              | 78              | 38              | 0               | 260   | 0.61     | 2.86    | 0.52                | 0.44       |
| 3        | 66                   | 78              | 74              | 42              | 0               | 260   | 0.59     | 2.87    | 0.5                 | 0.41       |
| 4        | 68                   | 82              | 70              | 42              | 0               | 262   | 0.61     | 3.0     | 0.54                | 0.39       |
| 5        | 66                   | 80              | 76              | 40              | 0               | 262   | 0.62     | 3.06    | 0.53                | 0.45       |
| 6        | 68                   | 78              | 74              | 42              | 0               | 262   | 0.6      | 3.25    | 0.54                | 0.42       |
| 7        | 66                   | 80              | 80              | 42              | 0               | 268   | 0.61     | 3.03    | 0.53                | 0.41       |
| 8        | 62                   | 78              | 72              | 38              | 0               | 250   | 0.63     | 2.9     | 0.54                | 0.41       |
| 9        | 68                   | 76              | 74              | 36              | 0               | 254   | 0.6      | 2.17    | 0.46                | 0.44       |
| 10       | 72                   | 70              | 84              | 40              | 0               | 266   | 0.58     | 2.16    | 0.45                | 0.41       |

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

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



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

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

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 870(IR:502, SQ:148, MR:138, LR:82, 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>       | %    |
| 8                             | 4               | 4               | 4               | 0               | 20    | 1                        | 10.0 |
| 16                            | 4               | 6               | 6               | 0               | 32    | 2                        | 20.0 |
| 0                             | 0               | 2               | 4               | 0               | 6     | 3                        | 30.0 |

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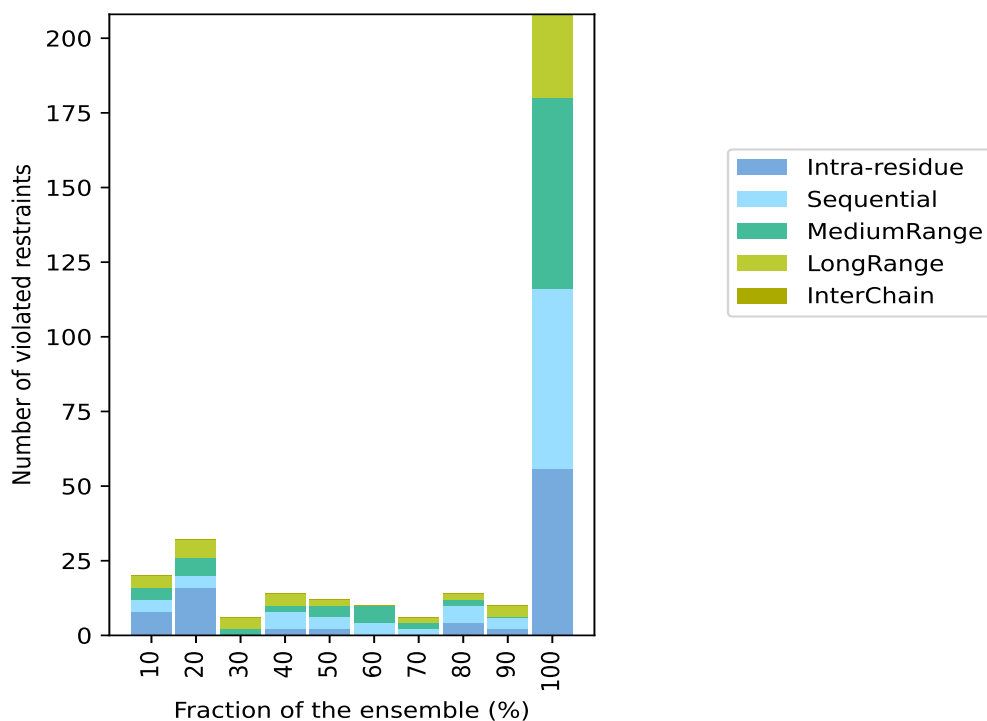
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| Number of violated restraints |                 |                 |                 |                 |       | Fraction of the ensemble |       |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|-------|
| IR <sup>1</sup>               | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total | Count <sup>6</sup>       | %     |
| 2                             | 6               | 2               | 4               | 0               | 14    | 4                        | 40.0  |
| 2                             | 4               | 4               | 2               | 0               | 12    | 5                        | 50.0  |
| 0                             | 4               | 6               | 0               | 0               | 10    | 6                        | 60.0  |
| 0                             | 2               | 2               | 2               | 0               | 6     | 7                        | 70.0  |
| 4                             | 6               | 2               | 2               | 0               | 14    | 8                        | 80.0  |
| 2                             | 4               | 0               | 4               | 0               | 10    | 9                        | 90.0  |
| 56                            | 60              | 64              | 28              | 0               | 208   | 10                       | 100.0 |

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

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

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

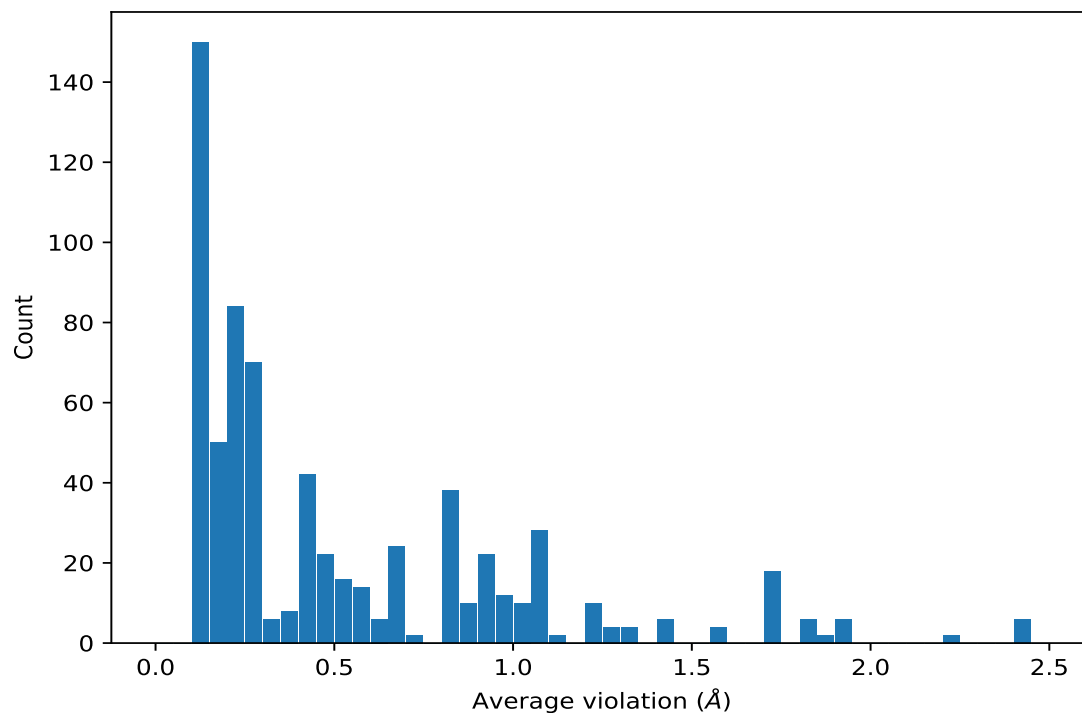


## 9.4 Most violated distance restraints in the ensemble ⓘ

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

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

in the ensemble



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

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

| Key     | Atom-1         | Atom-2         | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|----------------|----------------|---------------------|----------|---------------------|------------|
| (1,560) | 1:6:A:ARG:HG3  | 1:7:A:LEU:HD21 | 10                  | 2.44     | 1.09                | 2.9        |
| (1,560) | 1:6:A:ARG:HG3  | 1:7:A:LEU:HD22 | 10                  | 2.44     | 1.09                | 2.9        |
| (1,560) | 1:6:A:ARG:HG3  | 1:7:A:LEU:HD23 | 10                  | 2.44     | 1.09                | 2.9        |
| (3,82)  | 1:6:A:ARG:HG3  | 1:7:A:LEU:HD21 | 10                  | 2.44     | 1.09                | 2.9        |
| (3,82)  | 1:6:A:ARG:HG3  | 1:7:A:LEU:HD22 | 10                  | 2.44     | 1.09                | 2.9        |
| (3,82)  | 1:6:A:ARG:HG3  | 1:7:A:LEU:HD23 | 10                  | 2.44     | 1.09                | 2.9        |
| (1,399) | 1:1:A:GLU:HB3  | 1:4:A:ALA:H    | 10                  | 2.22     | 0.29                | 2.2        |
| (3,48)  | 1:1:A:GLU:HB3  | 1:4:A:ALA:H    | 10                  | 2.22     | 0.29                | 2.2        |
| (1,519) | 1:5:A:VAL:HG11 | 1:8:A:TYR:HA   | 10                  | 1.92     | 0.02                | 1.92       |
| (1,519) | 1:5:A:VAL:HG12 | 1:8:A:TYR:HA   | 10                  | 1.92     | 0.02                | 1.92       |
| (1,519) | 1:5:A:VAL:HG13 | 1:8:A:TYR:HA   | 10                  | 1.92     | 0.02                | 1.92       |
| (3,68)  | 1:5:A:VAL:HG11 | 1:8:A:TYR:HA   | 10                  | 1.92     | 0.02                | 1.92       |
| (3,68)  | 1:5:A:VAL:HG12 | 1:8:A:TYR:HA   | 10                  | 1.92     | 0.02                | 1.92       |
| (3,68)  | 1:5:A:VAL:HG13 | 1:8:A:TYR:HA   | 10                  | 1.92     | 0.02                | 1.92       |
| (1,352) | 1:11:A:TRP:HB2 | 1:11:A:TRP:HZ3 | 10                  | 1.9      | 0.01                | 1.9        |

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| Key     | Atom-1          | Atom-2         | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|----------------|---------------------|----------|---------------------|------------|
| (3,38)  | 1:11:A:TRP:HB2  | 1:11:A:TRP:HZ3 | 10                  | 1.9      | 0.01                | 1.9        |
| (1,542) | 1:5:A:VAL:HG21  | 1:6:A:ARG:HB3  | 10                  | 1.84     | 0.05                | 1.86       |
| (1,542) | 1:5:A:VAL:HG22  | 1:6:A:ARG:HB3  | 10                  | 1.84     | 0.05                | 1.86       |
| (1,542) | 1:5:A:VAL:HG23  | 1:6:A:ARG:HB3  | 10                  | 1.84     | 0.05                | 1.86       |
| (3,74)  | 1:5:A:VAL:HG21  | 1:6:A:ARG:HB3  | 10                  | 1.84     | 0.05                | 1.86       |
| (3,74)  | 1:5:A:VAL:HG22  | 1:6:A:ARG:HB3  | 10                  | 1.84     | 0.05                | 1.86       |
| (3,74)  | 1:5:A:VAL:HG23  | 1:6:A:ARG:HB3  | 10                  | 1.84     | 0.05                | 1.86       |
| (1,559) | 1:4:A:ALA:HB1   | 1:7:A:LEU:HD21 | 10                  | 1.73     | 0.39                | 1.91       |
| (1,559) | 1:4:A:ALA:HB1   | 1:7:A:LEU:HD22 | 10                  | 1.73     | 0.39                | 1.91       |
| (1,559) | 1:4:A:ALA:HB1   | 1:7:A:LEU:HD23 | 10                  | 1.73     | 0.39                | 1.91       |
| (1,559) | 1:4:A:ALA:HB2   | 1:7:A:LEU:HD21 | 10                  | 1.73     | 0.39                | 1.91       |
| (1,559) | 1:4:A:ALA:HB2   | 1:7:A:LEU:HD22 | 10                  | 1.73     | 0.39                | 1.91       |
| (1,559) | 1:4:A:ALA:HB2   | 1:7:A:LEU:HD23 | 10                  | 1.73     | 0.39                | 1.91       |
| (1,559) | 1:4:A:ALA:HB3   | 1:7:A:LEU:HD21 | 10                  | 1.73     | 0.39                | 1.91       |
| (1,559) | 1:4:A:ALA:HB3   | 1:7:A:LEU:HD22 | 10                  | 1.73     | 0.39                | 1.91       |
| (1,559) | 1:4:A:ALA:HB3   | 1:7:A:LEU:HD23 | 10                  | 1.73     | 0.39                | 1.91       |
| (3,81)  | 1:4:A:ALA:HB1   | 1:7:A:LEU:HD21 | 10                  | 1.73     | 0.39                | 1.91       |
| (3,81)  | 1:4:A:ALA:HB1   | 1:7:A:LEU:HD22 | 10                  | 1.73     | 0.39                | 1.91       |
| (3,81)  | 1:4:A:ALA:HB1   | 1:7:A:LEU:HD23 | 10                  | 1.73     | 0.39                | 1.91       |
| (3,81)  | 1:4:A:ALA:HB2   | 1:7:A:LEU:HD21 | 10                  | 1.73     | 0.39                | 1.91       |
| (3,81)  | 1:4:A:ALA:HB2   | 1:7:A:LEU:HD22 | 10                  | 1.73     | 0.39                | 1.91       |
| (3,81)  | 1:4:A:ALA:HB2   | 1:7:A:LEU:HD23 | 10                  | 1.73     | 0.39                | 1.91       |
| (3,81)  | 1:4:A:ALA:HB3   | 1:7:A:LEU:HD21 | 10                  | 1.73     | 0.39                | 1.91       |
| (3,81)  | 1:4:A:ALA:HB3   | 1:7:A:LEU:HD22 | 10                  | 1.73     | 0.39                | 1.91       |
| (3,81)  | 1:4:A:ALA:HB3   | 1:7:A:LEU:HD23 | 10                  | 1.73     | 0.39                | 1.91       |
| (1,384) | 1:11:A:TRP:HE3  | 1:11:A:TRP:HH2 | 10                  | 1.59     | 0.01                | 1.59       |
| (3,46)  | 1:11:A:TRP:HE3  | 1:11:A:TRP:HH2 | 10                  | 1.59     | 0.01                | 1.59       |
| (1,382) | 1:11:A:TRP:HD1  | 1:11:A:TRP:HZ2 | 10                  | 1.58     | 0.01                | 1.58       |
| (3,44)  | 1:11:A:TRP:HD1  | 1:11:A:TRP:HZ2 | 10                  | 1.58     | 0.01                | 1.58       |
| (1,565) | 1:12:A:LEU:HD11 | 1:16:A:GLY:H   | 10                  | 1.45     | 0.06                | 1.44       |
| (1,565) | 1:12:A:LEU:HD12 | 1:16:A:GLY:H   | 10                  | 1.45     | 0.06                | 1.44       |
| (1,565) | 1:12:A:LEU:HD13 | 1:16:A:GLY:H   | 10                  | 1.45     | 0.06                | 1.44       |
| (3,83)  | 1:12:A:LEU:HD11 | 1:16:A:GLY:H   | 10                  | 1.45     | 0.06                | 1.44       |
| (3,83)  | 1:12:A:LEU:HD12 | 1:16:A:GLY:H   | 10                  | 1.45     | 0.06                | 1.44       |
| (3,83)  | 1:12:A:LEU:HD13 | 1:16:A:GLY:H   | 10                  | 1.45     | 0.06                | 1.44       |
| (1,336) | 1:11:A:TRP:HZ2  | 1:21:A:ARG:HB3 | 10                  | 1.34     | 0.36                | 1.52       |
| (3,35)  | 1:11:A:TRP:HZ2  | 1:21:A:ARG:HB3 | 10                  | 1.34     | 0.36                | 1.52       |
| (1,482) | 1:6:A:ARG:HA    | 1:10:A:GLN:HB3 | 10                  | 1.31     | 0.37                | 1.42       |
| (3,65)  | 1:6:A:ARG:HA    | 1:10:A:GLN:HB3 | 10                  | 1.31     | 0.37                | 1.42       |
| (1,573) | 1:8:A:TYR:HD1   | 1:11:A:TRP:HB2 | 10                  | 1.29     | 0.05                | 1.31       |
| (1,573) | 1:8:A:TYR:HD2   | 1:11:A:TRP:HB2 | 10                  | 1.29     | 0.05                | 1.31       |
| (2,488) | 1:8:A:TYR:HD1   | 1:11:A:TRP:HB2 | 10                  | 1.29     | 0.05                | 1.31       |

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| Key     | Atom-1         | Atom-2         | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|----------------|----------------|---------------------|----------|---------------------|------------|
| (2,488) | 1:8:A:TYR:HD2  | 1:11:A:TRP:HB2 | 10                  | 1.29     | 0.05                | 1.31       |
| (1,591) | 1:5:A:VAL:HG11 | 1:9:A:ILE:HB   | 10                  | 1.23     | 0.06                | 1.25       |
| (1,591) | 1:5:A:VAL:HG12 | 1:9:A:ILE:HB   | 10                  | 1.23     | 0.06                | 1.25       |
| (1,591) | 1:5:A:VAL:HG13 | 1:9:A:ILE:HB   | 10                  | 1.23     | 0.06                | 1.25       |
| (3,90)  | 1:5:A:VAL:HG11 | 1:9:A:ILE:HB   | 10                  | 1.23     | 0.06                | 1.25       |
| (3,90)  | 1:5:A:VAL:HG12 | 1:9:A:ILE:HB   | 10                  | 1.23     | 0.06                | 1.25       |
| (3,90)  | 1:5:A:VAL:HG13 | 1:9:A:ILE:HB   | 10                  | 1.23     | 0.06                | 1.25       |
| (1,434) | 1:11:A:TRP:H   | 1:24:A:PRO:HG2 | 10                  | 1.23     | 0.36                | 1.34       |
| (2,378) | 1:11:A:TRP:H   | 1:24:A:PRO:HG2 | 10                  | 1.23     | 0.36                | 1.34       |
| (1,574) | 1:11:A:TRP:HB3 | 1:11:A:TRP:HD1 | 10                  | 1.21     | 0.01                | 1.21       |
| (3,86)  | 1:11:A:TRP:HB3 | 1:11:A:TRP:HD1 | 10                  | 1.21     | 0.01                | 1.21       |
| (1,489) | 1:21:A:ARG:HB2 | 1:22:A:PRO:HD3 | 10                  | 1.13     | 0.1                 | 1.12       |
| (2,424) | 1:21:A:ARG:HB2 | 1:22:A:PRO:HD3 | 10                  | 1.13     | 0.1                 | 1.12       |
| (1,59)  | 1:7:A:LEU:HA   | 1:7:A:LEU:HD11 | 10                  | 1.08     | 0.09                | 1.04       |
| (1,59)  | 1:7:A:LEU:HA   | 1:7:A:LEU:HD12 | 10                  | 1.08     | 0.09                | 1.04       |
| (1,59)  | 1:7:A:LEU:HA   | 1:7:A:LEU:HD13 | 10                  | 1.08     | 0.09                | 1.04       |
| (3,5)   | 1:7:A:LEU:HA   | 1:7:A:LEU:HD11 | 10                  | 1.08     | 0.09                | 1.04       |
| (3,5)   | 1:7:A:LEU:HA   | 1:7:A:LEU:HD12 | 10                  | 1.08     | 0.09                | 1.04       |
| (3,5)   | 1:7:A:LEU:HA   | 1:7:A:LEU:HD13 | 10                  | 1.08     | 0.09                | 1.04       |
| (1,512) | 1:1:A:GLU:HB2  | 1:2:A:GLU:HG2  | 10                  | 1.08     | 0.54                | 1.36       |
| (2,445) | 1:1:A:GLU:HB2  | 1:2:A:GLU:HG2  | 10                  | 1.08     | 0.54                | 1.36       |
| (1,87)  | 1:9:A:ILE:HA   | 1:9:A:ILE:HD11 | 10                  | 1.07     | 0.01                | 1.06       |
| (1,87)  | 1:9:A:ILE:HA   | 1:9:A:ILE:HD12 | 10                  | 1.07     | 0.01                | 1.06       |
| (1,87)  | 1:9:A:ILE:HA   | 1:9:A:ILE:HD13 | 10                  | 1.07     | 0.01                | 1.06       |
| (1,280) | 1:11:A:TRP:HE1 | 1:24:A:PRO:HD2 | 10                  | 1.07     | 0.11                | 1.04       |
| (2,261) | 1:11:A:TRP:HE1 | 1:24:A:PRO:HD2 | 10                  | 1.07     | 0.11                | 1.04       |
| (3,9)   | 1:9:A:ILE:HA   | 1:9:A:ILE:HD11 | 10                  | 1.07     | 0.01                | 1.06       |
| (3,9)   | 1:9:A:ILE:HA   | 1:9:A:ILE:HD12 | 10                  | 1.07     | 0.01                | 1.06       |
| (3,9)   | 1:9:A:ILE:HA   | 1:9:A:ILE:HD13 | 10                  | 1.07     | 0.01                | 1.06       |
| (1,318) | 1:7:A:LEU:HD11 | 1:8:A:TYR:HD1  | 10                  | 1.06     | 0.36                | 1.21       |
| (1,318) | 1:7:A:LEU:HD11 | 1:8:A:TYR:HD2  | 10                  | 1.06     | 0.36                | 1.21       |
| (1,318) | 1:7:A:LEU:HD12 | 1:8:A:TYR:HD1  | 10                  | 1.06     | 0.36                | 1.21       |
| (1,318) | 1:7:A:LEU:HD12 | 1:8:A:TYR:HD2  | 10                  | 1.06     | 0.36                | 1.21       |
| (1,318) | 1:7:A:LEU:HD13 | 1:8:A:TYR:HD1  | 10                  | 1.06     | 0.36                | 1.21       |
| (1,318) | 1:7:A:LEU:HD13 | 1:8:A:TYR:HD2  | 10                  | 1.06     | 0.36                | 1.21       |
| (3,30)  | 1:7:A:LEU:HD11 | 1:8:A:TYR:HD1  | 10                  | 1.06     | 0.36                | 1.21       |
| (3,30)  | 1:7:A:LEU:HD11 | 1:8:A:TYR:HD2  | 10                  | 1.06     | 0.36                | 1.21       |
| (3,30)  | 1:7:A:LEU:HD12 | 1:8:A:TYR:HD1  | 10                  | 1.06     | 0.36                | 1.21       |
| (3,30)  | 1:7:A:LEU:HD12 | 1:8:A:TYR:HD2  | 10                  | 1.06     | 0.36                | 1.21       |
| (3,30)  | 1:7:A:LEU:HD13 | 1:8:A:TYR:HD1  | 10                  | 1.06     | 0.36                | 1.21       |
| (3,30)  | 1:7:A:LEU:HD13 | 1:8:A:TYR:HD2  | 10                  | 1.06     | 0.36                | 1.21       |
| (1,428) | 1:5:A:VAL:HB   | 1:6:A:ARG:H    | 10                  | 1.04     | 0.03                | 1.04       |

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| Key     | Atom-1          | Atom-2         | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|----------------|---------------------|----------|---------------------|------------|
| (3,54)  | 1:5:A:VAL:HB    | 1:6:A:ARG:H    | 10                  | 1.04     | 0.03                | 1.04       |
| (1,418) | 1:21:A:ARG:H    | 1:22:A:PRO:HD2 | 10                  | 1.01     | 0.13                | 0.94       |
| (3,52)  | 1:21:A:ARG:H    | 1:22:A:PRO:HD2 | 10                  | 1.01     | 0.13                | 0.94       |
| (1,595) | 1:7:A:LEU:HD21  | 1:8:A:TYR:HB2  | 10                  | 1.01     | 0.35                | 1.17       |
| (1,595) | 1:7:A:LEU:HD22  | 1:8:A:TYR:HB2  | 10                  | 1.01     | 0.35                | 1.17       |
| (1,595) | 1:7:A:LEU:HD23  | 1:8:A:TYR:HB2  | 10                  | 1.01     | 0.35                | 1.17       |
| (3,91)  | 1:7:A:LEU:HD21  | 1:8:A:TYR:HB2  | 10                  | 1.01     | 0.35                | 1.17       |
| (3,91)  | 1:7:A:LEU:HD22  | 1:8:A:TYR:HB2  | 10                  | 1.01     | 0.35                | 1.17       |
| (3,91)  | 1:7:A:LEU:HD23  | 1:8:A:TYR:HB2  | 10                  | 1.01     | 0.35                | 1.17       |
| (1,536) | 1:12:A:LEU:HD11 | 1:16:A:GLY:HA2 | 10                  | 0.99     | 0.17                | 1.06       |
| (1,536) | 1:12:A:LEU:HD12 | 1:16:A:GLY:HA2 | 10                  | 0.99     | 0.17                | 1.06       |
| (1,536) | 1:12:A:LEU:HD13 | 1:16:A:GLY:HA2 | 10                  | 0.99     | 0.17                | 1.06       |
| (3,72)  | 1:12:A:LEU:HD11 | 1:16:A:GLY:HA2 | 10                  | 0.99     | 0.17                | 1.06       |
| (3,72)  | 1:12:A:LEU:HD12 | 1:16:A:GLY:HA2 | 10                  | 0.99     | 0.17                | 1.06       |
| (3,72)  | 1:12:A:LEU:HD13 | 1:16:A:GLY:HA2 | 10                  | 0.99     | 0.17                | 1.06       |
| (1,584) | 1:8:A:TYR:HB3   | 1:24:A:PRO:HG3 | 10                  | 0.99     | 0.37                | 0.86       |
| (3,89)  | 1:8:A:TYR:HB3   | 1:24:A:PRO:HG3 | 10                  | 0.99     | 0.37                | 0.86       |
| (1,304) | 1:8:A:TYR:HE1   | 1:24:A:PRO:HB3 | 10                  | 0.98     | 0.15                | 1.04       |
| (1,304) | 1:8:A:TYR:HE2   | 1:24:A:PRO:HB3 | 10                  | 0.98     | 0.15                | 1.04       |
| (2,281) | 1:8:A:TYR:HE1   | 1:24:A:PRO:HB3 | 10                  | 0.98     | 0.15                | 1.04       |
| (2,281) | 1:8:A:TYR:HE2   | 1:24:A:PRO:HB3 | 10                  | 0.98     | 0.15                | 1.04       |
| (1,575) | 1:8:A:TYR:HB3   | 1:11:A:TRP:HE3 | 10                  | 0.95     | 0.06                | 0.98       |
| (3,87)  | 1:8:A:TYR:HB3   | 1:11:A:TRP:HE3 | 10                  | 0.95     | 0.06                | 0.98       |
| (1,561) | 1:9:A:ILE:HG21  | 1:13:A:LYS:HG2 | 10                  | 0.94     | 0.02                | 0.93       |
| (1,561) | 1:9:A:ILE:HG22  | 1:13:A:LYS:HG2 | 10                  | 0.94     | 0.02                | 0.93       |
| (1,561) | 1:9:A:ILE:HG23  | 1:13:A:LYS:HG2 | 10                  | 0.94     | 0.02                | 0.93       |
| (2,479) | 1:9:A:ILE:HG21  | 1:13:A:LYS:HG2 | 10                  | 0.94     | 0.02                | 0.93       |
| (2,479) | 1:9:A:ILE:HG22  | 1:13:A:LYS:HG2 | 10                  | 0.94     | 0.02                | 0.93       |
| (2,479) | 1:9:A:ILE:HG23  | 1:13:A:LYS:HG2 | 10                  | 0.94     | 0.02                | 0.93       |
| (1,435) | 1:7:A:LEU:HB2   | 1:10:A:GLN:H   | 10                  | 0.92     | 0.08                | 0.87       |
| (3,57)  | 1:7:A:LEU:HB2   | 1:10:A:GLN:H   | 10                  | 0.92     | 0.08                | 0.87       |
| (1,554) | 1:7:A:LEU:HD21  | 1:24:A:PRO:HB2 | 10                  | 0.92     | 0.13                | 0.86       |
| (1,554) | 1:7:A:LEU:HD22  | 1:24:A:PRO:HB2 | 10                  | 0.92     | 0.13                | 0.86       |
| (1,554) | 1:7:A:LEU:HD23  | 1:24:A:PRO:HB2 | 10                  | 0.92     | 0.13                | 0.86       |
| (3,78)  | 1:7:A:LEU:HD21  | 1:24:A:PRO:HB2 | 10                  | 0.92     | 0.13                | 0.86       |
| (3,78)  | 1:7:A:LEU:HD22  | 1:24:A:PRO:HB2 | 10                  | 0.92     | 0.13                | 0.86       |
| (3,78)  | 1:7:A:LEU:HD23  | 1:24:A:PRO:HB2 | 10                  | 0.92     | 0.13                | 0.86       |
| (1,578) | 1:1:A:GLU:HB2   | 1:3:A:GLU:HA   | 10                  | 0.9      | 0.43                | 1.17       |
| (3,88)  | 1:1:A:GLU:HB2   | 1:3:A:GLU:HA   | 10                  | 0.9      | 0.43                | 1.17       |
| (1,152) | 1:13:A:LYS:H    | 1:13:A:LYS:HG2 | 10                  | 0.9      | 0.02                | 0.89       |
| (2,138) | 1:13:A:LYS:H    | 1:13:A:LYS:HG2 | 10                  | 0.9      | 0.02                | 0.89       |
| (1,504) | 1:16:A:GLY:HA2  | 1:17:A:PRO:HG2 | 10                  | 0.89     | 0.24                | 0.96       |

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| Key     | Atom-1         | Atom-2         | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|----------------|----------------|---------------------|----------|---------------------|------------|
| (1,504) | 1:16:A:GLY:HA2 | 1:17:A:PRO:HG3 | 10                  | 0.89     | 0.24                | 0.96       |
| (2,437) | 1:16:A:GLY:HA2 | 1:17:A:PRO:HG2 | 10                  | 0.89     | 0.24                | 0.96       |
| (2,437) | 1:16:A:GLY:HA2 | 1:17:A:PRO:HG3 | 10                  | 0.89     | 0.24                | 0.96       |
| (1,341) | 1:11:A:TRP:HH2 | 1:17:A:PRO:HB2 | 10                  | 0.89     | 0.05                | 0.88       |
| (2,305) | 1:11:A:TRP:HH2 | 1:17:A:PRO:HB2 | 10                  | 0.89     | 0.05                | 0.88       |
| (1,299) | 1:8:A:TYR:HD1  | 1:24:A:PRO:HD3 | 10                  | 0.88     | 0.03                | 0.88       |
| (1,299) | 1:8:A:TYR:HD2  | 1:24:A:PRO:HD3 | 10                  | 0.88     | 0.03                | 0.88       |
| (2,276) | 1:8:A:TYR:HD1  | 1:24:A:PRO:HD3 | 10                  | 0.88     | 0.03                | 0.88       |
| (2,276) | 1:8:A:TYR:HD2  | 1:24:A:PRO:HD3 | 10                  | 0.88     | 0.03                | 0.88       |
| (1,371) | 1:11:A:TRP:H   | 1:11:A:TRP:HD1 | 10                  | 0.84     | 0.04                | 0.85       |
| (3,42)  | 1:11:A:TRP:H   | 1:11:A:TRP:HD1 | 10                  | 0.84     | 0.04                | 0.85       |
| (1,317) | 1:5:A:VAL:HG21 | 1:8:A:TYR:HE1  | 10                  | 0.84     | 0.15                | 0.77       |
| (1,317) | 1:5:A:VAL:HG21 | 1:8:A:TYR:HE2  | 10                  | 0.84     | 0.15                | 0.77       |
| (1,317) | 1:5:A:VAL:HG22 | 1:8:A:TYR:HE1  | 10                  | 0.84     | 0.15                | 0.77       |
| (1,317) | 1:5:A:VAL:HG22 | 1:8:A:TYR:HE2  | 10                  | 0.84     | 0.15                | 0.77       |
| (1,317) | 1:5:A:VAL:HG23 | 1:8:A:TYR:HE1  | 10                  | 0.84     | 0.15                | 0.77       |
| (1,317) | 1:5:A:VAL:HG23 | 1:8:A:TYR:HE2  | 10                  | 0.84     | 0.15                | 0.77       |
| (3,29)  | 1:5:A:VAL:HG21 | 1:8:A:TYR:HE1  | 10                  | 0.84     | 0.15                | 0.77       |
| (3,29)  | 1:5:A:VAL:HG21 | 1:8:A:TYR:HE2  | 10                  | 0.84     | 0.15                | 0.77       |
| (3,29)  | 1:5:A:VAL:HG22 | 1:8:A:TYR:HE1  | 10                  | 0.84     | 0.15                | 0.77       |
| (3,29)  | 1:5:A:VAL:HG22 | 1:8:A:TYR:HE2  | 10                  | 0.84     | 0.15                | 0.77       |
| (3,29)  | 1:5:A:VAL:HG23 | 1:8:A:TYR:HE1  | 10                  | 0.84     | 0.15                | 0.77       |
| (3,29)  | 1:5:A:VAL:HG23 | 1:8:A:TYR:HE2  | 10                  | 0.84     | 0.15                | 0.77       |
| (1,546) | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG21 | 10                  | 0.83     | 0.07                | 0.86       |
| (1,546) | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG22 | 10                  | 0.83     | 0.07                | 0.86       |
| (1,546) | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG23 | 10                  | 0.83     | 0.07                | 0.86       |
| (1,546) | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG21 | 10                  | 0.83     | 0.07                | 0.86       |
| (1,546) | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG22 | 10                  | 0.83     | 0.07                | 0.86       |
| (1,546) | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG23 | 10                  | 0.83     | 0.07                | 0.86       |
| (1,546) | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG21 | 10                  | 0.83     | 0.07                | 0.86       |
| (1,546) | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG22 | 10                  | 0.83     | 0.07                | 0.86       |
| (1,546) | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG23 | 10                  | 0.83     | 0.07                | 0.86       |
| (3,76)  | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG21 | 10                  | 0.83     | 0.07                | 0.86       |
| (3,76)  | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG22 | 10                  | 0.83     | 0.07                | 0.86       |
| (3,76)  | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG23 | 10                  | 0.83     | 0.07                | 0.86       |
| (3,76)  | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG21 | 10                  | 0.83     | 0.07                | 0.86       |
| (3,76)  | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG22 | 10                  | 0.83     | 0.07                | 0.86       |
| (3,76)  | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG23 | 10                  | 0.83     | 0.07                | 0.86       |
| (3,76)  | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG21 | 10                  | 0.83     | 0.07                | 0.86       |
| (3,76)  | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG22 | 10                  | 0.83     | 0.07                | 0.86       |
| (3,76)  | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG23 | 10                  | 0.83     | 0.07                | 0.86       |
| (1,583) | 1:11:A:TRP:HB2 | 1:24:A:PRO:HD2 | 10                  | 0.82     | 0.11                | 0.85       |

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| Key     | Atom-1         | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (2,495) | 1:11:A:TRP:HB2 | 1:24:A:PRO:HD2  | 10                  | 0.82     | 0.11                | 0.85       |
| (1,432) | 1:3:A:GLU:HB3  | 1:6:A:ARG:H     | 10                  | 0.81     | 0.13                | 0.87       |
| (3,56)  | 1:3:A:GLU:HB3  | 1:6:A:ARG:H     | 10                  | 0.81     | 0.13                | 0.87       |
| (1,184) | 1:24:A:PRO:HA  | 1:25:A:SER:H    | 10                  | 0.8      | 0.05                | 0.79       |
| (3,16)  | 1:24:A:PRO:HA  | 1:25:A:SER:H    | 10                  | 0.8      | 0.05                | 0.79       |
| (1,324) | 1:11:A:TRP:HZ2 | 1:23:A:PRO:HB2  | 10                  | 0.73     | 0.02                | 0.72       |
| (2,293) | 1:11:A:TRP:HZ2 | 1:23:A:PRO:HB2  | 10                  | 0.73     | 0.02                | 0.72       |
| (1,446) | 1:9:A:ILE:HD11 | 1:10:A:GLN:H    | 10                  | 0.69     | 0.13                | 0.74       |
| (1,446) | 1:9:A:ILE:HD12 | 1:10:A:GLN:H    | 10                  | 0.69     | 0.13                | 0.74       |
| (1,446) | 1:9:A:ILE:HD13 | 1:10:A:GLN:H    | 10                  | 0.69     | 0.13                | 0.74       |
| (3,61)  | 1:9:A:ILE:HD11 | 1:10:A:GLN:H    | 10                  | 0.69     | 0.13                | 0.74       |
| (3,61)  | 1:9:A:ILE:HD12 | 1:10:A:GLN:H    | 10                  | 0.69     | 0.13                | 0.74       |
| (3,61)  | 1:9:A:ILE:HD13 | 1:10:A:GLN:H    | 10                  | 0.69     | 0.13                | 0.74       |
| (1,332) | 1:11:A:TRP:HZ2 | 1:23:A:PRO:HG2  | 10                  | 0.69     | 0.06                | 0.72       |
| (2,298) | 1:11:A:TRP:HZ2 | 1:23:A:PRO:HG2  | 10                  | 0.69     | 0.06                | 0.72       |
| (1,28)  | 1:5:A:VAL:H    | 1:5:A:VAL:HG21  | 10                  | 0.68     | 0.01                | 0.68       |
| (1,28)  | 1:5:A:VAL:H    | 1:5:A:VAL:HG22  | 10                  | 0.68     | 0.01                | 0.68       |
| (1,28)  | 1:5:A:VAL:H    | 1:5:A:VAL:HG23  | 10                  | 0.68     | 0.01                | 0.68       |
| (3,2)   | 1:5:A:VAL:H    | 1:5:A:VAL:HG21  | 10                  | 0.68     | 0.01                | 0.68       |
| (3,2)   | 1:5:A:VAL:H    | 1:5:A:VAL:HG22  | 10                  | 0.68     | 0.01                | 0.68       |
| (3,2)   | 1:5:A:VAL:H    | 1:5:A:VAL:HG23  | 10                  | 0.68     | 0.01                | 0.68       |
| (1,297) | 1:8:A:TYR:HB3  | 1:8:A:TYR:HE1   | 10                  | 0.67     | 0.01                | 0.67       |
| (1,297) | 1:8:A:TYR:HB3  | 1:8:A:TYR:HE2   | 10                  | 0.67     | 0.01                | 0.67       |
| (3,23)  | 1:8:A:TYR:HB3  | 1:8:A:TYR:HE1   | 10                  | 0.67     | 0.01                | 0.67       |
| (3,23)  | 1:8:A:TYR:HB3  | 1:8:A:TYR:HE2   | 10                  | 0.67     | 0.01                | 0.67       |
| (1,51)  | 1:6:A:ARG:H    | 1:6:A:ARG:HB3   | 10                  | 0.62     | 0.05                | 0.66       |
| (2,48)  | 1:6:A:ARG:H    | 1:6:A:ARG:HB3   | 10                  | 0.62     | 0.05                | 0.66       |
| (1,353) | 1:11:A:TRP:HB2 | 1:11:A:TRP:HE3  | 10                  | 0.62     | 0.01                | 0.62       |
| (2,315) | 1:11:A:TRP:HB2 | 1:11:A:TRP:HE3  | 10                  | 0.62     | 0.01                | 0.62       |
| (1,390) | 1:11:A:TRP:HB2 | 1:12:A:LEU:H    | 10                  | 0.58     | 0.01                | 0.59       |
| (2,344) | 1:11:A:TRP:HB2 | 1:12:A:LEU:H    | 10                  | 0.58     | 0.01                | 0.59       |
| (1,441) | 1:7:A:LEU:HB3  | 1:10:A:GLN:H    | 10                  | 0.57     | 0.18                | 0.48       |
| (3,59)  | 1:7:A:LEU:HB3  | 1:10:A:GLN:H    | 10                  | 0.57     | 0.18                | 0.48       |
| (1,326) | 1:11:A:TRP:HH2 | 1:12:A:LEU:HD11 | 10                  | 0.56     | 0.11                | 0.52       |
| (1,326) | 1:11:A:TRP:HH2 | 1:12:A:LEU:HD12 | 10                  | 0.56     | 0.11                | 0.52       |
| (1,326) | 1:11:A:TRP:HH2 | 1:12:A:LEU:HD13 | 10                  | 0.56     | 0.11                | 0.52       |
| (3,32)  | 1:11:A:TRP:HH2 | 1:12:A:LEU:HD11 | 10                  | 0.56     | 0.11                | 0.52       |
| (3,32)  | 1:11:A:TRP:HH2 | 1:12:A:LEU:HD12 | 10                  | 0.56     | 0.11                | 0.52       |
| (3,32)  | 1:11:A:TRP:HH2 | 1:12:A:LEU:HD13 | 10                  | 0.56     | 0.11                | 0.52       |
| (1,566) | 1:6:A:ARG:HB3  | 1:7:A:LEU:H     | 10                  | 0.53     | 0.05                | 0.55       |
| (2,483) | 1:6:A:ARG:HB3  | 1:7:A:LEU:H     | 10                  | 0.53     | 0.05                | 0.55       |
| (1,464) | 1:3:A:GLU:HA   | 1:6:A:ARG:HB3   | 10                  | 0.53     | 0.04                | 0.52       |

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| Key     | Atom-1         | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (2,402) | 1:3:A:GLU:HA   | 1:6:A:ARG:HB3   | 10                  | 0.53     | 0.04                | 0.52       |
| (1,398) | 1:3:A:GLU:HB2  | 1:4:A:ALA:H     | 10                  | 0.53     | 0.08                | 0.55       |
| (2,351) | 1:3:A:GLU:HB2  | 1:4:A:ALA:H     | 10                  | 0.53     | 0.08                | 0.55       |
| (1,429) | 1:10:A:GLN:HB2 | 1:11:A:TRP:H    | 10                  | 0.5      | 0.13                | 0.46       |
| (3,55)  | 1:10:A:GLN:HB2 | 1:11:A:TRP:H    | 10                  | 0.5      | 0.13                | 0.46       |
| (1,313) | 1:8:A:TYR:HD1  | 1:9:A:ILE:HG13  | 10                  | 0.49     | 0.17                | 0.42       |
| (1,313) | 1:8:A:TYR:HD2  | 1:9:A:ILE:HG13  | 10                  | 0.49     | 0.17                | 0.42       |
| (3,27)  | 1:8:A:TYR:HD1  | 1:9:A:ILE:HG13  | 10                  | 0.49     | 0.17                | 0.42       |
| (3,27)  | 1:8:A:TYR:HD2  | 1:9:A:ILE:HG13  | 10                  | 0.49     | 0.17                | 0.42       |
| (1,408) | 1:4:A:ALA:H    | 1:5:A:VAL:HG21  | 10                  | 0.48     | 0.23                | 0.42       |
| (1,408) | 1:4:A:ALA:H    | 1:5:A:VAL:HG22  | 10                  | 0.48     | 0.23                | 0.42       |
| (1,408) | 1:4:A:ALA:H    | 1:5:A:VAL:HG23  | 10                  | 0.48     | 0.23                | 0.42       |
| (3,51)  | 1:4:A:ALA:H    | 1:5:A:VAL:HG21  | 10                  | 0.48     | 0.23                | 0.42       |
| (3,51)  | 1:4:A:ALA:H    | 1:5:A:VAL:HG22  | 10                  | 0.48     | 0.23                | 0.42       |
| (3,51)  | 1:4:A:ALA:H    | 1:5:A:VAL:HG23  | 10                  | 0.48     | 0.23                | 0.42       |
| (1,237) | 1:22:A:PRO:HB3 | 1:22:A:PRO:HD2  | 10                  | 0.45     | 0.02                | 0.45       |
| (3,19)  | 1:22:A:PRO:HB3 | 1:22:A:PRO:HD2  | 10                  | 0.45     | 0.02                | 0.45       |
| (1,600) | 1:9:A:ILE:H    | 1:9:A:ILE:HG21  | 10                  | 0.45     | 0.01                | 0.44       |
| (1,600) | 1:9:A:ILE:H    | 1:9:A:ILE:HG22  | 10                  | 0.45     | 0.01                | 0.44       |
| (1,600) | 1:9:A:ILE:H    | 1:9:A:ILE:HG23  | 10                  | 0.45     | 0.01                | 0.44       |
| (3,92)  | 1:9:A:ILE:H    | 1:9:A:ILE:HG21  | 10                  | 0.45     | 0.01                | 0.44       |
| (3,92)  | 1:9:A:ILE:H    | 1:9:A:ILE:HG22  | 10                  | 0.45     | 0.01                | 0.44       |
| (3,92)  | 1:9:A:ILE:H    | 1:9:A:ILE:HG23  | 10                  | 0.45     | 0.01                | 0.44       |
| (1,377) | 1:8:A:TYR:HE1  | 1:11:A:TRP:HE3  | 10                  | 0.43     | 0.08                | 0.44       |
| (1,377) | 1:8:A:TYR:HE2  | 1:11:A:TRP:HE3  | 10                  | 0.43     | 0.08                | 0.44       |
| (3,43)  | 1:8:A:TYR:HE1  | 1:11:A:TRP:HE3  | 10                  | 0.43     | 0.08                | 0.44       |
| (3,43)  | 1:8:A:TYR:HE2  | 1:11:A:TRP:HE3  | 10                  | 0.43     | 0.08                | 0.44       |
| (1,520) | 1:5:A:VAL:HG21 | 1:8:A:TYR:HA    | 10                  | 0.42     | 0.03                | 0.41       |
| (1,520) | 1:5:A:VAL:HG22 | 1:8:A:TYR:HA    | 10                  | 0.42     | 0.03                | 0.41       |
| (1,520) | 1:5:A:VAL:HG23 | 1:8:A:TYR:HA    | 10                  | 0.42     | 0.03                | 0.41       |
| (3,69)  | 1:5:A:VAL:HG21 | 1:8:A:TYR:HA    | 10                  | 0.42     | 0.03                | 0.41       |
| (3,69)  | 1:5:A:VAL:HG22 | 1:8:A:TYR:HA    | 10                  | 0.42     | 0.03                | 0.41       |
| (3,69)  | 1:5:A:VAL:HG23 | 1:8:A:TYR:HA    | 10                  | 0.42     | 0.03                | 0.41       |
| (1,300) | 1:8:A:TYR:HE1  | 1:24:A:PRO:HD3  | 10                  | 0.41     | 0.07                | 0.41       |
| (1,300) | 1:8:A:TYR:HE2  | 1:24:A:PRO:HD3  | 10                  | 0.41     | 0.07                | 0.41       |
| (2,277) | 1:8:A:TYR:HE1  | 1:24:A:PRO:HD3  | 10                  | 0.41     | 0.07                | 0.41       |
| (2,277) | 1:8:A:TYR:HE2  | 1:24:A:PRO:HD3  | 10                  | 0.41     | 0.07                | 0.41       |
| (1,134) | 1:12:A:LEU:H   | 1:12:A:LEU:HD21 | 10                  | 0.41     | 0.01                | 0.4        |
| (1,134) | 1:12:A:LEU:H   | 1:12:A:LEU:HD22 | 10                  | 0.41     | 0.01                | 0.4        |
| (1,134) | 1:12:A:LEU:H   | 1:12:A:LEU:HD23 | 10                  | 0.41     | 0.01                | 0.4        |
| (3,13)  | 1:12:A:LEU:H   | 1:12:A:LEU:HD21 | 10                  | 0.41     | 0.01                | 0.4        |
| (3,13)  | 1:12:A:LEU:H   | 1:12:A:LEU:HD22 | 10                  | 0.41     | 0.01                | 0.4        |

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| Key     | Atom-1         | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (3,13)  | 1:12:A:LEU:H   | 1:12:A:LEU:HD23 | 10                  | 0.41     | 0.01                | 0.4        |
| (1,93)  | 1:9:A:ILE:HG13 | 1:9:A:ILE:HG21  | 10                  | 0.4      | 0.01                | 0.41       |
| (1,93)  | 1:9:A:ILE:HG13 | 1:9:A:ILE:HG22  | 10                  | 0.4      | 0.01                | 0.41       |
| (1,93)  | 1:9:A:ILE:HG13 | 1:9:A:ILE:HG23  | 10                  | 0.4      | 0.01                | 0.41       |
| (3,10)  | 1:9:A:ILE:HG13 | 1:9:A:ILE:HG21  | 10                  | 0.4      | 0.01                | 0.41       |
| (3,10)  | 1:9:A:ILE:HG13 | 1:9:A:ILE:HG22  | 10                  | 0.4      | 0.01                | 0.41       |
| (3,10)  | 1:9:A:ILE:HG13 | 1:9:A:ILE:HG23  | 10                  | 0.4      | 0.01                | 0.41       |
| (1,22)  | 1:5:A:VAL:HA   | 1:5:A:VAL:HG11  | 10                  | 0.4      | 0.01                | 0.4        |
| (1,22)  | 1:5:A:VAL:HA   | 1:5:A:VAL:HG12  | 10                  | 0.4      | 0.01                | 0.4        |
| (1,22)  | 1:5:A:VAL:HA   | 1:5:A:VAL:HG13  | 10                  | 0.4      | 0.01                | 0.4        |
| (3,1)   | 1:5:A:VAL:HA   | 1:5:A:VAL:HG11  | 10                  | 0.4      | 0.01                | 0.4        |
| (3,1)   | 1:5:A:VAL:HA   | 1:5:A:VAL:HG12  | 10                  | 0.4      | 0.01                | 0.4        |
| (3,1)   | 1:5:A:VAL:HA   | 1:5:A:VAL:HG13  | 10                  | 0.4      | 0.01                | 0.4        |
| (1,323) | 1:8:A:TYR:HD1  | 1:23:A:PRO:HB2  | 10                  | 0.4      | 0.1                 | 0.36       |
| (1,323) | 1:8:A:TYR:HD2  | 1:23:A:PRO:HB2  | 10                  | 0.4      | 0.1                 | 0.36       |
| (2,292) | 1:8:A:TYR:HD1  | 1:23:A:PRO:HB2  | 10                  | 0.4      | 0.1                 | 0.36       |
| (2,292) | 1:8:A:TYR:HD2  | 1:23:A:PRO:HB2  | 10                  | 0.4      | 0.1                 | 0.36       |
| (1,224) | 1:21:A:ARG:H   | 1:21:A:ARG:HB3  | 10                  | 0.38     | 0.03                | 0.38       |
| (2,206) | 1:21:A:ARG:H   | 1:21:A:ARG:HB3  | 10                  | 0.38     | 0.03                | 0.38       |
| (1,132) | 1:12:A:LEU:H   | 1:12:A:LEU:HB3  | 10                  | 0.37     | 0.0                 | 0.37       |
| (3,12)  | 1:12:A:LEU:H   | 1:12:A:LEU:HB3  | 10                  | 0.37     | 0.0                 | 0.37       |
| (1,444) | 1:11:A:TRP:H   | 1:12:A:LEU:HD11 | 10                  | 0.33     | 0.02                | 0.34       |
| (1,444) | 1:11:A:TRP:H   | 1:12:A:LEU:HD12 | 10                  | 0.33     | 0.02                | 0.34       |
| (1,444) | 1:11:A:TRP:H   | 1:12:A:LEU:HD13 | 10                  | 0.33     | 0.02                | 0.34       |
| (3,60)  | 1:11:A:TRP:H   | 1:12:A:LEU:HD11 | 10                  | 0.33     | 0.02                | 0.34       |
| (3,60)  | 1:11:A:TRP:H   | 1:12:A:LEU:HD12 | 10                  | 0.33     | 0.02                | 0.34       |
| (3,60)  | 1:11:A:TRP:H   | 1:12:A:LEU:HD13 | 10                  | 0.33     | 0.02                | 0.34       |
| (1,491) | 1:22:A:PRO:HG2 | 1:23:A:PRO:HD2  | 10                  | 0.3      | 0.04                | 0.29       |
| (1,491) | 1:22:A:PRO:HG2 | 1:23:A:PRO:HD3  | 10                  | 0.3      | 0.04                | 0.29       |
| (1,491) | 1:22:A:PRO:HG3 | 1:23:A:PRO:HD2  | 10                  | 0.3      | 0.04                | 0.29       |
| (1,491) | 1:22:A:PRO:HG3 | 1:23:A:PRO:HD3  | 10                  | 0.3      | 0.04                | 0.29       |
| (3,67)  | 1:22:A:PRO:HG2 | 1:23:A:PRO:HD2  | 10                  | 0.3      | 0.04                | 0.29       |
| (3,67)  | 1:22:A:PRO:HG2 | 1:23:A:PRO:HD3  | 10                  | 0.3      | 0.04                | 0.29       |
| (3,67)  | 1:22:A:PRO:HG3 | 1:23:A:PRO:HD2  | 10                  | 0.3      | 0.04                | 0.29       |
| (3,67)  | 1:22:A:PRO:HG3 | 1:23:A:PRO:HD3  | 10                  | 0.3      | 0.04                | 0.29       |
| (1,543) | 1:5:A:VAL:HG21 | 1:6:A:ARG:HG3   | 10                  | 0.29     | 0.05                | 0.29       |
| (1,543) | 1:5:A:VAL:HG22 | 1:6:A:ARG:HG3   | 10                  | 0.29     | 0.05                | 0.29       |
| (1,543) | 1:5:A:VAL:HG23 | 1:6:A:ARG:HG3   | 10                  | 0.29     | 0.05                | 0.29       |
| (3,75)  | 1:5:A:VAL:HG21 | 1:6:A:ARG:HG3   | 10                  | 0.29     | 0.05                | 0.29       |
| (3,75)  | 1:5:A:VAL:HG22 | 1:6:A:ARG:HG3   | 10                  | 0.29     | 0.05                | 0.29       |
| (3,75)  | 1:5:A:VAL:HG23 | 1:6:A:ARG:HG3   | 10                  | 0.29     | 0.05                | 0.29       |
| (1,141) | 1:13:A:LYS:HB2 | 1:13:A:LYS:HE2  | 10                  | 0.29     | 0.01                | 0.29       |

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| Key     | Atom-1         | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,141) | 1:13:A:LYS:HB3 | 1:13:A:LYS:HE2  | 10                  | 0.29     | 0.01                | 0.29       |
| (1,141) | 1:13:A:LYS:HB3 | 1:13:A:LYS:HE3  | 10                  | 0.29     | 0.01                | 0.29       |
| (2,127) | 1:13:A:LYS:HB2 | 1:13:A:LYS:HE2  | 10                  | 0.29     | 0.01                | 0.29       |
| (2,127) | 1:13:A:LYS:HB3 | 1:13:A:LYS:HE2  | 10                  | 0.29     | 0.01                | 0.29       |
| (2,127) | 1:13:A:LYS:HB3 | 1:13:A:LYS:HE3  | 10                  | 0.29     | 0.01                | 0.29       |
| (1,310) | 1:8:A:TYR:HE1  | 1:12:A:LEU:HG   | 10                  | 0.28     | 0.07                | 0.29       |
| (1,310) | 1:8:A:TYR:HE2  | 1:12:A:LEU:HG   | 10                  | 0.28     | 0.07                | 0.29       |
| (3,25)  | 1:8:A:TYR:HE1  | 1:12:A:LEU:HG   | 10                  | 0.28     | 0.07                | 0.29       |
| (3,25)  | 1:8:A:TYR:HE2  | 1:12:A:LEU:HG   | 10                  | 0.28     | 0.07                | 0.29       |
| (1,321) | 1:8:A:TYR:HE1  | 1:12:A:LEU:HD21 | 10                  | 0.27     | 0.06                | 0.3        |
| (1,321) | 1:8:A:TYR:HE1  | 1:12:A:LEU:HD22 | 10                  | 0.27     | 0.06                | 0.3        |
| (1,321) | 1:8:A:TYR:HE1  | 1:12:A:LEU:HD23 | 10                  | 0.27     | 0.06                | 0.3        |
| (1,321) | 1:8:A:TYR:HE2  | 1:12:A:LEU:HD21 | 10                  | 0.27     | 0.06                | 0.3        |
| (1,321) | 1:8:A:TYR:HE2  | 1:12:A:LEU:HD22 | 10                  | 0.27     | 0.06                | 0.3        |
| (1,321) | 1:8:A:TYR:HE2  | 1:12:A:LEU:HD23 | 10                  | 0.27     | 0.06                | 0.3        |
| (3,31)  | 1:8:A:TYR:HE1  | 1:12:A:LEU:HD21 | 10                  | 0.27     | 0.06                | 0.3        |
| (3,31)  | 1:8:A:TYR:HE1  | 1:12:A:LEU:HD22 | 10                  | 0.27     | 0.06                | 0.3        |
| (3,31)  | 1:8:A:TYR:HE1  | 1:12:A:LEU:HD23 | 10                  | 0.27     | 0.06                | 0.3        |
| (3,31)  | 1:8:A:TYR:HE2  | 1:12:A:LEU:HD21 | 10                  | 0.27     | 0.06                | 0.3        |
| (3,31)  | 1:8:A:TYR:HE2  | 1:12:A:LEU:HD22 | 10                  | 0.27     | 0.06                | 0.3        |
| (3,31)  | 1:8:A:TYR:HE2  | 1:12:A:LEU:HD23 | 10                  | 0.27     | 0.06                | 0.3        |
| (1,570) | 1:7:A:LEU:HA   | 1:8:A:TYR:H     | 10                  | 0.27     | 0.01                | 0.27       |
| (3,85)  | 1:7:A:LEU:HA   | 1:8:A:TYR:H     | 10                  | 0.27     | 0.01                | 0.27       |
| (1,421) | 1:14:A:ASP:H   | 1:15:A:GLY:HA2  | 10                  | 0.27     | 0.01                | 0.26       |
| (3,53)  | 1:14:A:ASP:H   | 1:15:A:GLY:HA2  | 10                  | 0.27     | 0.01                | 0.26       |
| (1,555) | 1:7:A:LEU:HD21 | 1:10:A:GLN:HB3  | 10                  | 0.27     | 0.02                | 0.26       |
| (1,555) | 1:7:A:LEU:HD22 | 1:10:A:GLN:HB3  | 10                  | 0.27     | 0.02                | 0.26       |
| (1,555) | 1:7:A:LEU:HD23 | 1:10:A:GLN:HB3  | 10                  | 0.27     | 0.02                | 0.26       |
| (3,79)  | 1:7:A:LEU:HD21 | 1:10:A:GLN:HB3  | 10                  | 0.27     | 0.02                | 0.26       |
| (3,79)  | 1:7:A:LEU:HD22 | 1:10:A:GLN:HB3  | 10                  | 0.27     | 0.02                | 0.26       |
| (3,79)  | 1:7:A:LEU:HD23 | 1:10:A:GLN:HB3  | 10                  | 0.27     | 0.02                | 0.26       |
| (1,401) | 1:9:A:ILE:H    | 1:9:A:ILE:HG12  | 10                  | 0.27     | 0.0                 | 0.27       |
| (3,49)  | 1:9:A:ILE:H    | 1:9:A:ILE:HG12  | 10                  | 0.27     | 0.0                 | 0.27       |
| (1,296) | 1:8:A:TYR:HB2  | 1:8:A:TYR:HE1   | 10                  | 0.26     | 0.02                | 0.25       |
| (1,296) | 1:8:A:TYR:HB2  | 1:8:A:TYR:HE2   | 10                  | 0.26     | 0.02                | 0.25       |
| (3,22)  | 1:8:A:TYR:HB2  | 1:8:A:TYR:HE1   | 10                  | 0.26     | 0.02                | 0.25       |
| (3,22)  | 1:8:A:TYR:HB2  | 1:8:A:TYR:HE2   | 10                  | 0.26     | 0.02                | 0.25       |
| (1,287) | 1:8:A:TYR:HA   | 1:8:A:TYR:HE1   | 10                  | 0.25     | 0.06                | 0.27       |
| (1,287) | 1:8:A:TYR:HA   | 1:8:A:TYR:HE2   | 10                  | 0.25     | 0.06                | 0.27       |
| (3,20)  | 1:8:A:TYR:HA   | 1:8:A:TYR:HE1   | 10                  | 0.25     | 0.06                | 0.27       |
| (3,20)  | 1:8:A:TYR:HA   | 1:8:A:TYR:HE2   | 10                  | 0.25     | 0.06                | 0.27       |
| (1,558) | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD11  | 10                  | 0.24     | 0.05                | 0.26       |

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| Key     | Atom-1         | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,558) | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD12  | 10                  | 0.24     | 0.05                | 0.26       |
| (1,558) | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD13  | 10                  | 0.24     | 0.05                | 0.26       |
| (1,558) | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD11  | 10                  | 0.24     | 0.05                | 0.26       |
| (1,558) | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD12  | 10                  | 0.24     | 0.05                | 0.26       |
| (1,558) | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD13  | 10                  | 0.24     | 0.05                | 0.26       |
| (1,558) | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD11  | 10                  | 0.24     | 0.05                | 0.26       |
| (1,558) | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD12  | 10                  | 0.24     | 0.05                | 0.26       |
| (1,558) | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD13  | 10                  | 0.24     | 0.05                | 0.26       |
| (3,80)  | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD11  | 10                  | 0.24     | 0.05                | 0.26       |
| (3,80)  | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD12  | 10                  | 0.24     | 0.05                | 0.26       |
| (3,80)  | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD13  | 10                  | 0.24     | 0.05                | 0.26       |
| (3,80)  | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD11  | 10                  | 0.24     | 0.05                | 0.26       |
| (3,80)  | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD12  | 10                  | 0.24     | 0.05                | 0.26       |
| (3,80)  | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD13  | 10                  | 0.24     | 0.05                | 0.26       |
| (3,80)  | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD11  | 10                  | 0.24     | 0.05                | 0.26       |
| (3,80)  | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD12  | 10                  | 0.24     | 0.05                | 0.26       |
| (3,80)  | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD13  | 10                  | 0.24     | 0.05                | 0.26       |
| (1,179) | 1:17:A:PRO:HB3 | 1:17:A:PRO:HD2  | 10                  | 0.23     | 0.04                | 0.24       |
| (2,164) | 1:17:A:PRO:HB3 | 1:17:A:PRO:HD2  | 10                  | 0.23     | 0.04                | 0.24       |
| (1,447) | 1:6:A:ARG:H    | 1:7:A:LEU:HD11  | 10                  | 0.22     | 0.03                | 0.21       |
| (1,447) | 1:6:A:ARG:H    | 1:7:A:LEU:HD12  | 10                  | 0.22     | 0.03                | 0.21       |
| (1,447) | 1:6:A:ARG:H    | 1:7:A:LEU:HD13  | 10                  | 0.22     | 0.03                | 0.21       |
| (3,62)  | 1:6:A:ARG:H    | 1:7:A:LEU:HD11  | 10                  | 0.22     | 0.03                | 0.21       |
| (3,62)  | 1:6:A:ARG:H    | 1:7:A:LEU:HD12  | 10                  | 0.22     | 0.03                | 0.21       |
| (3,62)  | 1:6:A:ARG:H    | 1:7:A:LEU:HD13  | 10                  | 0.22     | 0.03                | 0.21       |
| (1,437) | 1:13:A:LYS:HD2 | 1:14:A:ASP:H    | 10                  | 0.22     | 0.03                | 0.22       |
| (1,437) | 1:13:A:LYS:HD3 | 1:14:A:ASP:H    | 10                  | 0.22     | 0.03                | 0.22       |
| (3,58)  | 1:13:A:LYS:HD2 | 1:14:A:ASP:H    | 10                  | 0.22     | 0.03                | 0.22       |
| (3,58)  | 1:13:A:LYS:HD3 | 1:14:A:ASP:H    | 10                  | 0.22     | 0.03                | 0.22       |
| (1,329) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD21 | 10                  | 0.21     | 0.02                | 0.21       |
| (1,329) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD22 | 10                  | 0.21     | 0.02                | 0.21       |
| (1,329) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD23 | 10                  | 0.21     | 0.02                | 0.21       |
| (3,33)  | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD21 | 10                  | 0.21     | 0.02                | 0.21       |
| (3,33)  | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD22 | 10                  | 0.21     | 0.02                | 0.21       |
| (3,33)  | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD23 | 10                  | 0.21     | 0.02                | 0.21       |
| (1,480) | 1:6:A:ARG:HA   | 1:10:A:GLN:HB2  | 10                  | 0.2      | 0.06                | 0.18       |
| (3,64)  | 1:6:A:ARG:HA   | 1:10:A:GLN:HB2  | 10                  | 0.2      | 0.06                | 0.18       |
| (1,552) | 1:3:A:GLU:HG2  | 1:7:A:LEU:HD11  | 10                  | 0.2      | 0.07                | 0.2        |
| (1,552) | 1:3:A:GLU:HG2  | 1:7:A:LEU:HD12  | 10                  | 0.2      | 0.07                | 0.2        |
| (1,552) | 1:3:A:GLU:HG2  | 1:7:A:LEU:HD13  | 10                  | 0.2      | 0.07                | 0.2        |
| (1,552) | 1:3:A:GLU:HG3  | 1:7:A:LEU:HD11  | 10                  | 0.2      | 0.07                | 0.2        |
| (1,552) | 1:3:A:GLU:HG3  | 1:7:A:LEU:HD12  | 10                  | 0.2      | 0.07                | 0.2        |

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| Key     | Atom-1         | Atom-2         | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|----------------|----------------|---------------------|----------|---------------------|------------|
| (1,552) | 1:3:A:GLU:HG3  | 1:7:A:LEU:HD13 | 10                  | 0.2      | 0.07                | 0.2        |
| (3,77)  | 1:3:A:GLU:HG2  | 1:7:A:LEU:HD11 | 10                  | 0.2      | 0.07                | 0.2        |
| (3,77)  | 1:3:A:GLU:HG2  | 1:7:A:LEU:HD12 | 10                  | 0.2      | 0.07                | 0.2        |
| (3,77)  | 1:3:A:GLU:HG2  | 1:7:A:LEU:HD13 | 10                  | 0.2      | 0.07                | 0.2        |
| (3,77)  | 1:3:A:GLU:HG3  | 1:7:A:LEU:HD11 | 10                  | 0.2      | 0.07                | 0.2        |
| (3,77)  | 1:3:A:GLU:HG3  | 1:7:A:LEU:HD12 | 10                  | 0.2      | 0.07                | 0.2        |
| (3,77)  | 1:3:A:GLU:HG3  | 1:7:A:LEU:HD13 | 10                  | 0.2      | 0.07                | 0.2        |
| (1,539) | 1:2:A:GLU:HG2  | 1:5:A:VAL:HG21 | 10                  | 0.2      | 0.05                | 0.19       |
| (1,539) | 1:2:A:GLU:HG2  | 1:5:A:VAL:HG22 | 10                  | 0.2      | 0.05                | 0.19       |
| (1,539) | 1:2:A:GLU:HG2  | 1:5:A:VAL:HG23 | 10                  | 0.2      | 0.05                | 0.19       |
| (1,539) | 1:2:A:GLU:HG3  | 1:5:A:VAL:HG21 | 10                  | 0.2      | 0.05                | 0.19       |
| (1,539) | 1:2:A:GLU:HG3  | 1:5:A:VAL:HG22 | 10                  | 0.2      | 0.05                | 0.19       |
| (1,539) | 1:2:A:GLU:HG3  | 1:5:A:VAL:HG23 | 10                  | 0.2      | 0.05                | 0.19       |
| (3,73)  | 1:2:A:GLU:HG2  | 1:5:A:VAL:HG21 | 10                  | 0.2      | 0.05                | 0.19       |
| (3,73)  | 1:2:A:GLU:HG2  | 1:5:A:VAL:HG22 | 10                  | 0.2      | 0.05                | 0.19       |
| (3,73)  | 1:2:A:GLU:HG2  | 1:5:A:VAL:HG23 | 10                  | 0.2      | 0.05                | 0.19       |
| (3,73)  | 1:2:A:GLU:HG3  | 1:5:A:VAL:HG21 | 10                  | 0.2      | 0.05                | 0.19       |
| (3,73)  | 1:2:A:GLU:HG3  | 1:5:A:VAL:HG22 | 10                  | 0.2      | 0.05                | 0.19       |
| (3,73)  | 1:2:A:GLU:HG3  | 1:5:A:VAL:HG23 | 10                  | 0.2      | 0.05                | 0.19       |
| (1,532) | 1:5:A:VAL:HG11 | 1:8:A:TYR:HB2  | 10                  | 0.2      | 0.02                | 0.2        |
| (1,532) | 1:5:A:VAL:HG12 | 1:8:A:TYR:HB2  | 10                  | 0.2      | 0.02                | 0.2        |
| (1,532) | 1:5:A:VAL:HG13 | 1:8:A:TYR:HB2  | 10                  | 0.2      | 0.02                | 0.2        |
| (2,461) | 1:5:A:VAL:HG11 | 1:8:A:TYR:HB2  | 10                  | 0.2      | 0.02                | 0.2        |
| (2,461) | 1:5:A:VAL:HG12 | 1:8:A:TYR:HB2  | 10                  | 0.2      | 0.02                | 0.2        |
| (2,461) | 1:5:A:VAL:HG13 | 1:8:A:TYR:HB2  | 10                  | 0.2      | 0.02                | 0.2        |
| (1,411) | 1:5:A:VAL:HG21 | 1:7:A:LEU:H    | 10                  | 0.19     | 0.03                | 0.18       |
| (1,411) | 1:5:A:VAL:HG22 | 1:7:A:LEU:H    | 10                  | 0.19     | 0.03                | 0.18       |
| (1,411) | 1:5:A:VAL:HG23 | 1:7:A:LEU:H    | 10                  | 0.19     | 0.03                | 0.18       |
| (2,360) | 1:5:A:VAL:HG21 | 1:7:A:LEU:H    | 10                  | 0.19     | 0.03                | 0.18       |
| (2,360) | 1:5:A:VAL:HG22 | 1:7:A:LEU:H    | 10                  | 0.19     | 0.03                | 0.18       |
| (2,360) | 1:5:A:VAL:HG23 | 1:7:A:LEU:H    | 10                  | 0.19     | 0.03                | 0.18       |
| (1,315) | 1:4:A:ALA:HB1  | 1:8:A:TYR:HE1  | 10                  | 0.18     | 0.04                | 0.18       |
| (1,315) | 1:4:A:ALA:HB1  | 1:8:A:TYR:HE2  | 10                  | 0.18     | 0.04                | 0.18       |
| (1,315) | 1:4:A:ALA:HB2  | 1:8:A:TYR:HE1  | 10                  | 0.18     | 0.04                | 0.18       |
| (1,315) | 1:4:A:ALA:HB2  | 1:8:A:TYR:HE2  | 10                  | 0.18     | 0.04                | 0.18       |
| (1,315) | 1:4:A:ALA:HB3  | 1:8:A:TYR:HE1  | 10                  | 0.18     | 0.04                | 0.18       |
| (1,315) | 1:4:A:ALA:HB3  | 1:8:A:TYR:HE2  | 10                  | 0.18     | 0.04                | 0.18       |
| (3,28)  | 1:4:A:ALA:HB1  | 1:8:A:TYR:HE1  | 10                  | 0.18     | 0.04                | 0.18       |
| (3,28)  | 1:4:A:ALA:HB1  | 1:8:A:TYR:HE2  | 10                  | 0.18     | 0.04                | 0.18       |
| (3,28)  | 1:4:A:ALA:HB2  | 1:8:A:TYR:HE1  | 10                  | 0.18     | 0.04                | 0.18       |
| (3,28)  | 1:4:A:ALA:HB2  | 1:8:A:TYR:HE2  | 10                  | 0.18     | 0.04                | 0.18       |
| (3,28)  | 1:4:A:ALA:HB3  | 1:8:A:TYR:HE1  | 10                  | 0.18     | 0.04                | 0.18       |

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| Key     | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (3,28)  | 1:4:A:ALA:HB3   | 1:8:A:TYR:HE2   | 10                  | 0.18     | 0.04                | 0.18       |
| (1,601) | 1:10:A:GLN:HA   | 1:13:A:LYS:H    | 10                  | 0.18     | 0.04                | 0.18       |
| (3,93)  | 1:10:A:GLN:HA   | 1:13:A:LYS:H    | 10                  | 0.18     | 0.04                | 0.18       |
| (1,569) | 1:3:A:GLU:HA    | 1:7:A:LEU:H     | 10                  | 0.18     | 0.08                | 0.15       |
| (3,84)  | 1:3:A:GLU:HA    | 1:7:A:LEU:H     | 10                  | 0.18     | 0.08                | 0.15       |
| (1,357) | 1:11:A:TRP:HA   | 1:11:A:TRP:HE3  | 10                  | 0.17     | 0.02                | 0.18       |
| (3,40)  | 1:11:A:TRP:HA   | 1:11:A:TRP:HE3  | 10                  | 0.17     | 0.02                | 0.18       |
| (1,119) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD11 | 10                  | 0.15     | 0.01                | 0.15       |
| (1,119) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD12 | 10                  | 0.15     | 0.01                | 0.15       |
| (1,119) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD13 | 10                  | 0.15     | 0.01                | 0.15       |
| (3,11)  | 1:12:A:LEU:HA   | 1:12:A:LEU:HD11 | 10                  | 0.15     | 0.01                | 0.15       |
| (3,11)  | 1:12:A:LEU:HA   | 1:12:A:LEU:HD12 | 10                  | 0.15     | 0.01                | 0.15       |
| (3,11)  | 1:12:A:LEU:HA   | 1:12:A:LEU:HD13 | 10                  | 0.15     | 0.01                | 0.15       |
| (1,529) | 1:12:A:LEU:HD11 | 1:17:A:PRO:HD2  | 10                  | 0.15     | 0.02                | 0.15       |
| (1,529) | 1:12:A:LEU:HD12 | 1:17:A:PRO:HD2  | 10                  | 0.15     | 0.02                | 0.15       |
| (1,529) | 1:12:A:LEU:HD13 | 1:17:A:PRO:HD2  | 10                  | 0.15     | 0.02                | 0.15       |
| (3,71)  | 1:12:A:LEU:HD11 | 1:17:A:PRO:HD2  | 10                  | 0.15     | 0.02                | 0.15       |
| (3,71)  | 1:12:A:LEU:HD12 | 1:17:A:PRO:HD2  | 10                  | 0.15     | 0.02                | 0.15       |
| (3,71)  | 1:12:A:LEU:HD13 | 1:17:A:PRO:HD2  | 10                  | 0.15     | 0.02                | 0.15       |
| (1,183) | 1:17:A:PRO:HB3  | 1:17:A:PRO:HG2  | 10                  | 0.14     | 0.01                | 0.14       |
| (1,183) | 1:17:A:PRO:HB3  | 1:17:A:PRO:HG3  | 10                  | 0.14     | 0.01                | 0.14       |
| (2,168) | 1:17:A:PRO:HB3  | 1:17:A:PRO:HG2  | 10                  | 0.14     | 0.01                | 0.14       |
| (2,168) | 1:17:A:PRO:HB3  | 1:17:A:PRO:HG3  | 10                  | 0.14     | 0.01                | 0.14       |
| (1,474) | 1:5:A:VAL:HA    | 1:8:A:TYR:HB2   | 10                  | 0.14     | 0.01                | 0.14       |
| (3,63)  | 1:5:A:VAL:HA    | 1:8:A:TYR:HB2   | 10                  | 0.14     | 0.01                | 0.14       |
| (1,1)   | 1:2:A:GLU:HA    | 1:3:A:GLU:H     | 10                  | 0.14     | 0.03                | 0.13       |
| (2,1)   | 1:2:A:GLU:HA    | 1:3:A:GLU:H     | 10                  | 0.14     | 0.03                | 0.13       |
| (1,81)  | 1:8:A:TYR:HA    | 1:9:A:ILE:H     | 10                  | 0.13     | 0.01                | 0.13       |
| (3,8)   | 1:8:A:TYR:HA    | 1:9:A:ILE:H     | 10                  | 0.13     | 0.01                | 0.13       |
| (1,383) | 1:11:A:TRP:HH2  | 1:11:A:TRP:HZ3  | 10                  | 0.13     | 0.0                 | 0.13       |
| (3,45)  | 1:11:A:TRP:HH2  | 1:11:A:TRP:HZ3  | 10                  | 0.13     | 0.0                 | 0.13       |
| (1,526) | 1:5:A:VAL:HA    | 1:9:A:ILE:HD11  | 10                  | 0.12     | 0.01                | 0.12       |
| (1,526) | 1:5:A:VAL:HA    | 1:9:A:ILE:HD12  | 10                  | 0.12     | 0.01                | 0.12       |
| (1,526) | 1:5:A:VAL:HA    | 1:9:A:ILE:HD13  | 10                  | 0.12     | 0.01                | 0.12       |
| (2,456) | 1:5:A:VAL:HA    | 1:9:A:ILE:HD11  | 10                  | 0.12     | 0.01                | 0.12       |
| (2,456) | 1:5:A:VAL:HA    | 1:9:A:ILE:HD12  | 10                  | 0.12     | 0.01                | 0.12       |
| (2,456) | 1:5:A:VAL:HA    | 1:9:A:ILE:HD13  | 10                  | 0.12     | 0.01                | 0.12       |
| (1,349) | 1:11:A:TRP:HE3  | 1:12:A:LEU:HA   | 10                  | 0.12     | 0.01                | 0.12       |
| (2,312) | 1:11:A:TRP:HE3  | 1:12:A:LEU:HA   | 10                  | 0.12     | 0.01                | 0.12       |
| (1,476) | 1:16:A:GLY:HA2  | 1:17:A:PRO:HD2  | 9                   | 0.57     | 0.02                | 0.56       |
| (2,413) | 1:16:A:GLY:HA2  | 1:17:A:PRO:HD2  | 9                   | 0.57     | 0.02                | 0.56       |
| (1,486) | 1:16:A:GLY:HA2  | 1:17:A:PRO:HD3  | 9                   | 0.5      | 0.03                | 0.48       |

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| Key     | Atom-1         | Atom-2         | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|----------------|----------------|---------------------|----------|---------------------|------------|
| (2,421) | 1:16:A:GLY:HA2 | 1:17:A:PRO:HD3 | 9                   | 0.5      | 0.03                | 0.48       |
| (1,104) | 1:10:A:GLN:H   | 1:10:A:GLN:HG2 | 9                   | 0.26     | 0.05                | 0.27       |
| (1,104) | 1:10:A:GLN:H   | 1:10:A:GLN:HG3 | 9                   | 0.26     | 0.05                | 0.27       |
| (2,94)  | 1:10:A:GLN:H   | 1:10:A:GLN:HG2 | 9                   | 0.26     | 0.05                | 0.27       |
| (2,94)  | 1:10:A:GLN:H   | 1:10:A:GLN:HG3 | 9                   | 0.26     | 0.05                | 0.27       |
| (1,354) | 1:11:A:TRP:HH2 | 1:17:A:PRO:HD2 | 9                   | 0.25     | 0.01                | 0.25       |
| (3,39)  | 1:11:A:TRP:HH2 | 1:17:A:PRO:HD2 | 9                   | 0.25     | 0.01                | 0.25       |
| (1,303) | 1:8:A:TYR:HD1  | 1:24:A:PRO:HB3 | 9                   | 0.16     | 0.02                | 0.17       |
| (1,303) | 1:8:A:TYR:HD2  | 1:24:A:PRO:HB3 | 9                   | 0.16     | 0.02                | 0.17       |
| (2,280) | 1:8:A:TYR:HD1  | 1:24:A:PRO:HB3 | 9                   | 0.16     | 0.02                | 0.17       |
| (2,280) | 1:8:A:TYR:HD2  | 1:24:A:PRO:HB3 | 9                   | 0.16     | 0.02                | 0.17       |
| (1,308) | 1:11:A:TRP:HD1 | 1:21:A:ARG:HG2 | 8                   | 0.26     | 0.06                | 0.27       |
| (1,308) | 1:11:A:TRP:HD1 | 1:21:A:ARG:HG3 | 8                   | 0.26     | 0.06                | 0.27       |
| (3,24)  | 1:11:A:TRP:HD1 | 1:21:A:ARG:HG2 | 8                   | 0.26     | 0.06                | 0.27       |
| (3,24)  | 1:11:A:TRP:HD1 | 1:21:A:ARG:HG3 | 8                   | 0.26     | 0.06                | 0.27       |
| (1,138) | 1:13:A:LYS:HA  | 1:13:A:LYS:HD2 | 8                   | 0.24     | 0.02                | 0.24       |
| (1,138) | 1:13:A:LYS:HA  | 1:13:A:LYS:HD3 | 8                   | 0.24     | 0.02                | 0.24       |
| (3,14)  | 1:13:A:LYS:HA  | 1:13:A:LYS:HD2 | 8                   | 0.24     | 0.02                | 0.24       |
| (3,14)  | 1:13:A:LYS:HA  | 1:13:A:LYS:HD3 | 8                   | 0.24     | 0.02                | 0.24       |
| (1,413) | 1:7:A:LEU:HD21 | 1:8:A:TYR:H    | 8                   | 0.21     | 0.01                | 0.2        |
| (1,413) | 1:7:A:LEU:HD22 | 1:8:A:TYR:H    | 8                   | 0.21     | 0.01                | 0.2        |
| (1,413) | 1:7:A:LEU:HD23 | 1:8:A:TYR:H    | 8                   | 0.21     | 0.01                | 0.2        |
| (2,362) | 1:7:A:LEU:HD21 | 1:8:A:TYR:H    | 8                   | 0.21     | 0.01                | 0.2        |
| (2,362) | 1:7:A:LEU:HD22 | 1:8:A:TYR:H    | 8                   | 0.21     | 0.01                | 0.2        |
| (2,362) | 1:7:A:LEU:HD23 | 1:8:A:TYR:H    | 8                   | 0.21     | 0.01                | 0.2        |
| (1,218) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HG2 | 8                   | 0.16     | 0.01                | 0.16       |
| (1,218) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HG3 | 8                   | 0.16     | 0.01                | 0.16       |
| (2,201) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HG2 | 8                   | 0.16     | 0.01                | 0.16       |
| (2,201) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HG3 | 8                   | 0.16     | 0.01                | 0.16       |
| (1,370) | 1:4:A:ALA:H    | 1:5:A:VAL:H    | 8                   | 0.14     | 0.02                | 0.14       |
| (3,41)  | 1:4:A:ALA:H    | 1:5:A:VAL:H    | 8                   | 0.14     | 0.02                | 0.14       |
| (1,445) | 1:9:A:ILE:HG21 | 1:10:A:GLN:H   | 8                   | 0.14     | 0.02                | 0.14       |
| (1,445) | 1:9:A:ILE:HG22 | 1:10:A:GLN:H   | 8                   | 0.14     | 0.02                | 0.14       |
| (1,445) | 1:9:A:ILE:HG23 | 1:10:A:GLN:H   | 8                   | 0.14     | 0.02                | 0.14       |
| (2,385) | 1:9:A:ILE:HG21 | 1:10:A:GLN:H   | 8                   | 0.14     | 0.02                | 0.14       |
| (2,385) | 1:9:A:ILE:HG22 | 1:10:A:GLN:H   | 8                   | 0.14     | 0.02                | 0.14       |
| (2,385) | 1:9:A:ILE:HG23 | 1:10:A:GLN:H   | 8                   | 0.14     | 0.02                | 0.14       |
| (1,547) | 1:5:A:VAL:HG11 | 1:9:A:ILE:HG13 | 8                   | 0.12     | 0.01                | 0.12       |
| (1,547) | 1:5:A:VAL:HG12 | 1:9:A:ILE:HG13 | 8                   | 0.12     | 0.01                | 0.12       |
| (1,547) | 1:5:A:VAL:HG13 | 1:9:A:ILE:HG13 | 8                   | 0.12     | 0.01                | 0.12       |
| (2,471) | 1:5:A:VAL:HG11 | 1:9:A:ILE:HG13 | 8                   | 0.12     | 0.01                | 0.12       |
| (2,471) | 1:5:A:VAL:HG12 | 1:9:A:ILE:HG13 | 8                   | 0.12     | 0.01                | 0.12       |

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| Key     | Atom-1         | Atom-2         | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|----------------|----------------|---------------------|----------|---------------------|------------|
| (2,471) | 1:5:A:VAL:HG13 | 1:9:A:ILE:HG13 | 8                   | 0.12     | 0.01                | 0.12       |
| (1,585) | 1:1:A:GLU:HB3  | 1:2:A:GLU:HG2  | 7                   | 0.92     | 0.16                | 0.99       |
| (2,496) | 1:1:A:GLU:HB3  | 1:2:A:GLU:HG2  | 7                   | 0.92     | 0.16                | 0.99       |
| (1,550) | 1:9:A:ILE:HD11 | 1:13:A:LYS:HE3 | 7                   | 0.53     | 0.66                | 0.11       |
| (1,550) | 1:9:A:ILE:HD12 | 1:13:A:LYS:HE3 | 7                   | 0.53     | 0.66                | 0.11       |
| (1,550) | 1:9:A:ILE:HD13 | 1:13:A:LYS:HE3 | 7                   | 0.53     | 0.66                | 0.11       |
| (2,474) | 1:9:A:ILE:HD11 | 1:13:A:LYS:HE3 | 7                   | 0.53     | 0.66                | 0.11       |
| (2,474) | 1:9:A:ILE:HD12 | 1:13:A:LYS:HE3 | 7                   | 0.53     | 0.66                | 0.11       |
| (2,474) | 1:9:A:ILE:HD13 | 1:13:A:LYS:HE3 | 7                   | 0.53     | 0.66                | 0.11       |
| (1,301) | 1:11:A:TRP:HD1 | 1:23:A:PRO:HA  | 7                   | 0.12     | 0.01                | 0.12       |
| (2,278) | 1:11:A:TRP:HD1 | 1:23:A:PRO:HA  | 7                   | 0.12     | 0.01                | 0.12       |
| (1,466) | 1:11:A:TRP:HA  | 1:14:A:ASP:HB3 | 6                   | 0.59     | 0.21                | 0.68       |
| (2,404) | 1:11:A:TRP:HA  | 1:14:A:ASP:HB3 | 6                   | 0.59     | 0.21                | 0.68       |
| (1,449) | 1:24:A:PRO:HB3 | 1:25:A:SER:H   | 6                   | 0.24     | 0.02                | 0.24       |
| (2,387) | 1:24:A:PRO:HB3 | 1:25:A:SER:H   | 6                   | 0.24     | 0.02                | 0.24       |
| (1,490) | 1:22:A:PRO:HB3 | 1:23:A:PRO:HD2 | 6                   | 0.2      | 0.02                | 0.2        |
| (1,490) | 1:22:A:PRO:HB3 | 1:23:A:PRO:HD3 | 6                   | 0.2      | 0.02                | 0.2        |
| (3,66)  | 1:22:A:PRO:HB3 | 1:23:A:PRO:HD2 | 6                   | 0.2      | 0.02                | 0.2        |
| (3,66)  | 1:22:A:PRO:HB3 | 1:23:A:PRO:HD3 | 6                   | 0.2      | 0.02                | 0.2        |
| (1,521) | 1:6:A:ARG:HA   | 1:9:A:ILE:HG21 | 6                   | 0.16     | 0.06                | 0.12       |
| (1,521) | 1:6:A:ARG:HA   | 1:9:A:ILE:HG22 | 6                   | 0.16     | 0.06                | 0.12       |
| (1,521) | 1:6:A:ARG:HA   | 1:9:A:ILE:HG23 | 6                   | 0.16     | 0.06                | 0.12       |
| (3,70)  | 1:6:A:ARG:HA   | 1:9:A:ILE:HG21 | 6                   | 0.16     | 0.06                | 0.12       |
| (3,70)  | 1:6:A:ARG:HA   | 1:9:A:ILE:HG22 | 6                   | 0.16     | 0.06                | 0.12       |
| (3,70)  | 1:6:A:ARG:HA   | 1:9:A:ILE:HG23 | 6                   | 0.16     | 0.06                | 0.12       |
| (1,540) | 1:2:A:GLU:HB3  | 1:5:A:VAL:HG11 | 6                   | 0.12     | 0.02                | 0.12       |
| (1,540) | 1:2:A:GLU:HB3  | 1:5:A:VAL:HG12 | 6                   | 0.12     | 0.02                | 0.12       |
| (1,540) | 1:2:A:GLU:HB3  | 1:5:A:VAL:HG13 | 6                   | 0.12     | 0.02                | 0.12       |
| (2,467) | 1:2:A:GLU:HB3  | 1:5:A:VAL:HG11 | 6                   | 0.12     | 0.02                | 0.12       |
| (2,467) | 1:2:A:GLU:HB3  | 1:5:A:VAL:HG12 | 6                   | 0.12     | 0.02                | 0.12       |
| (2,467) | 1:2:A:GLU:HB3  | 1:5:A:VAL:HG13 | 6                   | 0.12     | 0.02                | 0.12       |
| (1,568) | 1:16:A:GLY:H   | 1:19:A:SER:HB3 | 5                   | 0.62     | 0.27                | 0.72       |
| (2,485) | 1:16:A:GLY:H   | 1:19:A:SER:HB3 | 5                   | 0.62     | 0.27                | 0.72       |
| (1,157) | 1:14:A:ASP:H   | 1:14:A:ASP:HB3 | 5                   | 0.45     | 0.17                | 0.53       |
| (2,142) | 1:14:A:ASP:H   | 1:14:A:ASP:HB3 | 5                   | 0.45     | 0.17                | 0.53       |
| (1,293) | 1:11:A:TRP:HD1 | 1:19:A:SER:HB3 | 5                   | 0.19     | 0.05                | 0.2        |
| (2,272) | 1:11:A:TRP:HD1 | 1:19:A:SER:HB3 | 5                   | 0.19     | 0.05                | 0.2        |
| (1,290) | 1:5:A:VAL:HA   | 1:8:A:TYR:HE1  | 5                   | 0.13     | 0.01                | 0.14       |
| (1,290) | 1:5:A:VAL:HA   | 1:8:A:TYR:HE2  | 5                   | 0.13     | 0.01                | 0.14       |
| (2,270) | 1:5:A:VAL:HA   | 1:8:A:TYR:HE1  | 5                   | 0.13     | 0.01                | 0.14       |
| (2,270) | 1:5:A:VAL:HA   | 1:8:A:TYR:HE2  | 5                   | 0.13     | 0.01                | 0.14       |
| (1,493) | 1:21:A:ARG:HG2 | 1:22:A:PRO:HD3 | 5                   | 0.12     | 0.01                | 0.12       |

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| Key     | Atom-1         | Atom-2         | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|----------------|----------------|---------------------|----------|---------------------|------------|
| (1,493) | 1:21:A:ARG:HG3 | 1:22:A:PRO:HD3 | 5                   | 0.12     | 0.01                | 0.12       |
| (2,426) | 1:21:A:ARG:HG2 | 1:22:A:PRO:HD3 | 5                   | 0.12     | 0.01                | 0.12       |
| (2,426) | 1:21:A:ARG:HG3 | 1:22:A:PRO:HD3 | 5                   | 0.12     | 0.01                | 0.12       |
| (1,443) | 1:5:A:VAL:HG21 | 1:6:A:ARG:H    | 5                   | 0.11     | 0.0                 | 0.11       |
| (1,443) | 1:5:A:VAL:HG22 | 1:6:A:ARG:H    | 5                   | 0.11     | 0.0                 | 0.11       |
| (1,443) | 1:5:A:VAL:HG23 | 1:6:A:ARG:H    | 5                   | 0.11     | 0.0                 | 0.11       |
| (2,384) | 1:5:A:VAL:HG21 | 1:6:A:ARG:H    | 5                   | 0.11     | 0.0                 | 0.11       |
| (2,384) | 1:5:A:VAL:HG22 | 1:6:A:ARG:H    | 5                   | 0.11     | 0.0                 | 0.11       |
| (2,384) | 1:5:A:VAL:HG23 | 1:6:A:ARG:H    | 5                   | 0.11     | 0.0                 | 0.11       |
| (1,238) | 1:22:A:PRO:HB3 | 1:22:A:PRO:HD3 | 4                   | 0.7      | 0.01                | 0.7        |
| (2,219) | 1:22:A:PRO:HB3 | 1:22:A:PRO:HD3 | 4                   | 0.7      | 0.01                | 0.7        |
| (1,485) | 1:21:A:ARG:HB2 | 1:22:A:PRO:HD2 | 4                   | 0.68     | 0.2                 | 0.68       |
| (2,420) | 1:21:A:ARG:HB2 | 1:22:A:PRO:HD2 | 4                   | 0.68     | 0.2                 | 0.68       |
| (1,448) | 1:23:A:PRO:HB3 | 1:25:A:SER:H   | 4                   | 0.41     | 0.27                | 0.33       |
| (2,386) | 1:23:A:PRO:HB3 | 1:25:A:SER:H   | 4                   | 0.41     | 0.27                | 0.33       |
| (1,477) | 1:14:A:ASP:HB2 | 1:19:A:SER:HB2 | 4                   | 0.18     | 0.04                | 0.18       |
| (2,414) | 1:14:A:ASP:HB2 | 1:19:A:SER:HB2 | 4                   | 0.18     | 0.04                | 0.18       |
| (1,306) | 1:11:A:TRP:HD1 | 1:21:A:ARG:HB3 | 4                   | 0.18     | 0.06                | 0.18       |
| (2,283) | 1:11:A:TRP:HD1 | 1:21:A:ARG:HB3 | 4                   | 0.18     | 0.06                | 0.18       |
| (1,488) | 1:22:A:PRO:HB2 | 1:23:A:PRO:HD2 | 4                   | 0.14     | 0.01                | 0.14       |
| (1,488) | 1:22:A:PRO:HB2 | 1:23:A:PRO:HD3 | 4                   | 0.14     | 0.01                | 0.14       |
| (2,423) | 1:22:A:PRO:HB2 | 1:23:A:PRO:HD2 | 4                   | 0.14     | 0.01                | 0.14       |
| (2,423) | 1:22:A:PRO:HB2 | 1:23:A:PRO:HD3 | 4                   | 0.14     | 0.01                | 0.14       |
| (1,545) | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG11 | 4                   | 0.12     | 0.01                | 0.12       |
| (1,545) | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG12 | 4                   | 0.12     | 0.01                | 0.12       |
| (1,545) | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG13 | 4                   | 0.12     | 0.01                | 0.12       |
| (1,545) | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG11 | 4                   | 0.12     | 0.01                | 0.12       |
| (1,545) | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG12 | 4                   | 0.12     | 0.01                | 0.12       |
| (1,545) | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG13 | 4                   | 0.12     | 0.01                | 0.12       |
| (1,545) | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG11 | 4                   | 0.12     | 0.01                | 0.12       |
| (1,545) | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG12 | 4                   | 0.12     | 0.01                | 0.12       |
| (1,545) | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG13 | 4                   | 0.12     | 0.01                | 0.12       |
| (2,470) | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG11 | 4                   | 0.12     | 0.01                | 0.12       |
| (2,470) | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG12 | 4                   | 0.12     | 0.01                | 0.12       |
| (2,470) | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG13 | 4                   | 0.12     | 0.01                | 0.12       |
| (2,470) | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG11 | 4                   | 0.12     | 0.01                | 0.12       |
| (2,470) | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG12 | 4                   | 0.12     | 0.01                | 0.12       |
| (2,470) | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG13 | 4                   | 0.12     | 0.01                | 0.12       |
| (2,470) | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG11 | 4                   | 0.12     | 0.01                | 0.12       |
| (2,470) | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG12 | 4                   | 0.12     | 0.01                | 0.12       |
| (2,470) | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG13 | 4                   | 0.12     | 0.01                | 0.12       |
| (1,282) | 1:11:A:TRP:HE1 | 1:19:A:SER:HB2 | 3                   | 0.17     | 0.05                | 0.21       |

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| Key     | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (2,263) | 1:11:A:TRP:HE1  | 1:19:A:SER:HB2  | 3                   | 0.17     | 0.05                | 0.21       |
| (1,319) | 1:8:A:TYR:HD1   | 1:12:A:LEU:HD21 | 3                   | 0.11     | 0.01                | 0.11       |
| (1,319) | 1:8:A:TYR:HD1   | 1:12:A:LEU:HD22 | 3                   | 0.11     | 0.01                | 0.11       |
| (1,319) | 1:8:A:TYR:HD1   | 1:12:A:LEU:HD23 | 3                   | 0.11     | 0.01                | 0.11       |
| (1,319) | 1:8:A:TYR:HD2   | 1:12:A:LEU:HD21 | 3                   | 0.11     | 0.01                | 0.11       |
| (1,319) | 1:8:A:TYR:HD2   | 1:12:A:LEU:HD22 | 3                   | 0.11     | 0.01                | 0.11       |
| (1,319) | 1:8:A:TYR:HD2   | 1:12:A:LEU:HD23 | 3                   | 0.11     | 0.01                | 0.11       |
| (1,344) | 1:11:A:TRP:HH2  | 1:16:A:GLY:HA2  | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,344) | 1:11:A:TRP:HZ2  | 1:16:A:GLY:HA2  | 3                   | 0.11     | 0.0                 | 0.11       |
| (2,289) | 1:8:A:TYR:HD1   | 1:12:A:LEU:HD21 | 3                   | 0.11     | 0.01                | 0.11       |
| (2,289) | 1:8:A:TYR:HD1   | 1:12:A:LEU:HD22 | 3                   | 0.11     | 0.01                | 0.11       |
| (2,289) | 1:8:A:TYR:HD1   | 1:12:A:LEU:HD23 | 3                   | 0.11     | 0.01                | 0.11       |
| (2,289) | 1:8:A:TYR:HD2   | 1:12:A:LEU:HD21 | 3                   | 0.11     | 0.01                | 0.11       |
| (2,289) | 1:8:A:TYR:HD2   | 1:12:A:LEU:HD22 | 3                   | 0.11     | 0.01                | 0.11       |
| (2,289) | 1:8:A:TYR:HD2   | 1:12:A:LEU:HD23 | 3                   | 0.11     | 0.01                | 0.11       |
| (2,308) | 1:11:A:TRP:HH2  | 1:16:A:GLY:HA2  | 3                   | 0.11     | 0.0                 | 0.11       |
| (2,308) | 1:11:A:TRP:HZ2  | 1:16:A:GLY:HA2  | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,514) | 1:7:A:LEU:HB3   | 1:24:A:PRO:HB2  | 2                   | 0.68     | 0.13                | 0.68       |
| (2,447) | 1:7:A:LEU:HB3   | 1:24:A:PRO:HB2  | 2                   | 0.68     | 0.13                | 0.68       |
| (1,57)  | 1:7:A:LEU:HA    | 1:7:A:LEU:HG    | 2                   | 0.46     | 0.01                | 0.46       |
| (3,4)   | 1:7:A:LEU:HA    | 1:7:A:LEU:HG    | 2                   | 0.46     | 0.01                | 0.46       |
| (1,214) | 1:21:A:ARG:HB3  | 1:21:A:ARG:HD2  | 2                   | 0.42     | 0.09                | 0.42       |
| (2,197) | 1:21:A:ARG:HB3  | 1:21:A:ARG:HD2  | 2                   | 0.42     | 0.09                | 0.42       |
| (1,69)  | 1:7:A:LEU:H     | 1:7:A:LEU:HB2   | 2                   | 0.4      | 0.01                | 0.4        |
| (3,6)   | 1:7:A:LEU:H     | 1:7:A:LEU:HB2   | 2                   | 0.4      | 0.01                | 0.4        |
| (1,215) | 1:21:A:ARG:HB3  | 1:21:A:ARG:HD3  | 2                   | 0.36     | 0.15                | 0.36       |
| (2,198) | 1:21:A:ARG:HB3  | 1:21:A:ARG:HD3  | 2                   | 0.36     | 0.15                | 0.36       |
| (1,197) | 1:19:A:SER:HA   | 1:19:A:SER:HB3  | 2                   | 0.36     | 0.0                 | 0.36       |
| (3,17)  | 1:19:A:SER:HA   | 1:19:A:SER:HB3  | 2                   | 0.36     | 0.0                 | 0.36       |
| (1,136) | 1:13:A:LYS:HA   | 1:13:A:LYS:HE2  | 2                   | 0.26     | 0.01                | 0.26       |
| (1,136) | 1:13:A:LYS:HA   | 1:13:A:LYS:HE3  | 2                   | 0.26     | 0.01                | 0.26       |
| (2,123) | 1:13:A:LYS:HA   | 1:13:A:LYS:HE2  | 2                   | 0.26     | 0.01                | 0.26       |
| (2,123) | 1:13:A:LYS:HA   | 1:13:A:LYS:HE3  | 2                   | 0.26     | 0.01                | 0.26       |
| (1,270) | 1:10:A:GLN:HE22 | 1:10:A:GLN:HG2  | 2                   | 0.16     | 0.01                | 0.16       |
| (1,270) | 1:10:A:GLN:HE22 | 1:10:A:GLN:HG3  | 2                   | 0.16     | 0.01                | 0.16       |
| (2,251) | 1:10:A:GLN:HE22 | 1:10:A:GLN:HG2  | 2                   | 0.16     | 0.01                | 0.16       |
| (2,251) | 1:10:A:GLN:HE22 | 1:10:A:GLN:HG3  | 2                   | 0.16     | 0.01                | 0.16       |
| (1,508) | 1:23:A:PRO:HB3  | 1:24:A:PRO:HD3  | 2                   | 0.14     | 0.02                | 0.14       |
| (1,551) | 1:7:A:LEU:HD21  | 1:10:A:GLN:HG2  | 2                   | 0.14     | 0.02                | 0.14       |
| (1,551) | 1:7:A:LEU:HD22  | 1:10:A:GLN:HG2  | 2                   | 0.14     | 0.02                | 0.14       |
| (1,551) | 1:7:A:LEU:HD23  | 1:10:A:GLN:HG2  | 2                   | 0.14     | 0.02                | 0.14       |
| (1,551) | 1:7:A:LEU:HD21  | 1:10:A:GLN:HG3  | 2                   | 0.14     | 0.02                | 0.14       |

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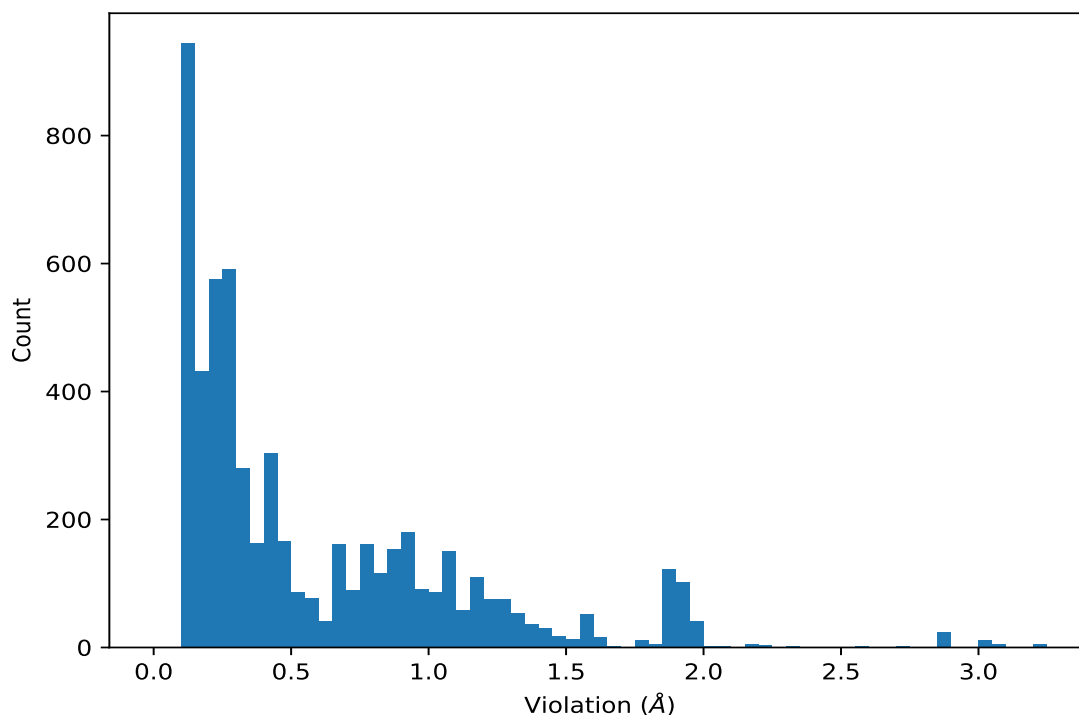
| Key     | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,551) | 1:7:A:LEU:HD22  | 1:10:A:GLN:HG3  | 2                   | 0.14     | 0.02                | 0.14       |
| (1,551) | 1:7:A:LEU:HD23  | 1:10:A:GLN:HG3  | 2                   | 0.14     | 0.02                | 0.14       |
| (2,441) | 1:23:A:PRO:HB3  | 1:24:A:PRO:HD3  | 2                   | 0.14     | 0.02                | 0.14       |
| (2,475) | 1:7:A:LEU:HD21  | 1:10:A:GLN:HG2  | 2                   | 0.14     | 0.02                | 0.14       |
| (2,475) | 1:7:A:LEU:HD22  | 1:10:A:GLN:HG2  | 2                   | 0.14     | 0.02                | 0.14       |
| (2,475) | 1:7:A:LEU:HD23  | 1:10:A:GLN:HG2  | 2                   | 0.14     | 0.02                | 0.14       |
| (2,475) | 1:7:A:LEU:HD21  | 1:10:A:GLN:HG3  | 2                   | 0.14     | 0.02                | 0.14       |
| (2,475) | 1:7:A:LEU:HD22  | 1:10:A:GLN:HG3  | 2                   | 0.14     | 0.02                | 0.14       |
| (2,475) | 1:7:A:LEU:HD23  | 1:10:A:GLN:HG3  | 2                   | 0.14     | 0.02                | 0.14       |
| (1,70)  | 1:7:A:LEU:H     | 1:7:A:LEU:HG    | 2                   | 0.13     | 0.0                 | 0.13       |
| (3,7)   | 1:7:A:LEU:H     | 1:7:A:LEU:HG    | 2                   | 0.13     | 0.0                 | 0.13       |
| (1,530) | 1:9:A:ILE:HA    | 1:12:A:LEU:HD21 | 2                   | 0.12     | 0.02                | 0.12       |
| (1,530) | 1:9:A:ILE:HA    | 1:12:A:LEU:HD22 | 2                   | 0.12     | 0.02                | 0.12       |
| (1,530) | 1:9:A:ILE:HA    | 1:12:A:LEU:HD23 | 2                   | 0.12     | 0.02                | 0.12       |
| (2,459) | 1:9:A:ILE:HA    | 1:12:A:LEU:HD21 | 2                   | 0.12     | 0.02                | 0.12       |
| (2,459) | 1:9:A:ILE:HA    | 1:12:A:LEU:HD22 | 2                   | 0.12     | 0.02                | 0.12       |
| (2,459) | 1:9:A:ILE:HA    | 1:12:A:LEU:HD23 | 2                   | 0.12     | 0.02                | 0.12       |
| (1,276) | 1:11:A:TRP:HE1  | 1:21:A:ARG:HG2  | 2                   | 0.12     | 0.01                | 0.12       |
| (1,276) | 1:11:A:TRP:HE1  | 1:21:A:ARG:HG3  | 2                   | 0.12     | 0.01                | 0.12       |
| (1,534) | 1:7:A:LEU:HD11  | 1:8:A:TYR:HB2   | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,534) | 1:7:A:LEU:HD12  | 1:8:A:TYR:HB2   | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,534) | 1:7:A:LEU:HD13  | 1:8:A:TYR:HB2   | 2                   | 0.12     | 0.0                 | 0.12       |
| (2,257) | 1:11:A:TRP:HE1  | 1:21:A:ARG:HG2  | 2                   | 0.12     | 0.01                | 0.12       |
| (2,257) | 1:11:A:TRP:HE1  | 1:21:A:ARG:HG3  | 2                   | 0.12     | 0.01                | 0.12       |
| (2,463) | 1:7:A:LEU:HD11  | 1:8:A:TYR:HB2   | 2                   | 0.12     | 0.0                 | 0.12       |
| (2,463) | 1:7:A:LEU:HD12  | 1:8:A:TYR:HB2   | 2                   | 0.12     | 0.0                 | 0.12       |
| (2,463) | 1:7:A:LEU:HD13  | 1:8:A:TYR:HB2   | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,440) | 1:4:A:ALA:HB1   | 1:6:A:ARG:H     | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,440) | 1:4:A:ALA:HB2   | 1:6:A:ARG:H     | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,440) | 1:4:A:ALA:HB3   | 1:6:A:ARG:H     | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,598) | 1:12:A:LEU:HD11 | 1:17:A:PRO:HD3  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,598) | 1:12:A:LEU:HD12 | 1:17:A:PRO:HD3  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,598) | 1:12:A:LEU:HD13 | 1:17:A:PRO:HD3  | 2                   | 0.11     | 0.0                 | 0.11       |
| (2,382) | 1:4:A:ALA:HB1   | 1:6:A:ARG:H     | 2                   | 0.11     | 0.0                 | 0.11       |
| (2,382) | 1:4:A:ALA:HB2   | 1:6:A:ARG:H     | 2                   | 0.11     | 0.0                 | 0.11       |
| (2,382) | 1:4:A:ALA:HB3   | 1:6:A:ARG:H     | 2                   | 0.11     | 0.0                 | 0.11       |
| (2,507) | 1:12:A:LEU:HD11 | 1:17:A:PRO:HD3  | 2                   | 0.11     | 0.0                 | 0.11       |
| (2,507) | 1:12:A:LEU:HD12 | 1:17:A:PRO:HD3  | 2                   | 0.11     | 0.0                 | 0.11       |
| (2,507) | 1:12:A:LEU:HD13 | 1:17:A:PRO:HD3  | 2                   | 0.11     | 0.0                 | 0.11       |

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

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

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

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



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

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

| Key     | Atom-1        | Atom-2         | Model ID | Violation (Å) |
|---------|---------------|----------------|----------|---------------|
| (3,82)  | 1:6:A:ARG:HG3 | 1:7:A:LEU:HD21 | 6        | 3.25          |
| (3,82)  | 1:6:A:ARG:HG3 | 1:7:A:LEU:HD22 | 6        | 3.25          |
| (3,82)  | 1:6:A:ARG:HG3 | 1:7:A:LEU:HD23 | 6        | 3.25          |
| (1,560) | 1:6:A:ARG:HG3 | 1:7:A:LEU:HD21 | 6        | 3.25          |
| (1,560) | 1:6:A:ARG:HG3 | 1:7:A:LEU:HD22 | 6        | 3.25          |
| (1,560) | 1:6:A:ARG:HG3 | 1:7:A:LEU:HD23 | 6        | 3.25          |
| (3,82)  | 1:6:A:ARG:HG3 | 1:7:A:LEU:HD21 | 5        | 3.06          |
| (3,82)  | 1:6:A:ARG:HG3 | 1:7:A:LEU:HD22 | 5        | 3.06          |
| (3,82)  | 1:6:A:ARG:HG3 | 1:7:A:LEU:HD23 | 5        | 3.06          |
| (1,560) | 1:6:A:ARG:HG3 | 1:7:A:LEU:HD21 | 5        | 3.06          |

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| Key     | Atom-1        | Atom-2         | Model ID | Violation (Å) |
|---------|---------------|----------------|----------|---------------|
| (1,560) | 1:6:A:ARG:HG3 | 1:7:A:LEU:HD22 | 5        | 3.06          |
| (1,560) | 1:6:A:ARG:HG3 | 1:7:A:LEU:HD23 | 5        | 3.06          |
| (3,82)  | 1:6:A:ARG:HG3 | 1:7:A:LEU:HD21 | 7        | 3.03          |
| (3,82)  | 1:6:A:ARG:HG3 | 1:7:A:LEU:HD22 | 7        | 3.03          |
| (3,82)  | 1:6:A:ARG:HG3 | 1:7:A:LEU:HD23 | 7        | 3.03          |
| (1,560) | 1:6:A:ARG:HG3 | 1:7:A:LEU:HD21 | 7        | 3.03          |
| (1,560) | 1:6:A:ARG:HG3 | 1:7:A:LEU:HD22 | 7        | 3.03          |
| (1,560) | 1:6:A:ARG:HG3 | 1:7:A:LEU:HD23 | 7        | 3.03          |
| (3,82)  | 1:6:A:ARG:HG3 | 1:7:A:LEU:HD21 | 4        | 3.0           |
| (3,82)  | 1:6:A:ARG:HG3 | 1:7:A:LEU:HD22 | 4        | 3.0           |
| (3,82)  | 1:6:A:ARG:HG3 | 1:7:A:LEU:HD23 | 4        | 3.0           |
| (1,560) | 1:6:A:ARG:HG3 | 1:7:A:LEU:HD21 | 4        | 3.0           |
| (1,560) | 1:6:A:ARG:HG3 | 1:7:A:LEU:HD22 | 4        | 3.0           |
| (1,560) | 1:6:A:ARG:HG3 | 1:7:A:LEU:HD23 | 4        | 3.0           |
| (3,82)  | 1:6:A:ARG:HG3 | 1:7:A:LEU:HD21 | 1        | 2.9           |
| (3,82)  | 1:6:A:ARG:HG3 | 1:7:A:LEU:HD22 | 1        | 2.9           |
| (3,82)  | 1:6:A:ARG:HG3 | 1:7:A:LEU:HD23 | 1        | 2.9           |
| (3,82)  | 1:6:A:ARG:HG3 | 1:7:A:LEU:HD21 | 8        | 2.9           |
| (3,82)  | 1:6:A:ARG:HG3 | 1:7:A:LEU:HD22 | 8        | 2.9           |
| (3,82)  | 1:6:A:ARG:HG3 | 1:7:A:LEU:HD23 | 8        | 2.9           |
| (1,560) | 1:6:A:ARG:HG3 | 1:7:A:LEU:HD21 | 1        | 2.9           |
| (1,560) | 1:6:A:ARG:HG3 | 1:7:A:LEU:HD22 | 1        | 2.9           |
| (1,560) | 1:6:A:ARG:HG3 | 1:7:A:LEU:HD23 | 1        | 2.9           |
| (1,560) | 1:6:A:ARG:HG3 | 1:7:A:LEU:HD21 | 8        | 2.9           |
| (1,560) | 1:6:A:ARG:HG3 | 1:7:A:LEU:HD22 | 8        | 2.9           |
| (1,560) | 1:6:A:ARG:HG3 | 1:7:A:LEU:HD23 | 8        | 2.9           |
| (3,82)  | 1:6:A:ARG:HG3 | 1:7:A:LEU:HD21 | 3        | 2.87          |
| (3,82)  | 1:6:A:ARG:HG3 | 1:7:A:LEU:HD22 | 3        | 2.87          |
| (3,82)  | 1:6:A:ARG:HG3 | 1:7:A:LEU:HD23 | 3        | 2.87          |
| (1,560) | 1:6:A:ARG:HG3 | 1:7:A:LEU:HD21 | 3        | 2.87          |
| (1,560) | 1:6:A:ARG:HG3 | 1:7:A:LEU:HD22 | 3        | 2.87          |
| (1,560) | 1:6:A:ARG:HG3 | 1:7:A:LEU:HD23 | 3        | 2.87          |
| (3,82)  | 1:6:A:ARG:HG3 | 1:7:A:LEU:HD21 | 2        | 2.86          |
| (3,82)  | 1:6:A:ARG:HG3 | 1:7:A:LEU:HD22 | 2        | 2.86          |
| (3,82)  | 1:6:A:ARG:HG3 | 1:7:A:LEU:HD23 | 2        | 2.86          |
| (1,560) | 1:6:A:ARG:HG3 | 1:7:A:LEU:HD21 | 2        | 2.86          |
| (1,560) | 1:6:A:ARG:HG3 | 1:7:A:LEU:HD22 | 2        | 2.86          |
| (1,560) | 1:6:A:ARG:HG3 | 1:7:A:LEU:HD23 | 2        | 2.86          |
| (3,48)  | 1:1:A:GLU:HB3 | 1:4:A:ALA:H    | 4        | 2.73          |
| (1,399) | 1:1:A:GLU:HB3 | 1:4:A:ALA:H    | 4        | 2.73          |
| (3,48)  | 1:1:A:GLU:HB3 | 1:4:A:ALA:H    | 6        | 2.56          |
| (1,399) | 1:1:A:GLU:HB3 | 1:4:A:ALA:H    | 6        | 2.56          |

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| Key     | Atom-1        | Atom-2         | Model ID | Violation (Å) |
|---------|---------------|----------------|----------|---------------|
| (3,48)  | 1:1:A:GLU:HB3 | 1:4:A:ALA:H    | 7        | 2.31          |
| (1,399) | 1:1:A:GLU:HB3 | 1:4:A:ALA:H    | 7        | 2.31          |
| (3,48)  | 1:1:A:GLU:HB3 | 1:4:A:ALA:H    | 5        | 2.24          |
| (1,399) | 1:1:A:GLU:HB3 | 1:4:A:ALA:H    | 5        | 2.24          |
| (3,48)  | 1:1:A:GLU:HB3 | 1:4:A:ALA:H    | 2        | 2.2           |
| (1,399) | 1:1:A:GLU:HB3 | 1:4:A:ALA:H    | 2        | 2.2           |
| (3,48)  | 1:1:A:GLU:HB3 | 1:4:A:ALA:H    | 8        | 2.19          |
| (1,399) | 1:1:A:GLU:HB3 | 1:4:A:ALA:H    | 8        | 2.19          |
| (3,48)  | 1:1:A:GLU:HB3 | 1:4:A:ALA:H    | 9        | 2.17          |
| (1,399) | 1:1:A:GLU:HB3 | 1:4:A:ALA:H    | 9        | 2.17          |
| (3,48)  | 1:1:A:GLU:HB3 | 1:4:A:ALA:H    | 10       | 2.16          |
| (1,399) | 1:1:A:GLU:HB3 | 1:4:A:ALA:H    | 10       | 2.16          |
| (3,89)  | 1:8:A:TYR:HB3 | 1:24:A:PRO:HG3 | 8        | 2.09          |
| (1,584) | 1:8:A:TYR:HB3 | 1:24:A:PRO:HG3 | 8        | 2.09          |
| (3,48)  | 1:1:A:GLU:HB3 | 1:4:A:ALA:H    | 1        | 2.01          |
| (1,399) | 1:1:A:GLU:HB3 | 1:4:A:ALA:H    | 1        | 2.01          |
| (3,81)  | 1:4:A:ALA:HB1 | 1:7:A:LEU:HD21 | 8        | 1.97          |
| (3,81)  | 1:4:A:ALA:HB1 | 1:7:A:LEU:HD22 | 8        | 1.97          |
| (3,81)  | 1:4:A:ALA:HB1 | 1:7:A:LEU:HD23 | 8        | 1.97          |
| (3,81)  | 1:4:A:ALA:HB2 | 1:7:A:LEU:HD21 | 8        | 1.97          |
| (3,81)  | 1:4:A:ALA:HB2 | 1:7:A:LEU:HD22 | 8        | 1.97          |
| (3,81)  | 1:4:A:ALA:HB2 | 1:7:A:LEU:HD23 | 8        | 1.97          |
| (3,81)  | 1:4:A:ALA:HB3 | 1:7:A:LEU:HD21 | 8        | 1.97          |
| (3,81)  | 1:4:A:ALA:HB3 | 1:7:A:LEU:HD22 | 8        | 1.97          |
| (3,81)  | 1:4:A:ALA:HB3 | 1:7:A:LEU:HD23 | 8        | 1.97          |
| (1,559) | 1:4:A:ALA:HB1 | 1:7:A:LEU:HD21 | 8        | 1.97          |
| (1,559) | 1:4:A:ALA:HB1 | 1:7:A:LEU:HD22 | 8        | 1.97          |
| (1,559) | 1:4:A:ALA:HB1 | 1:7:A:LEU:HD23 | 8        | 1.97          |
| (1,559) | 1:4:A:ALA:HB2 | 1:7:A:LEU:HD21 | 8        | 1.97          |
| (1,559) | 1:4:A:ALA:HB2 | 1:7:A:LEU:HD22 | 8        | 1.97          |
| (1,559) | 1:4:A:ALA:HB2 | 1:7:A:LEU:HD23 | 8        | 1.97          |
| (1,559) | 1:4:A:ALA:HB3 | 1:7:A:LEU:HD21 | 8        | 1.97          |
| (1,559) | 1:4:A:ALA:HB3 | 1:7:A:LEU:HD22 | 8        | 1.97          |
| (1,559) | 1:4:A:ALA:HB3 | 1:7:A:LEU:HD23 | 8        | 1.97          |
| (3,81)  | 1:4:A:ALA:HB1 | 1:7:A:LEU:HD21 | 6        | 1.96          |
| (3,81)  | 1:4:A:ALA:HB1 | 1:7:A:LEU:HD22 | 6        | 1.96          |
| (3,81)  | 1:4:A:ALA:HB1 | 1:7:A:LEU:HD23 | 6        | 1.96          |
| (3,81)  | 1:4:A:ALA:HB2 | 1:7:A:LEU:HD21 | 6        | 1.96          |
| (3,81)  | 1:4:A:ALA:HB2 | 1:7:A:LEU:HD22 | 6        | 1.96          |
| (3,81)  | 1:4:A:ALA:HB2 | 1:7:A:LEU:HD23 | 6        | 1.96          |
| (3,81)  | 1:4:A:ALA:HB3 | 1:7:A:LEU:HD21 | 6        | 1.96          |
| (3,81)  | 1:4:A:ALA:HB3 | 1:7:A:LEU:HD22 | 6        | 1.96          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (3,81)  | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD23 | 6        | 1.96          |
| (3,68)  | 1:5:A:VAL:HG11 | 1:8:A:TYR:HA   | 10       | 1.96          |
| (3,68)  | 1:5:A:VAL:HG12 | 1:8:A:TYR:HA   | 10       | 1.96          |
| (3,68)  | 1:5:A:VAL:HG13 | 1:8:A:TYR:HA   | 10       | 1.96          |
| (1,559) | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD21 | 6        | 1.96          |
| (1,559) | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD22 | 6        | 1.96          |
| (1,559) | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD23 | 6        | 1.96          |
| (1,559) | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD21 | 6        | 1.96          |
| (1,559) | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD22 | 6        | 1.96          |
| (1,559) | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD23 | 6        | 1.96          |
| (1,559) | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD21 | 6        | 1.96          |
| (1,559) | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD22 | 6        | 1.96          |
| (1,559) | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD23 | 6        | 1.96          |
| (1,519) | 1:5:A:VAL:HG11 | 1:8:A:TYR:HA   | 10       | 1.96          |
| (1,519) | 1:5:A:VAL:HG12 | 1:8:A:TYR:HA   | 10       | 1.96          |
| (1,519) | 1:5:A:VAL:HG13 | 1:8:A:TYR:HA   | 10       | 1.96          |
| (3,81)  | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD21 | 5        | 1.95          |
| (3,81)  | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD22 | 5        | 1.95          |
| (3,81)  | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD23 | 5        | 1.95          |
| (3,81)  | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD21 | 5        | 1.95          |
| (3,81)  | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD22 | 5        | 1.95          |
| (3,81)  | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD23 | 5        | 1.95          |
| (3,81)  | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD21 | 5        | 1.95          |
| (3,81)  | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD22 | 5        | 1.95          |
| (3,81)  | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD23 | 5        | 1.95          |
| (3,81)  | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD21 | 7        | 1.95          |
| (3,81)  | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD22 | 7        | 1.95          |
| (3,81)  | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD23 | 7        | 1.95          |
| (3,81)  | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD21 | 7        | 1.95          |
| (3,81)  | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD22 | 7        | 1.95          |
| (3,81)  | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD23 | 7        | 1.95          |
| (3,81)  | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD21 | 7        | 1.95          |
| (3,81)  | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD22 | 7        | 1.95          |
| (3,81)  | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD23 | 7        | 1.95          |
| (1,559) | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD21 | 5        | 1.95          |
| (1,559) | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD22 | 5        | 1.95          |
| (1,559) | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD23 | 5        | 1.95          |
| (1,559) | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD21 | 5        | 1.95          |
| (1,559) | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD22 | 5        | 1.95          |
| (1,559) | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD23 | 5        | 1.95          |
| (1,559) | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD21 | 5        | 1.95          |
| (1,559) | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD22 | 5        | 1.95          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,559) | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD23 | 5        | 1.95          |
| (1,559) | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD21 | 7        | 1.95          |
| (1,559) | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD22 | 7        | 1.95          |
| (1,559) | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD23 | 7        | 1.95          |
| (1,559) | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD21 | 7        | 1.95          |
| (1,559) | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD22 | 7        | 1.95          |
| (1,559) | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD23 | 7        | 1.95          |
| (1,559) | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD21 | 7        | 1.95          |
| (1,559) | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD22 | 7        | 1.95          |
| (1,559) | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD23 | 7        | 1.95          |
| (3,68)  | 1:5:A:VAL:HG11 | 1:8:A:TYR:HA   | 9        | 1.94          |
| (3,68)  | 1:5:A:VAL:HG12 | 1:8:A:TYR:HA   | 9        | 1.94          |
| (3,68)  | 1:5:A:VAL:HG13 | 1:8:A:TYR:HA   | 9        | 1.94          |
| (1,519) | 1:5:A:VAL:HG11 | 1:8:A:TYR:HA   | 9        | 1.94          |
| (1,519) | 1:5:A:VAL:HG12 | 1:8:A:TYR:HA   | 9        | 1.94          |
| (1,519) | 1:5:A:VAL:HG13 | 1:8:A:TYR:HA   | 9        | 1.94          |
| (3,81)  | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD21 | 2        | 1.92          |
| (3,81)  | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD22 | 2        | 1.92          |
| (3,81)  | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD23 | 2        | 1.92          |
| (3,81)  | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD21 | 2        | 1.92          |
| (3,81)  | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD22 | 2        | 1.92          |
| (3,81)  | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD23 | 2        | 1.92          |
| (3,81)  | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD21 | 2        | 1.92          |
| (3,81)  | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD22 | 2        | 1.92          |
| (3,81)  | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD23 | 2        | 1.92          |
| (3,68)  | 1:5:A:VAL:HG11 | 1:8:A:TYR:HA   | 1        | 1.92          |
| (3,68)  | 1:5:A:VAL:HG12 | 1:8:A:TYR:HA   | 1        | 1.92          |
| (3,68)  | 1:5:A:VAL:HG13 | 1:8:A:TYR:HA   | 1        | 1.92          |
| (3,68)  | 1:5:A:VAL:HG11 | 1:8:A:TYR:HA   | 3        | 1.92          |
| (3,68)  | 1:5:A:VAL:HG12 | 1:8:A:TYR:HA   | 3        | 1.92          |
| (3,68)  | 1:5:A:VAL:HG13 | 1:8:A:TYR:HA   | 3        | 1.92          |
| (3,68)  | 1:5:A:VAL:HG11 | 1:8:A:TYR:HA   | 8        | 1.92          |
| (3,68)  | 1:5:A:VAL:HG12 | 1:8:A:TYR:HA   | 8        | 1.92          |
| (3,68)  | 1:5:A:VAL:HG13 | 1:8:A:TYR:HA   | 8        | 1.92          |
| (1,559) | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD21 | 2        | 1.92          |
| (1,559) | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD22 | 2        | 1.92          |
| (1,559) | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD23 | 2        | 1.92          |
| (1,559) | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD21 | 2        | 1.92          |
| (1,559) | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD22 | 2        | 1.92          |
| (1,559) | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD23 | 2        | 1.92          |
| (1,559) | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD21 | 2        | 1.92          |
| (1,559) | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD22 | 2        | 1.92          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,559) | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD23 | 2        | 1.92          |
| (1,519) | 1:5:A:VAL:HG11 | 1:8:A:TYR:HA   | 1        | 1.92          |
| (1,519) | 1:5:A:VAL:HG12 | 1:8:A:TYR:HA   | 1        | 1.92          |
| (1,519) | 1:5:A:VAL:HG13 | 1:8:A:TYR:HA   | 1        | 1.92          |
| (1,519) | 1:5:A:VAL:HG11 | 1:8:A:TYR:HA   | 3        | 1.92          |
| (1,519) | 1:5:A:VAL:HG12 | 1:8:A:TYR:HA   | 3        | 1.92          |
| (1,519) | 1:5:A:VAL:HG13 | 1:8:A:TYR:HA   | 3        | 1.92          |
| (1,519) | 1:5:A:VAL:HG11 | 1:8:A:TYR:HA   | 8        | 1.92          |
| (1,519) | 1:5:A:VAL:HG12 | 1:8:A:TYR:HA   | 8        | 1.92          |
| (1,519) | 1:5:A:VAL:HG13 | 1:8:A:TYR:HA   | 8        | 1.92          |
| (3,68)  | 1:5:A:VAL:HG11 | 1:8:A:TYR:HA   | 2        | 1.91          |
| (3,68)  | 1:5:A:VAL:HG12 | 1:8:A:TYR:HA   | 2        | 1.91          |
| (3,68)  | 1:5:A:VAL:HG13 | 1:8:A:TYR:HA   | 2        | 1.91          |
| (3,68)  | 1:5:A:VAL:HG11 | 1:8:A:TYR:HA   | 5        | 1.91          |
| (3,68)  | 1:5:A:VAL:HG12 | 1:8:A:TYR:HA   | 5        | 1.91          |
| (3,68)  | 1:5:A:VAL:HG13 | 1:8:A:TYR:HA   | 5        | 1.91          |
| (3,68)  | 1:5:A:VAL:HG11 | 1:8:A:TYR:HA   | 6        | 1.91          |
| (3,68)  | 1:5:A:VAL:HG12 | 1:8:A:TYR:HA   | 6        | 1.91          |
| (3,68)  | 1:5:A:VAL:HG13 | 1:8:A:TYR:HA   | 6        | 1.91          |
| (3,68)  | 1:5:A:VAL:HG11 | 1:8:A:TYR:HA   | 7        | 1.91          |
| (3,68)  | 1:5:A:VAL:HG12 | 1:8:A:TYR:HA   | 7        | 1.91          |
| (3,68)  | 1:5:A:VAL:HG13 | 1:8:A:TYR:HA   | 7        | 1.91          |
| (1,519) | 1:5:A:VAL:HG11 | 1:8:A:TYR:HA   | 2        | 1.91          |
| (1,519) | 1:5:A:VAL:HG12 | 1:8:A:TYR:HA   | 2        | 1.91          |
| (1,519) | 1:5:A:VAL:HG13 | 1:8:A:TYR:HA   | 2        | 1.91          |
| (1,519) | 1:5:A:VAL:HG11 | 1:8:A:TYR:HA   | 5        | 1.91          |
| (1,519) | 1:5:A:VAL:HG12 | 1:8:A:TYR:HA   | 5        | 1.91          |
| (1,519) | 1:5:A:VAL:HG13 | 1:8:A:TYR:HA   | 5        | 1.91          |
| (1,519) | 1:5:A:VAL:HG11 | 1:8:A:TYR:HA   | 6        | 1.91          |
| (1,519) | 1:5:A:VAL:HG12 | 1:8:A:TYR:HA   | 6        | 1.91          |
| (1,519) | 1:5:A:VAL:HG13 | 1:8:A:TYR:HA   | 6        | 1.91          |
| (1,519) | 1:5:A:VAL:HG11 | 1:8:A:TYR:HA   | 7        | 1.91          |
| (1,519) | 1:5:A:VAL:HG12 | 1:8:A:TYR:HA   | 7        | 1.91          |
| (1,519) | 1:5:A:VAL:HG13 | 1:8:A:TYR:HA   | 7        | 1.91          |
| (3,81)  | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD21 | 3        | 1.9           |
| (3,81)  | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD22 | 3        | 1.9           |
| (3,81)  | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD23 | 3        | 1.9           |
| (3,81)  | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD21 | 3        | 1.9           |
| (3,81)  | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD22 | 3        | 1.9           |
| (3,81)  | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD23 | 3        | 1.9           |
| (3,81)  | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD21 | 3        | 1.9           |
| (3,81)  | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD22 | 3        | 1.9           |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (3,81)  | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD23 | 3        | 1.9           |
| (3,68)  | 1:5:A:VAL:HG11 | 1:8:A:TYR:HA   | 4        | 1.9           |
| (3,68)  | 1:5:A:VAL:HG12 | 1:8:A:TYR:HA   | 4        | 1.9           |
| (3,68)  | 1:5:A:VAL:HG13 | 1:8:A:TYR:HA   | 4        | 1.9           |
| (3,38)  | 1:11:A:TRP:HB2 | 1:11:A:TRP:HZ3 | 1        | 1.9           |
| (3,38)  | 1:11:A:TRP:HB2 | 1:11:A:TRP:HZ3 | 2        | 1.9           |
| (3,38)  | 1:11:A:TRP:HB2 | 1:11:A:TRP:HZ3 | 4        | 1.9           |
| (3,38)  | 1:11:A:TRP:HB2 | 1:11:A:TRP:HZ3 | 5        | 1.9           |
| (3,38)  | 1:11:A:TRP:HB2 | 1:11:A:TRP:HZ3 | 6        | 1.9           |
| (3,38)  | 1:11:A:TRP:HB2 | 1:11:A:TRP:HZ3 | 7        | 1.9           |
| (3,38)  | 1:11:A:TRP:HB2 | 1:11:A:TRP:HZ3 | 8        | 1.9           |
| (1,559) | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD21 | 3        | 1.9           |
| (1,559) | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD22 | 3        | 1.9           |
| (1,559) | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD23 | 3        | 1.9           |
| (1,559) | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD21 | 3        | 1.9           |
| (1,559) | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD22 | 3        | 1.9           |
| (1,559) | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD23 | 3        | 1.9           |
| (1,559) | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD21 | 3        | 1.9           |
| (1,559) | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD22 | 3        | 1.9           |
| (1,559) | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD23 | 3        | 1.9           |
| (1,519) | 1:5:A:VAL:HG11 | 1:8:A:TYR:HA   | 4        | 1.9           |
| (1,519) | 1:5:A:VAL:HG12 | 1:8:A:TYR:HA   | 4        | 1.9           |
| (1,519) | 1:5:A:VAL:HG13 | 1:8:A:TYR:HA   | 4        | 1.9           |
| (1,352) | 1:11:A:TRP:HB2 | 1:11:A:TRP:HZ3 | 1        | 1.9           |
| (1,352) | 1:11:A:TRP:HB2 | 1:11:A:TRP:HZ3 | 2        | 1.9           |
| (1,352) | 1:11:A:TRP:HB2 | 1:11:A:TRP:HZ3 | 4        | 1.9           |
| (1,352) | 1:11:A:TRP:HB2 | 1:11:A:TRP:HZ3 | 5        | 1.9           |
| (1,352) | 1:11:A:TRP:HB2 | 1:11:A:TRP:HZ3 | 6        | 1.9           |
| (1,352) | 1:11:A:TRP:HB2 | 1:11:A:TRP:HZ3 | 7        | 1.9           |
| (1,352) | 1:11:A:TRP:HB2 | 1:11:A:TRP:HZ3 | 8        | 1.9           |
| (3,74)  | 1:5:A:VAL:HG21 | 1:6:A:ARG:HB3  | 7        | 1.89          |
| (3,74)  | 1:5:A:VAL:HG22 | 1:6:A:ARG:HB3  | 7        | 1.89          |
| (3,74)  | 1:5:A:VAL:HG23 | 1:6:A:ARG:HB3  | 7        | 1.89          |
| (3,38)  | 1:11:A:TRP:HB2 | 1:11:A:TRP:HZ3 | 3        | 1.89          |
| (3,38)  | 1:11:A:TRP:HB2 | 1:11:A:TRP:HZ3 | 9        | 1.89          |
| (1,542) | 1:5:A:VAL:HG21 | 1:6:A:ARG:HB3  | 7        | 1.89          |
| (1,542) | 1:5:A:VAL:HG22 | 1:6:A:ARG:HB3  | 7        | 1.89          |
| (1,542) | 1:5:A:VAL:HG23 | 1:6:A:ARG:HB3  | 7        | 1.89          |
| (1,352) | 1:11:A:TRP:HB2 | 1:11:A:TRP:HZ3 | 3        | 1.89          |
| (1,352) | 1:11:A:TRP:HB2 | 1:11:A:TRP:HZ3 | 9        | 1.89          |
| (3,74)  | 1:5:A:VAL:HG21 | 1:6:A:ARG:HB3  | 2        | 1.88          |
| (3,74)  | 1:5:A:VAL:HG22 | 1:6:A:ARG:HB3  | 2        | 1.88          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (3,74)  | 1:5:A:VAL:HG23 | 1:6:A:ARG:HB3  | 2        | 1.88          |
| (3,74)  | 1:5:A:VAL:HG21 | 1:6:A:ARG:HB3  | 8        | 1.88          |
| (3,74)  | 1:5:A:VAL:HG22 | 1:6:A:ARG:HB3  | 8        | 1.88          |
| (3,74)  | 1:5:A:VAL:HG23 | 1:6:A:ARG:HB3  | 8        | 1.88          |
| (3,38)  | 1:11:A:TRP:HB2 | 1:11:A:TRP:HZ3 | 10       | 1.88          |
| (1,542) | 1:5:A:VAL:HG21 | 1:6:A:ARG:HB3  | 2        | 1.88          |
| (1,542) | 1:5:A:VAL:HG22 | 1:6:A:ARG:HB3  | 2        | 1.88          |
| (1,542) | 1:5:A:VAL:HG23 | 1:6:A:ARG:HB3  | 2        | 1.88          |
| (1,542) | 1:5:A:VAL:HG21 | 1:6:A:ARG:HB3  | 8        | 1.88          |
| (1,542) | 1:5:A:VAL:HG22 | 1:6:A:ARG:HB3  | 8        | 1.88          |
| (1,542) | 1:5:A:VAL:HG23 | 1:6:A:ARG:HB3  | 8        | 1.88          |
| (1,352) | 1:11:A:TRP:HB2 | 1:11:A:TRP:HZ3 | 10       | 1.88          |
| (3,81)  | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD21 | 4        | 1.87          |
| (3,81)  | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD22 | 4        | 1.87          |
| (3,81)  | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD23 | 4        | 1.87          |
| (3,81)  | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD21 | 4        | 1.87          |
| (3,81)  | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD22 | 4        | 1.87          |
| (3,81)  | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD23 | 4        | 1.87          |
| (3,81)  | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD21 | 4        | 1.87          |
| (3,81)  | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD22 | 4        | 1.87          |
| (3,81)  | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD23 | 4        | 1.87          |
| (3,74)  | 1:5:A:VAL:HG21 | 1:6:A:ARG:HB3  | 6        | 1.87          |
| (3,74)  | 1:5:A:VAL:HG22 | 1:6:A:ARG:HB3  | 6        | 1.87          |
| (3,74)  | 1:5:A:VAL:HG23 | 1:6:A:ARG:HB3  | 6        | 1.87          |
| (1,559) | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD21 | 4        | 1.87          |
| (1,559) | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD22 | 4        | 1.87          |
| (1,559) | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD23 | 4        | 1.87          |
| (1,559) | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD21 | 4        | 1.87          |
| (1,559) | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD22 | 4        | 1.87          |
| (1,559) | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD23 | 4        | 1.87          |
| (1,559) | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD21 | 4        | 1.87          |
| (1,559) | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD22 | 4        | 1.87          |
| (1,559) | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD23 | 4        | 1.87          |
| (1,542) | 1:5:A:VAL:HG21 | 1:6:A:ARG:HB3  | 6        | 1.87          |
| (1,542) | 1:5:A:VAL:HG22 | 1:6:A:ARG:HB3  | 6        | 1.87          |
| (1,542) | 1:5:A:VAL:HG23 | 1:6:A:ARG:HB3  | 6        | 1.87          |
| (3,81)  | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD21 | 1        | 1.86          |
| (3,81)  | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD22 | 1        | 1.86          |
| (3,81)  | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD23 | 1        | 1.86          |
| (3,81)  | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD21 | 1        | 1.86          |
| (3,81)  | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD22 | 1        | 1.86          |
| (3,81)  | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD23 | 1        | 1.86          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (3,81)  | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD21 | 1        | 1.86          |
| (3,81)  | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD22 | 1        | 1.86          |
| (3,81)  | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD23 | 1        | 1.86          |
| (3,74)  | 1:5:A:VAL:HG21 | 1:6:A:ARG:HB3  | 3        | 1.86          |
| (3,74)  | 1:5:A:VAL:HG22 | 1:6:A:ARG:HB3  | 3        | 1.86          |
| (3,74)  | 1:5:A:VAL:HG23 | 1:6:A:ARG:HB3  | 3        | 1.86          |
| (3,74)  | 1:5:A:VAL:HG21 | 1:6:A:ARG:HB3  | 4        | 1.86          |
| (3,74)  | 1:5:A:VAL:HG22 | 1:6:A:ARG:HB3  | 4        | 1.86          |
| (3,74)  | 1:5:A:VAL:HG23 | 1:6:A:ARG:HB3  | 4        | 1.86          |
| (1,559) | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD21 | 1        | 1.86          |
| (1,559) | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD22 | 1        | 1.86          |
| (1,559) | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD23 | 1        | 1.86          |
| (1,559) | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD21 | 1        | 1.86          |
| (1,559) | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD22 | 1        | 1.86          |
| (1,559) | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD23 | 1        | 1.86          |
| (1,559) | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD21 | 1        | 1.86          |
| (1,559) | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD22 | 1        | 1.86          |
| (1,559) | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD23 | 1        | 1.86          |
| (1,542) | 1:5:A:VAL:HG21 | 1:6:A:ARG:HB3  | 3        | 1.86          |
| (1,542) | 1:5:A:VAL:HG22 | 1:6:A:ARG:HB3  | 3        | 1.86          |
| (1,542) | 1:5:A:VAL:HG23 | 1:6:A:ARG:HB3  | 3        | 1.86          |
| (1,542) | 1:5:A:VAL:HG21 | 1:6:A:ARG:HB3  | 4        | 1.86          |
| (1,542) | 1:5:A:VAL:HG22 | 1:6:A:ARG:HB3  | 4        | 1.86          |
| (1,542) | 1:5:A:VAL:HG23 | 1:6:A:ARG:HB3  | 4        | 1.86          |
| (3,74)  | 1:5:A:VAL:HG21 | 1:6:A:ARG:HB3  | 5        | 1.85          |
| (3,74)  | 1:5:A:VAL:HG22 | 1:6:A:ARG:HB3  | 5        | 1.85          |
| (3,74)  | 1:5:A:VAL:HG23 | 1:6:A:ARG:HB3  | 5        | 1.85          |
| (1,542) | 1:5:A:VAL:HG21 | 1:6:A:ARG:HB3  | 5        | 1.85          |
| (1,542) | 1:5:A:VAL:HG22 | 1:6:A:ARG:HB3  | 5        | 1.85          |
| (1,542) | 1:5:A:VAL:HG23 | 1:6:A:ARG:HB3  | 5        | 1.85          |
| (3,74)  | 1:5:A:VAL:HG21 | 1:6:A:ARG:HB3  | 1        | 1.81          |
| (3,74)  | 1:5:A:VAL:HG22 | 1:6:A:ARG:HB3  | 1        | 1.81          |
| (3,74)  | 1:5:A:VAL:HG23 | 1:6:A:ARG:HB3  | 1        | 1.81          |
| (1,542) | 1:5:A:VAL:HG21 | 1:6:A:ARG:HB3  | 1        | 1.81          |
| (1,542) | 1:5:A:VAL:HG22 | 1:6:A:ARG:HB3  | 1        | 1.81          |
| (1,542) | 1:5:A:VAL:HG23 | 1:6:A:ARG:HB3  | 1        | 1.81          |
| (3,74)  | 1:5:A:VAL:HG21 | 1:6:A:ARG:HB3  | 10       | 1.77          |
| (3,74)  | 1:5:A:VAL:HG22 | 1:6:A:ARG:HB3  | 10       | 1.77          |
| (3,74)  | 1:5:A:VAL:HG23 | 1:6:A:ARG:HB3  | 10       | 1.77          |
| (1,542) | 1:5:A:VAL:HG21 | 1:6:A:ARG:HB3  | 10       | 1.77          |
| (1,542) | 1:5:A:VAL:HG22 | 1:6:A:ARG:HB3  | 10       | 1.77          |
| (1,542) | 1:5:A:VAL:HG23 | 1:6:A:ARG:HB3  | 10       | 1.77          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (3,74)  | 1:5:A:VAL:HG21  | 1:6:A:ARG:HB3  | 9        | 1.75          |
| (3,74)  | 1:5:A:VAL:HG22  | 1:6:A:ARG:HB3  | 9        | 1.75          |
| (3,74)  | 1:5:A:VAL:HG23  | 1:6:A:ARG:HB3  | 9        | 1.75          |
| (1,542) | 1:5:A:VAL:HG21  | 1:6:A:ARG:HB3  | 9        | 1.75          |
| (1,542) | 1:5:A:VAL:HG22  | 1:6:A:ARG:HB3  | 9        | 1.75          |
| (1,542) | 1:5:A:VAL:HG23  | 1:6:A:ARG:HB3  | 9        | 1.75          |
| (3,65)  | 1:6:A:ARG:HA    | 1:10:A:GLN:HB3 | 2        | 1.68          |
| (1,482) | 1:6:A:ARG:HA    | 1:10:A:GLN:HB3 | 2        | 1.68          |
| (3,65)  | 1:6:A:ARG:HA    | 1:10:A:GLN:HB3 | 3        | 1.64          |
| (1,482) | 1:6:A:ARG:HA    | 1:10:A:GLN:HB3 | 3        | 1.64          |
| (3,46)  | 1:11:A:TRP:HE3  | 1:11:A:TRP:HH2 | 1        | 1.6           |
| (3,46)  | 1:11:A:TRP:HE3  | 1:11:A:TRP:HH2 | 4        | 1.6           |
| (3,46)  | 1:11:A:TRP:HE3  | 1:11:A:TRP:HH2 | 8        | 1.6           |
| (3,46)  | 1:11:A:TRP:HE3  | 1:11:A:TRP:HH2 | 9        | 1.6           |
| (2,474) | 1:9:A:ILE:HD11  | 1:13:A:LYS:HE3 | 7        | 1.6           |
| (2,474) | 1:9:A:ILE:HD12  | 1:13:A:LYS:HE3 | 7        | 1.6           |
| (2,474) | 1:9:A:ILE:HD13  | 1:13:A:LYS:HE3 | 7        | 1.6           |
| (1,550) | 1:9:A:ILE:HD11  | 1:13:A:LYS:HE3 | 7        | 1.6           |
| (1,550) | 1:9:A:ILE:HD12  | 1:13:A:LYS:HE3 | 7        | 1.6           |
| (1,550) | 1:9:A:ILE:HD13  | 1:13:A:LYS:HE3 | 7        | 1.6           |
| (1,384) | 1:11:A:TRP:HE3  | 1:11:A:TRP:HH2 | 1        | 1.6           |
| (1,384) | 1:11:A:TRP:HE3  | 1:11:A:TRP:HH2 | 4        | 1.6           |
| (1,384) | 1:11:A:TRP:HE3  | 1:11:A:TRP:HH2 | 8        | 1.6           |
| (1,384) | 1:11:A:TRP:HE3  | 1:11:A:TRP:HH2 | 9        | 1.6           |
| (3,83)  | 1:12:A:LEU:HD11 | 1:16:A:GLY:H   | 6        | 1.59          |
| (3,83)  | 1:12:A:LEU:HD12 | 1:16:A:GLY:H   | 6        | 1.59          |
| (3,83)  | 1:12:A:LEU:HD13 | 1:16:A:GLY:H   | 6        | 1.59          |
| (3,46)  | 1:11:A:TRP:HE3  | 1:11:A:TRP:HH2 | 2        | 1.59          |
| (3,46)  | 1:11:A:TRP:HE3  | 1:11:A:TRP:HH2 | 5        | 1.59          |
| (3,44)  | 1:11:A:TRP:HD1  | 1:11:A:TRP:HZ2 | 7        | 1.59          |
| (3,44)  | 1:11:A:TRP:HD1  | 1:11:A:TRP:HZ2 | 10       | 1.59          |
| (3,35)  | 1:11:A:TRP:HZ2  | 1:21:A:ARG:HB3 | 9        | 1.59          |
| (1,565) | 1:12:A:LEU:HD11 | 1:16:A:GLY:H   | 6        | 1.59          |
| (1,565) | 1:12:A:LEU:HD12 | 1:16:A:GLY:H   | 6        | 1.59          |
| (1,565) | 1:12:A:LEU:HD13 | 1:16:A:GLY:H   | 6        | 1.59          |
| (1,384) | 1:11:A:TRP:HE3  | 1:11:A:TRP:HH2 | 2        | 1.59          |
| (1,384) | 1:11:A:TRP:HE3  | 1:11:A:TRP:HH2 | 5        | 1.59          |
| (1,382) | 1:11:A:TRP:HD1  | 1:11:A:TRP:HZ2 | 7        | 1.59          |
| (1,382) | 1:11:A:TRP:HD1  | 1:11:A:TRP:HZ2 | 10       | 1.59          |
| (1,336) | 1:11:A:TRP:HZ2  | 1:21:A:ARG:HB3 | 9        | 1.59          |
| (3,48)  | 1:1:A:GLU:HB3   | 1:4:A:ALA:H    | 3        | 1.58          |
| (3,46)  | 1:11:A:TRP:HE3  | 1:11:A:TRP:HH2 | 3        | 1.58          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (3,46)  | 1:11:A:TRP:HE3 | 1:11:A:TRP:HH2 | 7        | 1.58          |
| (3,46)  | 1:11:A:TRP:HE3 | 1:11:A:TRP:HH2 | 10       | 1.58          |
| (3,44)  | 1:11:A:TRP:HD1 | 1:11:A:TRP:HZ2 | 1        | 1.58          |
| (3,44)  | 1:11:A:TRP:HD1 | 1:11:A:TRP:HZ2 | 2        | 1.58          |
| (3,44)  | 1:11:A:TRP:HD1 | 1:11:A:TRP:HZ2 | 3        | 1.58          |
| (3,44)  | 1:11:A:TRP:HD1 | 1:11:A:TRP:HZ2 | 4        | 1.58          |
| (3,44)  | 1:11:A:TRP:HD1 | 1:11:A:TRP:HZ2 | 6        | 1.58          |
| (3,44)  | 1:11:A:TRP:HD1 | 1:11:A:TRP:HZ2 | 8        | 1.58          |
| (3,44)  | 1:11:A:TRP:HD1 | 1:11:A:TRP:HZ2 | 9        | 1.58          |
| (1,399) | 1:1:A:GLU:HB3  | 1:4:A:ALA:H    | 3        | 1.58          |
| (1,384) | 1:11:A:TRP:HE3 | 1:11:A:TRP:HH2 | 3        | 1.58          |
| (1,384) | 1:11:A:TRP:HE3 | 1:11:A:TRP:HH2 | 7        | 1.58          |
| (1,384) | 1:11:A:TRP:HE3 | 1:11:A:TRP:HH2 | 10       | 1.58          |
| (1,382) | 1:11:A:TRP:HD1 | 1:11:A:TRP:HZ2 | 1        | 1.58          |
| (1,382) | 1:11:A:TRP:HD1 | 1:11:A:TRP:HZ2 | 2        | 1.58          |
| (1,382) | 1:11:A:TRP:HD1 | 1:11:A:TRP:HZ2 | 3        | 1.58          |
| (1,382) | 1:11:A:TRP:HD1 | 1:11:A:TRP:HZ2 | 4        | 1.58          |
| (1,382) | 1:11:A:TRP:HD1 | 1:11:A:TRP:HZ2 | 6        | 1.58          |
| (1,382) | 1:11:A:TRP:HD1 | 1:11:A:TRP:HZ2 | 8        | 1.58          |
| (1,382) | 1:11:A:TRP:HD1 | 1:11:A:TRP:HZ2 | 9        | 1.58          |
| (3,46)  | 1:11:A:TRP:HE3 | 1:11:A:TRP:HH2 | 6        | 1.57          |
| (3,44)  | 1:11:A:TRP:HD1 | 1:11:A:TRP:HZ2 | 5        | 1.57          |
| (3,35)  | 1:11:A:TRP:HZ2 | 1:21:A:ARG:HB3 | 5        | 1.57          |
| (1,384) | 1:11:A:TRP:HE3 | 1:11:A:TRP:HH2 | 6        | 1.57          |
| (1,382) | 1:11:A:TRP:HD1 | 1:11:A:TRP:HZ2 | 5        | 1.57          |
| (1,336) | 1:11:A:TRP:HZ2 | 1:21:A:ARG:HB3 | 5        | 1.57          |
| (3,35)  | 1:11:A:TRP:HZ2 | 1:21:A:ARG:HB3 | 4        | 1.56          |
| (1,336) | 1:11:A:TRP:HZ2 | 1:21:A:ARG:HB3 | 4        | 1.56          |
| (2,474) | 1:9:A:ILE:HD11 | 1:13:A:LYS:HE3 | 9        | 1.55          |
| (2,474) | 1:9:A:ILE:HD12 | 1:13:A:LYS:HE3 | 9        | 1.55          |
| (2,474) | 1:9:A:ILE:HD13 | 1:13:A:LYS:HE3 | 9        | 1.55          |
| (1,550) | 1:9:A:ILE:HD11 | 1:13:A:LYS:HE3 | 9        | 1.55          |
| (1,550) | 1:9:A:ILE:HD12 | 1:13:A:LYS:HE3 | 9        | 1.55          |
| (1,550) | 1:9:A:ILE:HD13 | 1:13:A:LYS:HE3 | 9        | 1.55          |
| (3,35)  | 1:11:A:TRP:HZ2 | 1:21:A:ARG:HB3 | 2        | 1.53          |
| (2,445) | 1:1:A:GLU:HB2  | 1:2:A:GLU:HG2  | 5        | 1.53          |
| (1,512) | 1:1:A:GLU:HB2  | 1:2:A:GLU:HG2  | 5        | 1.53          |
| (1,336) | 1:11:A:TRP:HZ2 | 1:21:A:ARG:HB3 | 2        | 1.53          |
| (3,35)  | 1:11:A:TRP:HZ2 | 1:21:A:ARG:HB3 | 8        | 1.52          |
| (1,336) | 1:11:A:TRP:HZ2 | 1:21:A:ARG:HB3 | 8        | 1.52          |
| (3,35)  | 1:11:A:TRP:HZ2 | 1:21:A:ARG:HB3 | 3        | 1.51          |
| (1,336) | 1:11:A:TRP:HZ2 | 1:21:A:ARG:HB3 | 3        | 1.51          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (3,65)  | 1:6:A:ARG:HA    | 1:10:A:GLN:HB3 | 1        | 1.5           |
| (2,445) | 1:1:A:GLU:HB2   | 1:2:A:GLU:HG2  | 9        | 1.5           |
| (2,445) | 1:1:A:GLU:HB2   | 1:2:A:GLU:HG2  | 10       | 1.5           |
| (1,512) | 1:1:A:GLU:HB2   | 1:2:A:GLU:HG2  | 9        | 1.5           |
| (1,512) | 1:1:A:GLU:HB2   | 1:2:A:GLU:HG2  | 10       | 1.5           |
| (1,482) | 1:6:A:ARG:HA    | 1:10:A:GLN:HB3 | 1        | 1.5           |
| (3,83)  | 1:12:A:LEU:HD11 | 1:16:A:GLY:H   | 5        | 1.49          |
| (3,83)  | 1:12:A:LEU:HD12 | 1:16:A:GLY:H   | 5        | 1.49          |
| (3,83)  | 1:12:A:LEU:HD13 | 1:16:A:GLY:H   | 5        | 1.49          |
| (1,565) | 1:12:A:LEU:HD11 | 1:16:A:GLY:H   | 5        | 1.49          |
| (1,565) | 1:12:A:LEU:HD12 | 1:16:A:GLY:H   | 5        | 1.49          |
| (1,565) | 1:12:A:LEU:HD13 | 1:16:A:GLY:H   | 5        | 1.49          |
| (3,65)  | 1:6:A:ARG:HA    | 1:10:A:GLN:HB3 | 8        | 1.48          |
| (1,482) | 1:6:A:ARG:HA    | 1:10:A:GLN:HB3 | 8        | 1.48          |
| (3,35)  | 1:11:A:TRP:HZ2  | 1:21:A:ARG:HB3 | 7        | 1.47          |
| (2,445) | 1:1:A:GLU:HB2   | 1:2:A:GLU:HG2  | 4        | 1.47          |
| (1,512) | 1:1:A:GLU:HB2   | 1:2:A:GLU:HG2  | 4        | 1.47          |
| (1,336) | 1:11:A:TRP:HZ2  | 1:21:A:ARG:HB3 | 7        | 1.47          |
| (3,83)  | 1:12:A:LEU:HD11 | 1:16:A:GLY:H   | 9        | 1.46          |
| (3,83)  | 1:12:A:LEU:HD12 | 1:16:A:GLY:H   | 9        | 1.46          |
| (3,83)  | 1:12:A:LEU:HD13 | 1:16:A:GLY:H   | 9        | 1.46          |
| (1,565) | 1:12:A:LEU:HD11 | 1:16:A:GLY:H   | 9        | 1.46          |
| (1,565) | 1:12:A:LEU:HD12 | 1:16:A:GLY:H   | 9        | 1.46          |
| (1,565) | 1:12:A:LEU:HD13 | 1:16:A:GLY:H   | 9        | 1.46          |
| (3,83)  | 1:12:A:LEU:HD11 | 1:16:A:GLY:H   | 1        | 1.45          |
| (3,83)  | 1:12:A:LEU:HD12 | 1:16:A:GLY:H   | 1        | 1.45          |
| (3,83)  | 1:12:A:LEU:HD13 | 1:16:A:GLY:H   | 1        | 1.45          |
| (3,83)  | 1:12:A:LEU:HD11 | 1:16:A:GLY:H   | 4        | 1.45          |
| (3,83)  | 1:12:A:LEU:HD12 | 1:16:A:GLY:H   | 4        | 1.45          |
| (3,83)  | 1:12:A:LEU:HD13 | 1:16:A:GLY:H   | 4        | 1.45          |
| (1,565) | 1:12:A:LEU:HD11 | 1:16:A:GLY:H   | 1        | 1.45          |
| (1,565) | 1:12:A:LEU:HD12 | 1:16:A:GLY:H   | 1        | 1.45          |
| (1,565) | 1:12:A:LEU:HD13 | 1:16:A:GLY:H   | 1        | 1.45          |
| (1,565) | 1:12:A:LEU:HD11 | 1:16:A:GLY:H   | 4        | 1.45          |
| (1,565) | 1:12:A:LEU:HD12 | 1:16:A:GLY:H   | 4        | 1.45          |
| (1,565) | 1:12:A:LEU:HD13 | 1:16:A:GLY:H   | 4        | 1.45          |
| (3,83)  | 1:12:A:LEU:HD11 | 1:16:A:GLY:H   | 2        | 1.44          |
| (3,83)  | 1:12:A:LEU:HD12 | 1:16:A:GLY:H   | 2        | 1.44          |
| (3,83)  | 1:12:A:LEU:HD13 | 1:16:A:GLY:H   | 2        | 1.44          |
| (1,565) | 1:12:A:LEU:HD11 | 1:16:A:GLY:H   | 2        | 1.44          |
| (1,565) | 1:12:A:LEU:HD12 | 1:16:A:GLY:H   | 2        | 1.44          |
| (1,565) | 1:12:A:LEU:HD13 | 1:16:A:GLY:H   | 2        | 1.44          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (3,65)  | 1:6:A:ARG:HA    | 1:10:A:GLN:HB3 | 4        | 1.43          |
| (1,482) | 1:6:A:ARG:HA    | 1:10:A:GLN:HB3 | 4        | 1.43          |
| (3,83)  | 1:12:A:LEU:HD11 | 1:16:A:GLY:H   | 7        | 1.42          |
| (3,83)  | 1:12:A:LEU:HD12 | 1:16:A:GLY:H   | 7        | 1.42          |
| (3,83)  | 1:12:A:LEU:HD13 | 1:16:A:GLY:H   | 7        | 1.42          |
| (1,565) | 1:12:A:LEU:HD11 | 1:16:A:GLY:H   | 7        | 1.42          |
| (1,565) | 1:12:A:LEU:HD12 | 1:16:A:GLY:H   | 7        | 1.42          |
| (1,565) | 1:12:A:LEU:HD13 | 1:16:A:GLY:H   | 7        | 1.42          |
| (3,65)  | 1:6:A:ARG:HA    | 1:10:A:GLN:HB3 | 7        | 1.41          |
| (2,445) | 1:1:A:GLU:HB2   | 1:2:A:GLU:HG2  | 8        | 1.41          |
| (1,512) | 1:1:A:GLU:HB2   | 1:2:A:GLU:HG2  | 8        | 1.41          |
| (1,482) | 1:6:A:ARG:HA    | 1:10:A:GLN:HB3 | 7        | 1.41          |
| (3,83)  | 1:12:A:LEU:HD11 | 1:16:A:GLY:H   | 3        | 1.39          |
| (3,83)  | 1:12:A:LEU:HD12 | 1:16:A:GLY:H   | 3        | 1.39          |
| (3,83)  | 1:12:A:LEU:HD13 | 1:16:A:GLY:H   | 3        | 1.39          |
| (3,83)  | 1:12:A:LEU:HD11 | 1:16:A:GLY:H   | 8        | 1.39          |
| (3,83)  | 1:12:A:LEU:HD12 | 1:16:A:GLY:H   | 8        | 1.39          |
| (3,83)  | 1:12:A:LEU:HD13 | 1:16:A:GLY:H   | 8        | 1.39          |
| (3,83)  | 1:12:A:LEU:HD11 | 1:16:A:GLY:H   | 10       | 1.39          |
| (3,83)  | 1:12:A:LEU:HD12 | 1:16:A:GLY:H   | 10       | 1.39          |
| (3,83)  | 1:12:A:LEU:HD13 | 1:16:A:GLY:H   | 10       | 1.39          |
| (3,65)  | 1:6:A:ARG:HA    | 1:10:A:GLN:HB3 | 6        | 1.39          |
| (2,378) | 1:11:A:TRP:H    | 1:24:A:PRO:HG2 | 1        | 1.39          |
| (1,565) | 1:12:A:LEU:HD11 | 1:16:A:GLY:H   | 3        | 1.39          |
| (1,565) | 1:12:A:LEU:HD12 | 1:16:A:GLY:H   | 3        | 1.39          |
| (1,565) | 1:12:A:LEU:HD13 | 1:16:A:GLY:H   | 3        | 1.39          |
| (1,565) | 1:12:A:LEU:HD11 | 1:16:A:GLY:H   | 8        | 1.39          |
| (1,565) | 1:12:A:LEU:HD12 | 1:16:A:GLY:H   | 8        | 1.39          |
| (1,565) | 1:12:A:LEU:HD13 | 1:16:A:GLY:H   | 8        | 1.39          |
| (1,565) | 1:12:A:LEU:HD11 | 1:16:A:GLY:H   | 10       | 1.39          |
| (1,565) | 1:12:A:LEU:HD12 | 1:16:A:GLY:H   | 10       | 1.39          |
| (1,565) | 1:12:A:LEU:HD13 | 1:16:A:GLY:H   | 10       | 1.39          |
| (1,482) | 1:6:A:ARG:HA    | 1:10:A:GLN:HB3 | 6        | 1.39          |
| (1,434) | 1:11:A:TRP:H    | 1:24:A:PRO:HG2 | 1        | 1.39          |
| (3,35)  | 1:11:A:TRP:HZ2  | 1:21:A:ARG:HB3 | 10       | 1.38          |
| (2,378) | 1:11:A:TRP:H    | 1:24:A:PRO:HG2 | 6        | 1.38          |
| (2,261) | 1:11:A:TRP:HE1  | 1:24:A:PRO:HD2 | 8        | 1.38          |
| (1,434) | 1:11:A:TRP:H    | 1:24:A:PRO:HG2 | 6        | 1.38          |
| (1,336) | 1:11:A:TRP:HZ2  | 1:21:A:ARG:HB3 | 10       | 1.38          |
| (1,280) | 1:11:A:TRP:HE1  | 1:24:A:PRO:HD2 | 8        | 1.38          |
| (3,65)  | 1:6:A:ARG:HA    | 1:10:A:GLN:HB3 | 5        | 1.37          |
| (2,378) | 1:11:A:TRP:H    | 1:24:A:PRO:HG2 | 4        | 1.37          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,482) | 1:6:A:ARG:HA   | 1:10:A:GLN:HB3 | 5        | 1.37          |
| (1,434) | 1:11:A:TRP:H   | 1:24:A:PRO:HG2 | 4        | 1.37          |
| (3,88)  | 1:1:A:GLU:HB2  | 1:3:A:GLU:HA   | 6        | 1.35          |
| (2,378) | 1:11:A:TRP:H   | 1:24:A:PRO:HG2 | 5        | 1.35          |
| (1,578) | 1:1:A:GLU:HB2  | 1:3:A:GLU:HA   | 6        | 1.35          |
| (1,434) | 1:11:A:TRP:H   | 1:24:A:PRO:HG2 | 5        | 1.35          |
| (2,488) | 1:8:A:TYR:HD1  | 1:11:A:TRP:HB2 | 2        | 1.34          |
| (2,488) | 1:8:A:TYR:HD2  | 1:11:A:TRP:HB2 | 2        | 1.34          |
| (2,378) | 1:11:A:TRP:H   | 1:24:A:PRO:HG2 | 2        | 1.34          |
| (2,378) | 1:11:A:TRP:H   | 1:24:A:PRO:HG2 | 3        | 1.34          |
| (2,378) | 1:11:A:TRP:H   | 1:24:A:PRO:HG2 | 7        | 1.34          |
| (1,573) | 1:8:A:TYR:HD1  | 1:11:A:TRP:HB2 | 2        | 1.34          |
| (1,573) | 1:8:A:TYR:HD2  | 1:11:A:TRP:HB2 | 2        | 1.34          |
| (1,434) | 1:11:A:TRP:H   | 1:24:A:PRO:HG2 | 2        | 1.34          |
| (1,434) | 1:11:A:TRP:H   | 1:24:A:PRO:HG2 | 3        | 1.34          |
| (1,434) | 1:11:A:TRP:H   | 1:24:A:PRO:HG2 | 7        | 1.34          |
| (3,90)  | 1:5:A:VAL:HG11 | 1:9:A:ILE:HB   | 1        | 1.32          |
| (3,90)  | 1:5:A:VAL:HG12 | 1:9:A:ILE:HB   | 1        | 1.32          |
| (3,90)  | 1:5:A:VAL:HG13 | 1:9:A:ILE:HB   | 1        | 1.32          |
| (2,488) | 1:8:A:TYR:HD1  | 1:11:A:TRP:HB2 | 3        | 1.32          |
| (2,488) | 1:8:A:TYR:HD2  | 1:11:A:TRP:HB2 | 3        | 1.32          |
| (2,488) | 1:8:A:TYR:HD1  | 1:11:A:TRP:HB2 | 4        | 1.32          |
| (2,488) | 1:8:A:TYR:HD2  | 1:11:A:TRP:HB2 | 4        | 1.32          |
| (2,488) | 1:8:A:TYR:HD1  | 1:11:A:TRP:HB2 | 5        | 1.32          |
| (2,488) | 1:8:A:TYR:HD2  | 1:11:A:TRP:HB2 | 5        | 1.32          |
| (2,378) | 1:11:A:TRP:H   | 1:24:A:PRO:HG2 | 9        | 1.32          |
| (1,591) | 1:5:A:VAL:HG11 | 1:9:A:ILE:HB   | 1        | 1.32          |
| (1,591) | 1:5:A:VAL:HG12 | 1:9:A:ILE:HB   | 1        | 1.32          |
| (1,591) | 1:5:A:VAL:HG13 | 1:9:A:ILE:HB   | 1        | 1.32          |
| (1,573) | 1:8:A:TYR:HD1  | 1:11:A:TRP:HB2 | 3        | 1.32          |
| (1,573) | 1:8:A:TYR:HD2  | 1:11:A:TRP:HB2 | 3        | 1.32          |
| (1,573) | 1:8:A:TYR:HD1  | 1:11:A:TRP:HB2 | 4        | 1.32          |
| (1,573) | 1:8:A:TYR:HD2  | 1:11:A:TRP:HB2 | 4        | 1.32          |
| (1,573) | 1:8:A:TYR:HD1  | 1:11:A:TRP:HB2 | 5        | 1.32          |
| (1,573) | 1:8:A:TYR:HD2  | 1:11:A:TRP:HB2 | 5        | 1.32          |
| (1,434) | 1:11:A:TRP:H   | 1:24:A:PRO:HG2 | 9        | 1.32          |
| (3,30)  | 1:7:A:LEU:HD11 | 1:8:A:TYR:HD1  | 4        | 1.31          |
| (3,30)  | 1:7:A:LEU:HD11 | 1:8:A:TYR:HD2  | 4        | 1.31          |
| (3,30)  | 1:7:A:LEU:HD12 | 1:8:A:TYR:HD1  | 4        | 1.31          |
| (3,30)  | 1:7:A:LEU:HD12 | 1:8:A:TYR:HD2  | 4        | 1.31          |
| (3,30)  | 1:7:A:LEU:HD13 | 1:8:A:TYR:HD1  | 4        | 1.31          |
| (3,30)  | 1:7:A:LEU:HD13 | 1:8:A:TYR:HD2  | 4        | 1.31          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (2,488) | 1:8:A:TYR:HD1  | 1:11:A:TRP:HB2 | 7        | 1.31          |
| (2,488) | 1:8:A:TYR:HD2  | 1:11:A:TRP:HB2 | 7        | 1.31          |
| (2,445) | 1:1:A:GLU:HB2  | 1:2:A:GLU:HG2  | 6        | 1.31          |
| (2,424) | 1:21:A:ARG:HB2 | 1:22:A:PRO:HD3 | 6        | 1.31          |
| (1,573) | 1:8:A:TYR:HD1  | 1:11:A:TRP:HB2 | 7        | 1.31          |
| (1,573) | 1:8:A:TYR:HD2  | 1:11:A:TRP:HB2 | 7        | 1.31          |
| (1,512) | 1:1:A:GLU:HB2  | 1:2:A:GLU:HG2  | 6        | 1.31          |
| (1,489) | 1:21:A:ARG:HB2 | 1:22:A:PRO:HD3 | 6        | 1.31          |
| (1,318) | 1:7:A:LEU:HD11 | 1:8:A:TYR:HD1  | 4        | 1.31          |
| (1,318) | 1:7:A:LEU:HD11 | 1:8:A:TYR:HD2  | 4        | 1.31          |
| (1,318) | 1:7:A:LEU:HD12 | 1:8:A:TYR:HD1  | 4        | 1.31          |
| (1,318) | 1:7:A:LEU:HD12 | 1:8:A:TYR:HD2  | 4        | 1.31          |
| (1,318) | 1:7:A:LEU:HD13 | 1:8:A:TYR:HD1  | 4        | 1.31          |
| (1,318) | 1:7:A:LEU:HD13 | 1:8:A:TYR:HD2  | 4        | 1.31          |
| (2,488) | 1:8:A:TYR:HD1  | 1:11:A:TRP:HB2 | 6        | 1.3           |
| (2,488) | 1:8:A:TYR:HD2  | 1:11:A:TRP:HB2 | 6        | 1.3           |
| (1,573) | 1:8:A:TYR:HD1  | 1:11:A:TRP:HB2 | 6        | 1.3           |
| (1,573) | 1:8:A:TYR:HD2  | 1:11:A:TRP:HB2 | 6        | 1.3           |
| (3,90)  | 1:5:A:VAL:HG11 | 1:9:A:ILE:HB   | 10       | 1.29          |
| (3,90)  | 1:5:A:VAL:HG12 | 1:9:A:ILE:HB   | 10       | 1.29          |
| (3,90)  | 1:5:A:VAL:HG13 | 1:9:A:ILE:HB   | 10       | 1.29          |
| (3,30)  | 1:7:A:LEU:HD11 | 1:8:A:TYR:HD1  | 1        | 1.29          |
| (3,30)  | 1:7:A:LEU:HD11 | 1:8:A:TYR:HD2  | 1        | 1.29          |
| (3,30)  | 1:7:A:LEU:HD12 | 1:8:A:TYR:HD1  | 1        | 1.29          |
| (3,30)  | 1:7:A:LEU:HD12 | 1:8:A:TYR:HD2  | 1        | 1.29          |
| (3,30)  | 1:7:A:LEU:HD13 | 1:8:A:TYR:HD1  | 1        | 1.29          |
| (3,30)  | 1:7:A:LEU:HD13 | 1:8:A:TYR:HD2  | 1        | 1.29          |
| (3,30)  | 1:7:A:LEU:HD11 | 1:8:A:TYR:HD1  | 2        | 1.29          |
| (3,30)  | 1:7:A:LEU:HD11 | 1:8:A:TYR:HD2  | 2        | 1.29          |
| (3,30)  | 1:7:A:LEU:HD12 | 1:8:A:TYR:HD1  | 2        | 1.29          |
| (3,30)  | 1:7:A:LEU:HD12 | 1:8:A:TYR:HD2  | 2        | 1.29          |
| (3,30)  | 1:7:A:LEU:HD13 | 1:8:A:TYR:HD1  | 2        | 1.29          |
| (3,30)  | 1:7:A:LEU:HD13 | 1:8:A:TYR:HD2  | 2        | 1.29          |
| (2,488) | 1:8:A:TYR:HD1  | 1:11:A:TRP:HB2 | 8        | 1.29          |
| (2,488) | 1:8:A:TYR:HD2  | 1:11:A:TRP:HB2 | 8        | 1.29          |
| (2,424) | 1:21:A:ARG:HB2 | 1:22:A:PRO:HD3 | 1        | 1.29          |
| (1,591) | 1:5:A:VAL:HG11 | 1:9:A:ILE:HB   | 10       | 1.29          |
| (1,591) | 1:5:A:VAL:HG12 | 1:9:A:ILE:HB   | 10       | 1.29          |
| (1,591) | 1:5:A:VAL:HG13 | 1:9:A:ILE:HB   | 10       | 1.29          |
| (1,573) | 1:8:A:TYR:HD1  | 1:11:A:TRP:HB2 | 8        | 1.29          |
| (1,573) | 1:8:A:TYR:HD2  | 1:11:A:TRP:HB2 | 8        | 1.29          |
| (1,489) | 1:21:A:ARG:HB2 | 1:22:A:PRO:HD3 | 1        | 1.29          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,318) | 1:7:A:LEU:HD11 | 1:8:A:TYR:HD1  | 1        | 1.29          |
| (1,318) | 1:7:A:LEU:HD11 | 1:8:A:TYR:HD2  | 1        | 1.29          |
| (1,318) | 1:7:A:LEU:HD12 | 1:8:A:TYR:HD1  | 1        | 1.29          |
| (1,318) | 1:7:A:LEU:HD12 | 1:8:A:TYR:HD2  | 1        | 1.29          |
| (1,318) | 1:7:A:LEU:HD13 | 1:8:A:TYR:HD1  | 1        | 1.29          |
| (1,318) | 1:7:A:LEU:HD13 | 1:8:A:TYR:HD2  | 1        | 1.29          |
| (1,318) | 1:7:A:LEU:HD11 | 1:8:A:TYR:HD1  | 2        | 1.29          |
| (1,318) | 1:7:A:LEU:HD11 | 1:8:A:TYR:HD2  | 2        | 1.29          |
| (1,318) | 1:7:A:LEU:HD12 | 1:8:A:TYR:HD1  | 2        | 1.29          |
| (1,318) | 1:7:A:LEU:HD12 | 1:8:A:TYR:HD2  | 2        | 1.29          |
| (1,318) | 1:7:A:LEU:HD13 | 1:8:A:TYR:HD1  | 2        | 1.29          |
| (1,318) | 1:7:A:LEU:HD13 | 1:8:A:TYR:HD2  | 2        | 1.29          |
| (3,90)  | 1:5:A:VAL:HG11 | 1:9:A:ILE:HB   | 9        | 1.28          |
| (3,90)  | 1:5:A:VAL:HG12 | 1:9:A:ILE:HB   | 9        | 1.28          |
| (3,90)  | 1:5:A:VAL:HG13 | 1:9:A:ILE:HB   | 9        | 1.28          |
| (2,488) | 1:8:A:TYR:HD1  | 1:11:A:TRP:HB2 | 1        | 1.28          |
| (2,488) | 1:8:A:TYR:HD2  | 1:11:A:TRP:HB2 | 1        | 1.28          |
| (2,445) | 1:1:A:GLU:HB2  | 1:2:A:GLU:HG2  | 7        | 1.28          |
| (2,378) | 1:11:A:TRP:H   | 1:24:A:PRO:HG2 | 10       | 1.28          |
| (1,591) | 1:5:A:VAL:HG11 | 1:9:A:ILE:HB   | 9        | 1.28          |
| (1,591) | 1:5:A:VAL:HG12 | 1:9:A:ILE:HB   | 9        | 1.28          |
| (1,591) | 1:5:A:VAL:HG13 | 1:9:A:ILE:HB   | 9        | 1.28          |
| (1,573) | 1:8:A:TYR:HD1  | 1:11:A:TRP:HB2 | 1        | 1.28          |
| (1,573) | 1:8:A:TYR:HD2  | 1:11:A:TRP:HB2 | 1        | 1.28          |
| (1,512) | 1:1:A:GLU:HB2  | 1:2:A:GLU:HG2  | 7        | 1.28          |
| (1,434) | 1:11:A:TRP:H   | 1:24:A:PRO:HG2 | 10       | 1.28          |
| (3,90)  | 1:5:A:VAL:HG11 | 1:9:A:ILE:HB   | 2        | 1.26          |
| (3,90)  | 1:5:A:VAL:HG12 | 1:9:A:ILE:HB   | 2        | 1.26          |
| (3,90)  | 1:5:A:VAL:HG13 | 1:9:A:ILE:HB   | 2        | 1.26          |
| (3,90)  | 1:5:A:VAL:HG11 | 1:9:A:ILE:HB   | 4        | 1.26          |
| (3,90)  | 1:5:A:VAL:HG12 | 1:9:A:ILE:HB   | 4        | 1.26          |
| (3,90)  | 1:5:A:VAL:HG13 | 1:9:A:ILE:HB   | 4        | 1.26          |
| (3,52)  | 1:21:A:ARG:H   | 1:22:A:PRO:HD2 | 1        | 1.26          |
| (1,591) | 1:5:A:VAL:HG11 | 1:9:A:ILE:HB   | 2        | 1.26          |
| (1,591) | 1:5:A:VAL:HG12 | 1:9:A:ILE:HB   | 2        | 1.26          |
| (1,591) | 1:5:A:VAL:HG13 | 1:9:A:ILE:HB   | 2        | 1.26          |
| (1,591) | 1:5:A:VAL:HG11 | 1:9:A:ILE:HB   | 4        | 1.26          |
| (1,591) | 1:5:A:VAL:HG12 | 1:9:A:ILE:HB   | 4        | 1.26          |
| (1,591) | 1:5:A:VAL:HG13 | 1:9:A:ILE:HB   | 4        | 1.26          |
| (1,418) | 1:21:A:ARG:H   | 1:22:A:PRO:HD2 | 1        | 1.26          |
| (3,5)   | 1:7:A:LEU:HA   | 1:7:A:LEU:HD11 | 9        | 1.25          |
| (3,5)   | 1:7:A:LEU:HA   | 1:7:A:LEU:HD12 | 9        | 1.25          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (3,5)   | 1:7:A:LEU:HA   | 1:7:A:LEU:HD13 | 9        | 1.25          |
| (3,5)   | 1:7:A:LEU:HA   | 1:7:A:LEU:HD11 | 10       | 1.25          |
| (3,5)   | 1:7:A:LEU:HA   | 1:7:A:LEU:HD12 | 10       | 1.25          |
| (3,5)   | 1:7:A:LEU:HA   | 1:7:A:LEU:HD13 | 10       | 1.25          |
| (1,59)  | 1:7:A:LEU:HA   | 1:7:A:LEU:HD11 | 9        | 1.25          |
| (1,59)  | 1:7:A:LEU:HA   | 1:7:A:LEU:HD12 | 9        | 1.25          |
| (1,59)  | 1:7:A:LEU:HA   | 1:7:A:LEU:HD13 | 9        | 1.25          |
| (1,59)  | 1:7:A:LEU:HA   | 1:7:A:LEU:HD11 | 10       | 1.25          |
| (1,59)  | 1:7:A:LEU:HA   | 1:7:A:LEU:HD12 | 10       | 1.25          |
| (1,59)  | 1:7:A:LEU:HA   | 1:7:A:LEU:HD13 | 10       | 1.25          |
| (3,30)  | 1:7:A:LEU:HD11 | 1:8:A:TYR:HD1  | 7        | 1.24          |
| (3,30)  | 1:7:A:LEU:HD11 | 1:8:A:TYR:HD2  | 7        | 1.24          |
| (3,30)  | 1:7:A:LEU:HD12 | 1:8:A:TYR:HD1  | 7        | 1.24          |
| (3,30)  | 1:7:A:LEU:HD12 | 1:8:A:TYR:HD2  | 7        | 1.24          |
| (3,30)  | 1:7:A:LEU:HD13 | 1:8:A:TYR:HD1  | 7        | 1.24          |
| (3,30)  | 1:7:A:LEU:HD13 | 1:8:A:TYR:HD2  | 7        | 1.24          |
| (1,318) | 1:7:A:LEU:HD11 | 1:8:A:TYR:HD1  | 7        | 1.24          |
| (1,318) | 1:7:A:LEU:HD11 | 1:8:A:TYR:HD2  | 7        | 1.24          |
| (1,318) | 1:7:A:LEU:HD12 | 1:8:A:TYR:HD1  | 7        | 1.24          |
| (1,318) | 1:7:A:LEU:HD12 | 1:8:A:TYR:HD2  | 7        | 1.24          |
| (1,318) | 1:7:A:LEU:HD13 | 1:8:A:TYR:HD1  | 7        | 1.24          |
| (1,318) | 1:7:A:LEU:HD13 | 1:8:A:TYR:HD2  | 7        | 1.24          |
| (3,90)  | 1:5:A:VAL:HG11 | 1:9:A:ILE:HB   | 3        | 1.23          |
| (3,90)  | 1:5:A:VAL:HG12 | 1:9:A:ILE:HB   | 3        | 1.23          |
| (3,90)  | 1:5:A:VAL:HG13 | 1:9:A:ILE:HB   | 3        | 1.23          |
| (1,591) | 1:5:A:VAL:HG11 | 1:9:A:ILE:HB   | 3        | 1.23          |
| (1,591) | 1:5:A:VAL:HG12 | 1:9:A:ILE:HB   | 3        | 1.23          |
| (1,591) | 1:5:A:VAL:HG13 | 1:9:A:ILE:HB   | 3        | 1.23          |
| (3,88)  | 1:1:A:GLU:HB2  | 1:3:A:GLU:HA   | 8        | 1.22          |
| (3,86)  | 1:11:A:TRP:HB3 | 1:11:A:TRP:HD1 | 2        | 1.22          |
| (3,86)  | 1:11:A:TRP:HB3 | 1:11:A:TRP:HD1 | 4        | 1.22          |
| (3,86)  | 1:11:A:TRP:HB3 | 1:11:A:TRP:HD1 | 5        | 1.22          |
| (3,86)  | 1:11:A:TRP:HB3 | 1:11:A:TRP:HD1 | 7        | 1.22          |
| (3,30)  | 1:7:A:LEU:HD11 | 1:8:A:TYR:HD1  | 3        | 1.22          |
| (3,30)  | 1:7:A:LEU:HD11 | 1:8:A:TYR:HD2  | 3        | 1.22          |
| (3,30)  | 1:7:A:LEU:HD12 | 1:8:A:TYR:HD1  | 3        | 1.22          |
| (3,30)  | 1:7:A:LEU:HD12 | 1:8:A:TYR:HD2  | 3        | 1.22          |
| (3,30)  | 1:7:A:LEU:HD13 | 1:8:A:TYR:HD1  | 3        | 1.22          |
| (3,30)  | 1:7:A:LEU:HD13 | 1:8:A:TYR:HD2  | 3        | 1.22          |
| (1,578) | 1:1:A:GLU:HB2  | 1:3:A:GLU:HA   | 8        | 1.22          |
| (1,574) | 1:11:A:TRP:HB3 | 1:11:A:TRP:HD1 | 2        | 1.22          |
| (1,574) | 1:11:A:TRP:HB3 | 1:11:A:TRP:HD1 | 4        | 1.22          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,574) | 1:11:A:TRP:HB3 | 1:11:A:TRP:HD1 | 5        | 1.22          |
| (1,574) | 1:11:A:TRP:HB3 | 1:11:A:TRP:HD1 | 7        | 1.22          |
| (1,318) | 1:7:A:LEU:HD11 | 1:8:A:TYR:HD1  | 3        | 1.22          |
| (1,318) | 1:7:A:LEU:HD11 | 1:8:A:TYR:HD2  | 3        | 1.22          |
| (1,318) | 1:7:A:LEU:HD12 | 1:8:A:TYR:HD1  | 3        | 1.22          |
| (1,318) | 1:7:A:LEU:HD12 | 1:8:A:TYR:HD2  | 3        | 1.22          |
| (1,318) | 1:7:A:LEU:HD13 | 1:8:A:TYR:HD1  | 3        | 1.22          |
| (1,318) | 1:7:A:LEU:HD13 | 1:8:A:TYR:HD2  | 3        | 1.22          |
| (3,91)  | 1:7:A:LEU:HD21 | 1:8:A:TYR:HB2  | 1        | 1.21          |
| (3,91)  | 1:7:A:LEU:HD22 | 1:8:A:TYR:HB2  | 1        | 1.21          |
| (3,91)  | 1:7:A:LEU:HD23 | 1:8:A:TYR:HB2  | 1        | 1.21          |
| (3,91)  | 1:7:A:LEU:HD21 | 1:8:A:TYR:HB2  | 3        | 1.21          |
| (3,91)  | 1:7:A:LEU:HD22 | 1:8:A:TYR:HB2  | 3        | 1.21          |
| (3,91)  | 1:7:A:LEU:HD23 | 1:8:A:TYR:HB2  | 3        | 1.21          |
| (3,86)  | 1:11:A:TRP:HB3 | 1:11:A:TRP:HD1 | 3        | 1.21          |
| (3,86)  | 1:11:A:TRP:HB3 | 1:11:A:TRP:HD1 | 8        | 1.21          |
| (3,78)  | 1:7:A:LEU:HD21 | 1:24:A:PRO:HB2 | 10       | 1.21          |
| (3,78)  | 1:7:A:LEU:HD22 | 1:24:A:PRO:HB2 | 10       | 1.21          |
| (3,78)  | 1:7:A:LEU:HD23 | 1:24:A:PRO:HB2 | 10       | 1.21          |
| (3,52)  | 1:21:A:ARG:H   | 1:22:A:PRO:HD2 | 6        | 1.21          |
| (3,30)  | 1:7:A:LEU:HD11 | 1:8:A:TYR:HD1  | 6        | 1.21          |
| (3,30)  | 1:7:A:LEU:HD11 | 1:8:A:TYR:HD2  | 6        | 1.21          |
| (3,30)  | 1:7:A:LEU:HD12 | 1:8:A:TYR:HD1  | 6        | 1.21          |
| (3,30)  | 1:7:A:LEU:HD12 | 1:8:A:TYR:HD2  | 6        | 1.21          |
| (3,30)  | 1:7:A:LEU:HD13 | 1:8:A:TYR:HD1  | 6        | 1.21          |
| (3,30)  | 1:7:A:LEU:HD13 | 1:8:A:TYR:HD2  | 6        | 1.21          |
| (1,595) | 1:7:A:LEU:HD21 | 1:8:A:TYR:HB2  | 1        | 1.21          |
| (1,595) | 1:7:A:LEU:HD22 | 1:8:A:TYR:HB2  | 1        | 1.21          |
| (1,595) | 1:7:A:LEU:HD23 | 1:8:A:TYR:HB2  | 1        | 1.21          |
| (1,595) | 1:7:A:LEU:HD21 | 1:8:A:TYR:HB2  | 3        | 1.21          |
| (1,595) | 1:7:A:LEU:HD22 | 1:8:A:TYR:HB2  | 3        | 1.21          |
| (1,595) | 1:7:A:LEU:HD23 | 1:8:A:TYR:HB2  | 3        | 1.21          |
| (1,574) | 1:11:A:TRP:HB3 | 1:11:A:TRP:HD1 | 3        | 1.21          |
| (1,574) | 1:11:A:TRP:HB3 | 1:11:A:TRP:HD1 | 8        | 1.21          |
| (1,554) | 1:7:A:LEU:HD21 | 1:24:A:PRO:HB2 | 10       | 1.21          |
| (1,554) | 1:7:A:LEU:HD22 | 1:24:A:PRO:HB2 | 10       | 1.21          |
| (1,554) | 1:7:A:LEU:HD23 | 1:24:A:PRO:HB2 | 10       | 1.21          |
| (1,418) | 1:21:A:ARG:H   | 1:22:A:PRO:HD2 | 6        | 1.21          |
| (1,318) | 1:7:A:LEU:HD11 | 1:8:A:TYR:HD1  | 6        | 1.21          |
| (1,318) | 1:7:A:LEU:HD11 | 1:8:A:TYR:HD2  | 6        | 1.21          |
| (1,318) | 1:7:A:LEU:HD12 | 1:8:A:TYR:HD1  | 6        | 1.21          |
| (1,318) | 1:7:A:LEU:HD12 | 1:8:A:TYR:HD2  | 6        | 1.21          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,318) | 1:7:A:LEU:HD13 | 1:8:A:TYR:HD1  | 6        | 1.21          |
| (1,318) | 1:7:A:LEU:HD13 | 1:8:A:TYR:HD2  | 6        | 1.21          |
| (3,88)  | 1:1:A:GLU:HB2  | 1:3:A:GLU:HA   | 7        | 1.2           |
| (3,88)  | 1:1:A:GLU:HB2  | 1:3:A:GLU:HA   | 10       | 1.2           |
| (3,86)  | 1:11:A:TRP:HB3 | 1:11:A:TRP:HD1 | 9        | 1.2           |
| (3,86)  | 1:11:A:TRP:HB3 | 1:11:A:TRP:HD1 | 10       | 1.2           |
| (2,488) | 1:8:A:TYR:HD1  | 1:11:A:TRP:HB2 | 10       | 1.2           |
| (2,488) | 1:8:A:TYR:HD2  | 1:11:A:TRP:HB2 | 10       | 1.2           |
| (1,578) | 1:1:A:GLU:HB2  | 1:3:A:GLU:HA   | 7        | 1.2           |
| (1,578) | 1:1:A:GLU:HB2  | 1:3:A:GLU:HA   | 10       | 1.2           |
| (1,574) | 1:11:A:TRP:HB3 | 1:11:A:TRP:HD1 | 9        | 1.2           |
| (1,574) | 1:11:A:TRP:HB3 | 1:11:A:TRP:HD1 | 10       | 1.2           |
| (1,573) | 1:8:A:TYR:HD1  | 1:11:A:TRP:HB2 | 10       | 1.2           |
| (1,573) | 1:8:A:TYR:HD2  | 1:11:A:TRP:HB2 | 10       | 1.2           |
| (3,90)  | 1:5:A:VAL:HG11 | 1:9:A:ILE:HB   | 8        | 1.19          |
| (3,90)  | 1:5:A:VAL:HG12 | 1:9:A:ILE:HB   | 8        | 1.19          |
| (3,90)  | 1:5:A:VAL:HG13 | 1:9:A:ILE:HB   | 8        | 1.19          |
| (3,86)  | 1:11:A:TRP:HB3 | 1:11:A:TRP:HD1 | 1        | 1.19          |
| (3,86)  | 1:11:A:TRP:HB3 | 1:11:A:TRP:HD1 | 6        | 1.19          |
| (2,488) | 1:8:A:TYR:HD1  | 1:11:A:TRP:HB2 | 9        | 1.19          |
| (2,488) | 1:8:A:TYR:HD2  | 1:11:A:TRP:HB2 | 9        | 1.19          |
| (1,591) | 1:5:A:VAL:HG11 | 1:9:A:ILE:HB   | 8        | 1.19          |
| (1,591) | 1:5:A:VAL:HG12 | 1:9:A:ILE:HB   | 8        | 1.19          |
| (1,591) | 1:5:A:VAL:HG13 | 1:9:A:ILE:HB   | 8        | 1.19          |
| (1,574) | 1:11:A:TRP:HB3 | 1:11:A:TRP:HD1 | 1        | 1.19          |
| (1,574) | 1:11:A:TRP:HB3 | 1:11:A:TRP:HD1 | 6        | 1.19          |
| (1,573) | 1:8:A:TYR:HD1  | 1:11:A:TRP:HB2 | 9        | 1.19          |
| (1,573) | 1:8:A:TYR:HD2  | 1:11:A:TRP:HB2 | 9        | 1.19          |
| (3,91)  | 1:7:A:LEU:HD21 | 1:8:A:TYR:HB2  | 4        | 1.18          |
| (3,91)  | 1:7:A:LEU:HD22 | 1:8:A:TYR:HB2  | 4        | 1.18          |
| (3,91)  | 1:7:A:LEU:HD23 | 1:8:A:TYR:HB2  | 4        | 1.18          |
| (3,91)  | 1:7:A:LEU:HD21 | 1:8:A:TYR:HB2  | 5        | 1.18          |
| (3,91)  | 1:7:A:LEU:HD22 | 1:8:A:TYR:HB2  | 5        | 1.18          |
| (3,91)  | 1:7:A:LEU:HD23 | 1:8:A:TYR:HB2  | 5        | 1.18          |
| (3,91)  | 1:7:A:LEU:HD21 | 1:8:A:TYR:HB2  | 7        | 1.18          |
| (3,91)  | 1:7:A:LEU:HD22 | 1:8:A:TYR:HB2  | 7        | 1.18          |
| (3,91)  | 1:7:A:LEU:HD23 | 1:8:A:TYR:HB2  | 7        | 1.18          |
| (3,90)  | 1:5:A:VAL:HG11 | 1:9:A:ILE:HB   | 5        | 1.18          |
| (3,90)  | 1:5:A:VAL:HG12 | 1:9:A:ILE:HB   | 5        | 1.18          |
| (3,90)  | 1:5:A:VAL:HG13 | 1:9:A:ILE:HB   | 5        | 1.18          |
| (3,90)  | 1:5:A:VAL:HG11 | 1:9:A:ILE:HB   | 7        | 1.18          |
| (3,90)  | 1:5:A:VAL:HG12 | 1:9:A:ILE:HB   | 7        | 1.18          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (3,90)  | 1:5:A:VAL:HG13 | 1:9:A:ILE:HB   | 7        | 1.18          |
| (3,88)  | 1:1:A:GLU:HB2  | 1:3:A:GLU:HA   | 5        | 1.18          |
| (1,595) | 1:7:A:LEU:HD21 | 1:8:A:TYR:HB2  | 4        | 1.18          |
| (1,595) | 1:7:A:LEU:HD22 | 1:8:A:TYR:HB2  | 4        | 1.18          |
| (1,595) | 1:7:A:LEU:HD23 | 1:8:A:TYR:HB2  | 4        | 1.18          |
| (1,595) | 1:7:A:LEU:HD21 | 1:8:A:TYR:HB2  | 5        | 1.18          |
| (1,595) | 1:7:A:LEU:HD22 | 1:8:A:TYR:HB2  | 5        | 1.18          |
| (1,595) | 1:7:A:LEU:HD23 | 1:8:A:TYR:HB2  | 5        | 1.18          |
| (1,595) | 1:7:A:LEU:HD21 | 1:8:A:TYR:HB2  | 7        | 1.18          |
| (1,595) | 1:7:A:LEU:HD22 | 1:8:A:TYR:HB2  | 7        | 1.18          |
| (1,595) | 1:7:A:LEU:HD23 | 1:8:A:TYR:HB2  | 7        | 1.18          |
| (1,591) | 1:5:A:VAL:HG11 | 1:9:A:ILE:HB   | 5        | 1.18          |
| (1,591) | 1:5:A:VAL:HG12 | 1:9:A:ILE:HB   | 5        | 1.18          |
| (1,591) | 1:5:A:VAL:HG13 | 1:9:A:ILE:HB   | 5        | 1.18          |
| (1,591) | 1:5:A:VAL:HG11 | 1:9:A:ILE:HB   | 7        | 1.18          |
| (1,591) | 1:5:A:VAL:HG12 | 1:9:A:ILE:HB   | 7        | 1.18          |
| (1,591) | 1:5:A:VAL:HG13 | 1:9:A:ILE:HB   | 7        | 1.18          |
| (1,578) | 1:1:A:GLU:HB2  | 1:3:A:GLU:HA   | 5        | 1.18          |
| (3,91)  | 1:7:A:LEU:HD21 | 1:8:A:TYR:HB2  | 2        | 1.17          |
| (3,91)  | 1:7:A:LEU:HD22 | 1:8:A:TYR:HB2  | 2        | 1.17          |
| (3,91)  | 1:7:A:LEU:HD23 | 1:8:A:TYR:HB2  | 2        | 1.17          |
| (3,91)  | 1:7:A:LEU:HD21 | 1:8:A:TYR:HB2  | 8        | 1.17          |
| (3,91)  | 1:7:A:LEU:HD22 | 1:8:A:TYR:HB2  | 8        | 1.17          |
| (3,91)  | 1:7:A:LEU:HD23 | 1:8:A:TYR:HB2  | 8        | 1.17          |
| (1,595) | 1:7:A:LEU:HD21 | 1:8:A:TYR:HB2  | 2        | 1.17          |
| (1,595) | 1:7:A:LEU:HD22 | 1:8:A:TYR:HB2  | 2        | 1.17          |
| (1,595) | 1:7:A:LEU:HD23 | 1:8:A:TYR:HB2  | 2        | 1.17          |
| (1,595) | 1:7:A:LEU:HD21 | 1:8:A:TYR:HB2  | 8        | 1.17          |
| (1,595) | 1:7:A:LEU:HD22 | 1:8:A:TYR:HB2  | 8        | 1.17          |
| (1,595) | 1:7:A:LEU:HD23 | 1:8:A:TYR:HB2  | 8        | 1.17          |
| (3,91)  | 1:7:A:LEU:HD21 | 1:8:A:TYR:HB2  | 6        | 1.16          |
| (3,91)  | 1:7:A:LEU:HD22 | 1:8:A:TYR:HB2  | 6        | 1.16          |
| (3,91)  | 1:7:A:LEU:HD23 | 1:8:A:TYR:HB2  | 6        | 1.16          |
| (3,88)  | 1:1:A:GLU:HB2  | 1:3:A:GLU:HA   | 9        | 1.16          |
| (3,51)  | 1:4:A:ALA:H    | 1:5:A:VAL:HG21 | 4        | 1.16          |
| (3,51)  | 1:4:A:ALA:H    | 1:5:A:VAL:HG22 | 4        | 1.16          |
| (3,51)  | 1:4:A:ALA:H    | 1:5:A:VAL:HG23 | 4        | 1.16          |
| (3,30)  | 1:7:A:LEU:HD11 | 1:8:A:TYR:HD1  | 5        | 1.16          |
| (3,30)  | 1:7:A:LEU:HD11 | 1:8:A:TYR:HD2  | 5        | 1.16          |
| (3,30)  | 1:7:A:LEU:HD12 | 1:8:A:TYR:HD1  | 5        | 1.16          |
| (3,30)  | 1:7:A:LEU:HD12 | 1:8:A:TYR:HD2  | 5        | 1.16          |
| (3,30)  | 1:7:A:LEU:HD13 | 1:8:A:TYR:HD1  | 5        | 1.16          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (3,30)  | 1:7:A:LEU:HD13 | 1:8:A:TYR:HD2  | 5        | 1.16          |
| (3,30)  | 1:7:A:LEU:HD11 | 1:8:A:TYR:HD1  | 8        | 1.16          |
| (3,30)  | 1:7:A:LEU:HD11 | 1:8:A:TYR:HD2  | 8        | 1.16          |
| (3,30)  | 1:7:A:LEU:HD12 | 1:8:A:TYR:HD1  | 8        | 1.16          |
| (3,30)  | 1:7:A:LEU:HD12 | 1:8:A:TYR:HD2  | 8        | 1.16          |
| (3,30)  | 1:7:A:LEU:HD13 | 1:8:A:TYR:HD1  | 8        | 1.16          |
| (3,30)  | 1:7:A:LEU:HD13 | 1:8:A:TYR:HD2  | 8        | 1.16          |
| (2,424) | 1:21:A:ARG:HB2 | 1:22:A:PRO:HD3 | 2        | 1.16          |
| (1,595) | 1:7:A:LEU:HD21 | 1:8:A:TYR:HB2  | 6        | 1.16          |
| (1,595) | 1:7:A:LEU:HD22 | 1:8:A:TYR:HB2  | 6        | 1.16          |
| (1,595) | 1:7:A:LEU:HD23 | 1:8:A:TYR:HB2  | 6        | 1.16          |
| (1,578) | 1:1:A:GLU:HB2  | 1:3:A:GLU:HA   | 9        | 1.16          |
| (1,489) | 1:21:A:ARG:HB2 | 1:22:A:PRO:HD3 | 2        | 1.16          |
| (1,408) | 1:4:A:ALA:H    | 1:5:A:VAL:HG21 | 4        | 1.16          |
| (1,408) | 1:4:A:ALA:H    | 1:5:A:VAL:HG22 | 4        | 1.16          |
| (1,408) | 1:4:A:ALA:H    | 1:5:A:VAL:HG23 | 4        | 1.16          |
| (1,318) | 1:7:A:LEU:HD11 | 1:8:A:TYR:HD1  | 5        | 1.16          |
| (1,318) | 1:7:A:LEU:HD11 | 1:8:A:TYR:HD2  | 5        | 1.16          |
| (1,318) | 1:7:A:LEU:HD12 | 1:8:A:TYR:HD1  | 5        | 1.16          |
| (1,318) | 1:7:A:LEU:HD12 | 1:8:A:TYR:HD2  | 5        | 1.16          |
| (1,318) | 1:7:A:LEU:HD13 | 1:8:A:TYR:HD1  | 5        | 1.16          |
| (1,318) | 1:7:A:LEU:HD13 | 1:8:A:TYR:HD2  | 5        | 1.16          |
| (1,318) | 1:7:A:LEU:HD11 | 1:8:A:TYR:HD1  | 8        | 1.16          |
| (1,318) | 1:7:A:LEU:HD11 | 1:8:A:TYR:HD2  | 8        | 1.16          |
| (1,318) | 1:7:A:LEU:HD12 | 1:8:A:TYR:HD1  | 8        | 1.16          |
| (1,318) | 1:7:A:LEU:HD12 | 1:8:A:TYR:HD2  | 8        | 1.16          |
| (1,318) | 1:7:A:LEU:HD13 | 1:8:A:TYR:HD1  | 8        | 1.16          |
| (1,318) | 1:7:A:LEU:HD13 | 1:8:A:TYR:HD2  | 8        | 1.16          |
| (3,90)  | 1:5:A:VAL:HG11 | 1:9:A:ILE:HB   | 6        | 1.14          |
| (3,90)  | 1:5:A:VAL:HG12 | 1:9:A:ILE:HB   | 6        | 1.14          |
| (3,90)  | 1:5:A:VAL:HG13 | 1:9:A:ILE:HB   | 6        | 1.14          |
| (2,424) | 1:21:A:ARG:HB2 | 1:22:A:PRO:HD3 | 5        | 1.14          |
| (2,424) | 1:21:A:ARG:HB2 | 1:22:A:PRO:HD3 | 10       | 1.14          |
| (1,591) | 1:5:A:VAL:HG11 | 1:9:A:ILE:HB   | 6        | 1.14          |
| (1,591) | 1:5:A:VAL:HG12 | 1:9:A:ILE:HB   | 6        | 1.14          |
| (1,591) | 1:5:A:VAL:HG13 | 1:9:A:ILE:HB   | 6        | 1.14          |
| (1,489) | 1:21:A:ARG:HB2 | 1:22:A:PRO:HD3 | 5        | 1.14          |
| (1,489) | 1:21:A:ARG:HB2 | 1:22:A:PRO:HD3 | 10       | 1.14          |
| (3,29)  | 1:5:A:VAL:HG21 | 1:8:A:TYR:HE1  | 10       | 1.13          |
| (3,29)  | 1:5:A:VAL:HG21 | 1:8:A:TYR:HE2  | 10       | 1.13          |
| (3,29)  | 1:5:A:VAL:HG22 | 1:8:A:TYR:HE1  | 10       | 1.13          |
| (3,29)  | 1:5:A:VAL:HG22 | 1:8:A:TYR:HE2  | 10       | 1.13          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (3,29)  | 1:5:A:VAL:HG23  | 1:8:A:TYR:HE1  | 10       | 1.13          |
| (3,29)  | 1:5:A:VAL:HG23  | 1:8:A:TYR:HE2  | 10       | 1.13          |
| (1,317) | 1:5:A:VAL:HG21  | 1:8:A:TYR:HE1  | 10       | 1.13          |
| (1,317) | 1:5:A:VAL:HG21  | 1:8:A:TYR:HE2  | 10       | 1.13          |
| (1,317) | 1:5:A:VAL:HG22  | 1:8:A:TYR:HE1  | 10       | 1.13          |
| (1,317) | 1:5:A:VAL:HG22  | 1:8:A:TYR:HE2  | 10       | 1.13          |
| (1,317) | 1:5:A:VAL:HG23  | 1:8:A:TYR:HE1  | 10       | 1.13          |
| (1,317) | 1:5:A:VAL:HG23  | 1:8:A:TYR:HE2  | 10       | 1.13          |
| (3,78)  | 1:7:A:LEU:HD21  | 1:24:A:PRO:HB2 | 9        | 1.11          |
| (3,78)  | 1:7:A:LEU:HD22  | 1:24:A:PRO:HB2 | 9        | 1.11          |
| (3,78)  | 1:7:A:LEU:HD23  | 1:24:A:PRO:HB2 | 9        | 1.11          |
| (3,9)   | 1:9:A:ILE:HA    | 1:9:A:ILE:HD11 | 10       | 1.11          |
| (3,9)   | 1:9:A:ILE:HA    | 1:9:A:ILE:HD12 | 10       | 1.11          |
| (3,9)   | 1:9:A:ILE:HA    | 1:9:A:ILE:HD13 | 10       | 1.11          |
| (2,281) | 1:8:A:TYR:HE1   | 1:24:A:PRO:HB3 | 2        | 1.11          |
| (2,281) | 1:8:A:TYR:HE2   | 1:24:A:PRO:HB3 | 2        | 1.11          |
| (1,554) | 1:7:A:LEU:HD21  | 1:24:A:PRO:HB2 | 9        | 1.11          |
| (1,554) | 1:7:A:LEU:HD22  | 1:24:A:PRO:HB2 | 9        | 1.11          |
| (1,554) | 1:7:A:LEU:HD23  | 1:24:A:PRO:HB2 | 9        | 1.11          |
| (1,304) | 1:8:A:TYR:HE1   | 1:24:A:PRO:HB3 | 2        | 1.11          |
| (1,304) | 1:8:A:TYR:HE2   | 1:24:A:PRO:HB3 | 2        | 1.11          |
| (1,87)  | 1:9:A:ILE:HA    | 1:9:A:ILE:HD11 | 10       | 1.11          |
| (1,87)  | 1:9:A:ILE:HA    | 1:9:A:ILE:HD12 | 10       | 1.11          |
| (1,87)  | 1:9:A:ILE:HA    | 1:9:A:ILE:HD13 | 10       | 1.11          |
| (3,72)  | 1:12:A:LEU:HD11 | 1:16:A:GLY:HA2 | 1        | 1.1           |
| (3,72)  | 1:12:A:LEU:HD12 | 1:16:A:GLY:HA2 | 1        | 1.1           |
| (3,72)  | 1:12:A:LEU:HD13 | 1:16:A:GLY:HA2 | 1        | 1.1           |
| (3,52)  | 1:21:A:ARG:H    | 1:22:A:PRO:HD2 | 5        | 1.1           |
| (2,424) | 1:21:A:ARG:HB2  | 1:22:A:PRO:HD3 | 7        | 1.1           |
| (2,424) | 1:21:A:ARG:HB2  | 1:22:A:PRO:HD3 | 8        | 1.1           |
| (2,281) | 1:8:A:TYR:HE1   | 1:24:A:PRO:HB3 | 4        | 1.1           |
| (2,281) | 1:8:A:TYR:HE2   | 1:24:A:PRO:HB3 | 4        | 1.1           |
| (2,261) | 1:11:A:TRP:HE1  | 1:24:A:PRO:HD2 | 3        | 1.1           |
| (2,261) | 1:11:A:TRP:HE1  | 1:24:A:PRO:HD2 | 4        | 1.1           |
| (1,536) | 1:12:A:LEU:HD11 | 1:16:A:GLY:HA2 | 1        | 1.1           |
| (1,536) | 1:12:A:LEU:HD12 | 1:16:A:GLY:HA2 | 1        | 1.1           |
| (1,536) | 1:12:A:LEU:HD13 | 1:16:A:GLY:HA2 | 1        | 1.1           |
| (1,489) | 1:21:A:ARG:HB2  | 1:22:A:PRO:HD3 | 7        | 1.1           |
| (1,489) | 1:21:A:ARG:HB2  | 1:22:A:PRO:HD3 | 8        | 1.1           |
| (1,418) | 1:21:A:ARG:H    | 1:22:A:PRO:HD2 | 5        | 1.1           |
| (1,304) | 1:8:A:TYR:HE1   | 1:24:A:PRO:HB3 | 4        | 1.1           |
| (1,304) | 1:8:A:TYR:HE2   | 1:24:A:PRO:HB3 | 4        | 1.1           |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,280) | 1:11:A:TRP:HE1  | 1:24:A:PRO:HD2 | 3        | 1.1           |
| (1,280) | 1:11:A:TRP:HE1  | 1:24:A:PRO:HD2 | 4        | 1.1           |
| (3,72)  | 1:12:A:LEU:HD11 | 1:16:A:GLY:HA2 | 9        | 1.09          |
| (3,72)  | 1:12:A:LEU:HD12 | 1:16:A:GLY:HA2 | 9        | 1.09          |
| (3,72)  | 1:12:A:LEU:HD13 | 1:16:A:GLY:HA2 | 9        | 1.09          |
| (3,57)  | 1:7:A:LEU:HB2   | 1:10:A:GLN:H   | 10       | 1.09          |
| (2,496) | 1:1:A:GLU:HB3   | 1:2:A:GLU:HG2  | 5        | 1.09          |
| (2,496) | 1:1:A:GLU:HB3   | 1:2:A:GLU:HG2  | 6        | 1.09          |
| (2,281) | 1:8:A:TYR:HE1   | 1:24:A:PRO:HB3 | 8        | 1.09          |
| (2,281) | 1:8:A:TYR:HE2   | 1:24:A:PRO:HB3 | 8        | 1.09          |
| (1,585) | 1:1:A:GLU:HB3   | 1:2:A:GLU:HG2  | 5        | 1.09          |
| (1,585) | 1:1:A:GLU:HB3   | 1:2:A:GLU:HG2  | 6        | 1.09          |
| (1,536) | 1:12:A:LEU:HD11 | 1:16:A:GLY:HA2 | 9        | 1.09          |
| (1,536) | 1:12:A:LEU:HD12 | 1:16:A:GLY:HA2 | 9        | 1.09          |
| (1,536) | 1:12:A:LEU:HD13 | 1:16:A:GLY:HA2 | 9        | 1.09          |
| (1,435) | 1:7:A:LEU:HB2   | 1:10:A:GLN:H   | 10       | 1.09          |
| (1,304) | 1:8:A:TYR:HE1   | 1:24:A:PRO:HB3 | 8        | 1.09          |
| (1,304) | 1:8:A:TYR:HE2   | 1:24:A:PRO:HB3 | 8        | 1.09          |
| (3,72)  | 1:12:A:LEU:HD11 | 1:16:A:GLY:HA2 | 4        | 1.08          |
| (3,72)  | 1:12:A:LEU:HD12 | 1:16:A:GLY:HA2 | 4        | 1.08          |
| (3,72)  | 1:12:A:LEU:HD13 | 1:16:A:GLY:HA2 | 4        | 1.08          |
| (3,72)  | 1:12:A:LEU:HD11 | 1:16:A:GLY:HA2 | 5        | 1.08          |
| (3,72)  | 1:12:A:LEU:HD12 | 1:16:A:GLY:HA2 | 5        | 1.08          |
| (3,72)  | 1:12:A:LEU:HD13 | 1:16:A:GLY:HA2 | 5        | 1.08          |
| (3,54)  | 1:5:A:VAL:HB    | 1:6:A:ARG:H    | 4        | 1.08          |
| (3,52)  | 1:21:A:ARG:H    | 1:22:A:PRO:HD2 | 2        | 1.08          |
| (3,29)  | 1:5:A:VAL:HG21  | 1:8:A:TYR:HE1  | 9        | 1.08          |
| (3,29)  | 1:5:A:VAL:HG21  | 1:8:A:TYR:HE2  | 9        | 1.08          |
| (3,29)  | 1:5:A:VAL:HG22  | 1:8:A:TYR:HE1  | 9        | 1.08          |
| (3,29)  | 1:5:A:VAL:HG22  | 1:8:A:TYR:HE2  | 9        | 1.08          |
| (3,29)  | 1:5:A:VAL:HG23  | 1:8:A:TYR:HE1  | 9        | 1.08          |
| (3,29)  | 1:5:A:VAL:HG23  | 1:8:A:TYR:HE2  | 9        | 1.08          |
| (3,9)   | 1:9:A:ILE:HA    | 1:9:A:ILE:HD11 | 9        | 1.08          |
| (3,9)   | 1:9:A:ILE:HA    | 1:9:A:ILE:HD12 | 9        | 1.08          |
| (3,9)   | 1:9:A:ILE:HA    | 1:9:A:ILE:HD13 | 9        | 1.08          |
| (2,496) | 1:1:A:GLU:HB3   | 1:2:A:GLU:HG2  | 9        | 1.08          |
| (1,585) | 1:1:A:GLU:HB3   | 1:2:A:GLU:HG2  | 9        | 1.08          |
| (1,536) | 1:12:A:LEU:HD11 | 1:16:A:GLY:HA2 | 4        | 1.08          |
| (1,536) | 1:12:A:LEU:HD12 | 1:16:A:GLY:HA2 | 4        | 1.08          |
| (1,536) | 1:12:A:LEU:HD13 | 1:16:A:GLY:HA2 | 4        | 1.08          |
| (1,536) | 1:12:A:LEU:HD11 | 1:16:A:GLY:HA2 | 5        | 1.08          |
| (1,536) | 1:12:A:LEU:HD12 | 1:16:A:GLY:HA2 | 5        | 1.08          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,536) | 1:12:A:LEU:HD13 | 1:16:A:GLY:HA2 | 5        | 1.08          |
| (1,428) | 1:5:A:VAL:HB    | 1:6:A:ARG:H    | 4        | 1.08          |
| (1,418) | 1:21:A:ARG:H    | 1:22:A:PRO:HD2 | 2        | 1.08          |
| (1,317) | 1:5:A:VAL:HG21  | 1:8:A:TYR:HE1  | 9        | 1.08          |
| (1,317) | 1:5:A:VAL:HG21  | 1:8:A:TYR:HE2  | 9        | 1.08          |
| (1,317) | 1:5:A:VAL:HG22  | 1:8:A:TYR:HE1  | 9        | 1.08          |
| (1,317) | 1:5:A:VAL:HG22  | 1:8:A:TYR:HE2  | 9        | 1.08          |
| (1,317) | 1:5:A:VAL:HG23  | 1:8:A:TYR:HE1  | 9        | 1.08          |
| (1,317) | 1:5:A:VAL:HG23  | 1:8:A:TYR:HE2  | 9        | 1.08          |
| (1,87)  | 1:9:A:ILE:HA    | 1:9:A:ILE:HD11 | 9        | 1.08          |
| (1,87)  | 1:9:A:ILE:HA    | 1:9:A:ILE:HD12 | 9        | 1.08          |
| (1,87)  | 1:9:A:ILE:HA    | 1:9:A:ILE:HD13 | 9        | 1.08          |
| (3,72)  | 1:12:A:LEU:HD11 | 1:16:A:GLY:HA2 | 7        | 1.07          |
| (3,72)  | 1:12:A:LEU:HD12 | 1:16:A:GLY:HA2 | 7        | 1.07          |
| (3,72)  | 1:12:A:LEU:HD13 | 1:16:A:GLY:HA2 | 7        | 1.07          |
| (3,54)  | 1:5:A:VAL:HB    | 1:6:A:ARG:H    | 1        | 1.07          |
| (3,9)   | 1:9:A:ILE:HA    | 1:9:A:ILE:HD11 | 1        | 1.07          |
| (3,9)   | 1:9:A:ILE:HA    | 1:9:A:ILE:HD12 | 1        | 1.07          |
| (3,9)   | 1:9:A:ILE:HA    | 1:9:A:ILE:HD13 | 1        | 1.07          |
| (3,9)   | 1:9:A:ILE:HA    | 1:9:A:ILE:HD11 | 2        | 1.07          |
| (3,9)   | 1:9:A:ILE:HA    | 1:9:A:ILE:HD12 | 2        | 1.07          |
| (3,9)   | 1:9:A:ILE:HA    | 1:9:A:ILE:HD13 | 2        | 1.07          |
| (3,9)   | 1:9:A:ILE:HA    | 1:9:A:ILE:HD11 | 3        | 1.07          |
| (3,9)   | 1:9:A:ILE:HA    | 1:9:A:ILE:HD12 | 3        | 1.07          |
| (3,9)   | 1:9:A:ILE:HA    | 1:9:A:ILE:HD13 | 3        | 1.07          |
| (2,281) | 1:8:A:TYR:HE1   | 1:24:A:PRO:HB3 | 7        | 1.07          |
| (2,281) | 1:8:A:TYR:HE2   | 1:24:A:PRO:HB3 | 7        | 1.07          |
| (1,536) | 1:12:A:LEU:HD11 | 1:16:A:GLY:HA2 | 7        | 1.07          |
| (1,536) | 1:12:A:LEU:HD12 | 1:16:A:GLY:HA2 | 7        | 1.07          |
| (1,536) | 1:12:A:LEU:HD13 | 1:16:A:GLY:HA2 | 7        | 1.07          |
| (1,428) | 1:5:A:VAL:HB    | 1:6:A:ARG:H    | 1        | 1.07          |
| (1,304) | 1:8:A:TYR:HE1   | 1:24:A:PRO:HB3 | 7        | 1.07          |
| (1,304) | 1:8:A:TYR:HE2   | 1:24:A:PRO:HB3 | 7        | 1.07          |
| (1,87)  | 1:9:A:ILE:HA    | 1:9:A:ILE:HD11 | 1        | 1.07          |
| (1,87)  | 1:9:A:ILE:HA    | 1:9:A:ILE:HD12 | 1        | 1.07          |
| (1,87)  | 1:9:A:ILE:HA    | 1:9:A:ILE:HD13 | 1        | 1.07          |
| (1,87)  | 1:9:A:ILE:HA    | 1:9:A:ILE:HD11 | 2        | 1.07          |
| (1,87)  | 1:9:A:ILE:HA    | 1:9:A:ILE:HD12 | 2        | 1.07          |
| (1,87)  | 1:9:A:ILE:HA    | 1:9:A:ILE:HD13 | 2        | 1.07          |
| (1,87)  | 1:9:A:ILE:HA    | 1:9:A:ILE:HD11 | 3        | 1.07          |
| (1,87)  | 1:9:A:ILE:HA    | 1:9:A:ILE:HD12 | 3        | 1.07          |
| (1,87)  | 1:9:A:ILE:HA    | 1:9:A:ILE:HD13 | 3        | 1.07          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (3,9)   | 1:9:A:ILE:HA    | 1:9:A:ILE:HD11 | 4        | 1.06          |
| (3,9)   | 1:9:A:ILE:HA    | 1:9:A:ILE:HD12 | 4        | 1.06          |
| (3,9)   | 1:9:A:ILE:HA    | 1:9:A:ILE:HD13 | 4        | 1.06          |
| (3,9)   | 1:9:A:ILE:HA    | 1:9:A:ILE:HD11 | 5        | 1.06          |
| (3,9)   | 1:9:A:ILE:HA    | 1:9:A:ILE:HD12 | 5        | 1.06          |
| (3,9)   | 1:9:A:ILE:HA    | 1:9:A:ILE:HD13 | 5        | 1.06          |
| (3,9)   | 1:9:A:ILE:HA    | 1:9:A:ILE:HD11 | 6        | 1.06          |
| (3,9)   | 1:9:A:ILE:HA    | 1:9:A:ILE:HD12 | 6        | 1.06          |
| (3,9)   | 1:9:A:ILE:HA    | 1:9:A:ILE:HD13 | 6        | 1.06          |
| (3,9)   | 1:9:A:ILE:HA    | 1:9:A:ILE:HD11 | 7        | 1.06          |
| (3,9)   | 1:9:A:ILE:HA    | 1:9:A:ILE:HD12 | 7        | 1.06          |
| (3,9)   | 1:9:A:ILE:HA    | 1:9:A:ILE:HD13 | 7        | 1.06          |
| (3,9)   | 1:9:A:ILE:HA    | 1:9:A:ILE:HD11 | 8        | 1.06          |
| (3,9)   | 1:9:A:ILE:HA    | 1:9:A:ILE:HD12 | 8        | 1.06          |
| (3,9)   | 1:9:A:ILE:HA    | 1:9:A:ILE:HD13 | 8        | 1.06          |
| (2,424) | 1:21:A:ARG:HB2  | 1:22:A:PRO:HD3 | 3        | 1.06          |
| (1,489) | 1:21:A:ARG:HB2  | 1:22:A:PRO:HD3 | 3        | 1.06          |
| (1,87)  | 1:9:A:ILE:HA    | 1:9:A:ILE:HD11 | 4        | 1.06          |
| (1,87)  | 1:9:A:ILE:HA    | 1:9:A:ILE:HD12 | 4        | 1.06          |
| (1,87)  | 1:9:A:ILE:HA    | 1:9:A:ILE:HD13 | 4        | 1.06          |
| (1,87)  | 1:9:A:ILE:HA    | 1:9:A:ILE:HD11 | 5        | 1.06          |
| (1,87)  | 1:9:A:ILE:HA    | 1:9:A:ILE:HD12 | 5        | 1.06          |
| (1,87)  | 1:9:A:ILE:HA    | 1:9:A:ILE:HD13 | 5        | 1.06          |
| (1,87)  | 1:9:A:ILE:HA    | 1:9:A:ILE:HD11 | 6        | 1.06          |
| (1,87)  | 1:9:A:ILE:HA    | 1:9:A:ILE:HD12 | 6        | 1.06          |
| (1,87)  | 1:9:A:ILE:HA    | 1:9:A:ILE:HD13 | 6        | 1.06          |
| (1,87)  | 1:9:A:ILE:HA    | 1:9:A:ILE:HD11 | 7        | 1.06          |
| (1,87)  | 1:9:A:ILE:HA    | 1:9:A:ILE:HD12 | 7        | 1.06          |
| (1,87)  | 1:9:A:ILE:HA    | 1:9:A:ILE:HD13 | 7        | 1.06          |
| (1,87)  | 1:9:A:ILE:HA    | 1:9:A:ILE:HD11 | 8        | 1.06          |
| (1,87)  | 1:9:A:ILE:HA    | 1:9:A:ILE:HD12 | 8        | 1.06          |
| (1,87)  | 1:9:A:ILE:HA    | 1:9:A:ILE:HD13 | 8        | 1.06          |
| (3,72)  | 1:12:A:LEU:HD11 | 1:16:A:GLY:HA2 | 8        | 1.05          |
| (3,72)  | 1:12:A:LEU:HD12 | 1:16:A:GLY:HA2 | 8        | 1.05          |
| (3,72)  | 1:12:A:LEU:HD13 | 1:16:A:GLY:HA2 | 8        | 1.05          |
| (3,57)  | 1:7:A:LEU:HB2   | 1:10:A:GLN:H   | 9        | 1.05          |
| (3,54)  | 1:5:A:VAL:HB    | 1:6:A:ARG:H    | 2        | 1.05          |
| (3,54)  | 1:5:A:VAL:HB    | 1:6:A:ARG:H    | 3        | 1.05          |
| (3,54)  | 1:5:A:VAL:HB    | 1:6:A:ARG:H    | 9        | 1.05          |
| (3,5)   | 1:7:A:LEU:HA    | 1:7:A:LEU:HD11 | 5        | 1.05          |
| (3,5)   | 1:7:A:LEU:HA    | 1:7:A:LEU:HD12 | 5        | 1.05          |
| (3,5)   | 1:7:A:LEU:HA    | 1:7:A:LEU:HD13 | 5        | 1.05          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (3,5)   | 1:7:A:LEU:HA    | 1:7:A:LEU:HD11 | 7        | 1.05          |
| (3,5)   | 1:7:A:LEU:HA    | 1:7:A:LEU:HD12 | 7        | 1.05          |
| (3,5)   | 1:7:A:LEU:HA    | 1:7:A:LEU:HD13 | 7        | 1.05          |
| (3,5)   | 1:7:A:LEU:HA    | 1:7:A:LEU:HD11 | 8        | 1.05          |
| (3,5)   | 1:7:A:LEU:HA    | 1:7:A:LEU:HD12 | 8        | 1.05          |
| (3,5)   | 1:7:A:LEU:HA    | 1:7:A:LEU:HD13 | 8        | 1.05          |
| (2,424) | 1:21:A:ARG:HB2  | 1:22:A:PRO:HD3 | 4        | 1.05          |
| (2,261) | 1:11:A:TRP:HE1  | 1:24:A:PRO:HD2 | 5        | 1.05          |
| (1,536) | 1:12:A:LEU:HD11 | 1:16:A:GLY:HA2 | 8        | 1.05          |
| (1,536) | 1:12:A:LEU:HD12 | 1:16:A:GLY:HA2 | 8        | 1.05          |
| (1,536) | 1:12:A:LEU:HD13 | 1:16:A:GLY:HA2 | 8        | 1.05          |
| (1,489) | 1:21:A:ARG:HB2  | 1:22:A:PRO:HD3 | 4        | 1.05          |
| (1,435) | 1:7:A:LEU:HB2   | 1:10:A:GLN:H   | 9        | 1.05          |
| (1,428) | 1:5:A:VAL:HB    | 1:6:A:ARG:H    | 2        | 1.05          |
| (1,428) | 1:5:A:VAL:HB    | 1:6:A:ARG:H    | 3        | 1.05          |
| (1,428) | 1:5:A:VAL:HB    | 1:6:A:ARG:H    | 9        | 1.05          |
| (1,280) | 1:11:A:TRP:HE1  | 1:24:A:PRO:HD2 | 5        | 1.05          |
| (1,59)  | 1:7:A:LEU:HA    | 1:7:A:LEU:HD11 | 5        | 1.05          |
| (1,59)  | 1:7:A:LEU:HA    | 1:7:A:LEU:HD12 | 5        | 1.05          |
| (1,59)  | 1:7:A:LEU:HA    | 1:7:A:LEU:HD13 | 5        | 1.05          |
| (1,59)  | 1:7:A:LEU:HA    | 1:7:A:LEU:HD11 | 7        | 1.05          |
| (1,59)  | 1:7:A:LEU:HA    | 1:7:A:LEU:HD12 | 7        | 1.05          |
| (1,59)  | 1:7:A:LEU:HA    | 1:7:A:LEU:HD13 | 7        | 1.05          |
| (1,59)  | 1:7:A:LEU:HA    | 1:7:A:LEU:HD11 | 8        | 1.05          |
| (1,59)  | 1:7:A:LEU:HA    | 1:7:A:LEU:HD12 | 8        | 1.05          |
| (1,59)  | 1:7:A:LEU:HA    | 1:7:A:LEU:HD13 | 8        | 1.05          |
| (3,54)  | 1:5:A:VAL:HB    | 1:6:A:ARG:H    | 10       | 1.04          |
| (3,5)   | 1:7:A:LEU:HA    | 1:7:A:LEU:HD11 | 3        | 1.04          |
| (3,5)   | 1:7:A:LEU:HA    | 1:7:A:LEU:HD12 | 3        | 1.04          |
| (3,5)   | 1:7:A:LEU:HA    | 1:7:A:LEU:HD13 | 3        | 1.04          |
| (3,5)   | 1:7:A:LEU:HA    | 1:7:A:LEU:HD11 | 6        | 1.04          |
| (3,5)   | 1:7:A:LEU:HA    | 1:7:A:LEU:HD12 | 6        | 1.04          |
| (3,5)   | 1:7:A:LEU:HA    | 1:7:A:LEU:HD13 | 6        | 1.04          |
| (2,281) | 1:8:A:TYR:HE1   | 1:24:A:PRO:HB3 | 3        | 1.04          |
| (2,281) | 1:8:A:TYR:HE2   | 1:24:A:PRO:HB3 | 3        | 1.04          |
| (2,281) | 1:8:A:TYR:HE1   | 1:24:A:PRO:HB3 | 5        | 1.04          |
| (2,281) | 1:8:A:TYR:HE2   | 1:24:A:PRO:HB3 | 5        | 1.04          |
| (2,261) | 1:11:A:TRP:HE1  | 1:24:A:PRO:HD2 | 1        | 1.04          |
| (2,261) | 1:11:A:TRP:HE1  | 1:24:A:PRO:HD2 | 2        | 1.04          |
| (2,261) | 1:11:A:TRP:HE1  | 1:24:A:PRO:HD2 | 7        | 1.04          |
| (1,428) | 1:5:A:VAL:HB    | 1:6:A:ARG:H    | 10       | 1.04          |
| (1,304) | 1:8:A:TYR:HE1   | 1:24:A:PRO:HB3 | 3        | 1.04          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,304) | 1:8:A:TYR:HE2  | 1:24:A:PRO:HB3 | 3        | 1.04          |
| (1,304) | 1:8:A:TYR:HE1  | 1:24:A:PRO:HB3 | 5        | 1.04          |
| (1,304) | 1:8:A:TYR:HE2  | 1:24:A:PRO:HB3 | 5        | 1.04          |
| (1,280) | 1:11:A:TRP:HE1 | 1:24:A:PRO:HD2 | 1        | 1.04          |
| (1,280) | 1:11:A:TRP:HE1 | 1:24:A:PRO:HD2 | 2        | 1.04          |
| (1,280) | 1:11:A:TRP:HE1 | 1:24:A:PRO:HD2 | 7        | 1.04          |
| (1,59)  | 1:7:A:LEU:HA   | 1:7:A:LEU:HD11 | 3        | 1.04          |
| (1,59)  | 1:7:A:LEU:HA   | 1:7:A:LEU:HD12 | 3        | 1.04          |
| (1,59)  | 1:7:A:LEU:HA   | 1:7:A:LEU:HD13 | 3        | 1.04          |
| (1,59)  | 1:7:A:LEU:HA   | 1:7:A:LEU:HD11 | 6        | 1.04          |
| (1,59)  | 1:7:A:LEU:HA   | 1:7:A:LEU:HD12 | 6        | 1.04          |
| (1,59)  | 1:7:A:LEU:HA   | 1:7:A:LEU:HD13 | 6        | 1.04          |
| (3,5)   | 1:7:A:LEU:HA   | 1:7:A:LEU:HD11 | 2        | 1.03          |
| (3,5)   | 1:7:A:LEU:HA   | 1:7:A:LEU:HD12 | 2        | 1.03          |
| (3,5)   | 1:7:A:LEU:HA   | 1:7:A:LEU:HD13 | 2        | 1.03          |
| (3,5)   | 1:7:A:LEU:HA   | 1:7:A:LEU:HD11 | 4        | 1.03          |
| (3,5)   | 1:7:A:LEU:HA   | 1:7:A:LEU:HD12 | 4        | 1.03          |
| (3,5)   | 1:7:A:LEU:HA   | 1:7:A:LEU:HD13 | 4        | 1.03          |
| (1,59)  | 1:7:A:LEU:HA   | 1:7:A:LEU:HD11 | 2        | 1.03          |
| (1,59)  | 1:7:A:LEU:HA   | 1:7:A:LEU:HD12 | 2        | 1.03          |
| (1,59)  | 1:7:A:LEU:HA   | 1:7:A:LEU:HD13 | 2        | 1.03          |
| (1,59)  | 1:7:A:LEU:HA   | 1:7:A:LEU:HD11 | 4        | 1.03          |
| (1,59)  | 1:7:A:LEU:HA   | 1:7:A:LEU:HD12 | 4        | 1.03          |
| (1,59)  | 1:7:A:LEU:HA   | 1:7:A:LEU:HD13 | 4        | 1.03          |
| (3,54)  | 1:5:A:VAL:HB   | 1:6:A:ARG:H    | 7        | 1.02          |
| (3,5)   | 1:7:A:LEU:HA   | 1:7:A:LEU:HD11 | 1        | 1.02          |
| (3,5)   | 1:7:A:LEU:HA   | 1:7:A:LEU:HD12 | 1        | 1.02          |
| (3,5)   | 1:7:A:LEU:HA   | 1:7:A:LEU:HD13 | 1        | 1.02          |
| (2,281) | 1:8:A:TYR:HE1  | 1:24:A:PRO:HB3 | 6        | 1.02          |
| (2,281) | 1:8:A:TYR:HE2  | 1:24:A:PRO:HB3 | 6        | 1.02          |
| (2,261) | 1:11:A:TRP:HE1 | 1:24:A:PRO:HD2 | 9        | 1.02          |
| (1,428) | 1:5:A:VAL:HB   | 1:6:A:ARG:H    | 7        | 1.02          |
| (1,304) | 1:8:A:TYR:HE1  | 1:24:A:PRO:HB3 | 6        | 1.02          |
| (1,304) | 1:8:A:TYR:HE2  | 1:24:A:PRO:HB3 | 6        | 1.02          |
| (1,280) | 1:11:A:TRP:HE1 | 1:24:A:PRO:HD2 | 9        | 1.02          |
| (1,59)  | 1:7:A:LEU:HA   | 1:7:A:LEU:HD11 | 1        | 1.02          |
| (1,59)  | 1:7:A:LEU:HA   | 1:7:A:LEU:HD12 | 1        | 1.02          |
| (1,59)  | 1:7:A:LEU:HA   | 1:7:A:LEU:HD13 | 1        | 1.02          |
| (3,87)  | 1:8:A:TYR:HB3  | 1:11:A:TRP:HE3 | 1        | 1.01          |
| (3,87)  | 1:8:A:TYR:HB3  | 1:11:A:TRP:HE3 | 4        | 1.01          |
| (3,54)  | 1:5:A:VAL:HB   | 1:6:A:ARG:H    | 6        | 1.01          |
| (3,54)  | 1:5:A:VAL:HB   | 1:6:A:ARG:H    | 8        | 1.01          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (2,437) | 1:16:A:GLY:HA2  | 1:17:A:PRO:HG2 | 10       | 1.01          |
| (2,437) | 1:16:A:GLY:HA2  | 1:17:A:PRO:HG3 | 10       | 1.01          |
| (1,575) | 1:8:A:TYR:HB3   | 1:11:A:TRP:HE3 | 1        | 1.01          |
| (1,575) | 1:8:A:TYR:HB3   | 1:11:A:TRP:HE3 | 4        | 1.01          |
| (1,504) | 1:16:A:GLY:HA2  | 1:17:A:PRO:HG2 | 10       | 1.01          |
| (1,504) | 1:16:A:GLY:HA2  | 1:17:A:PRO:HG3 | 10       | 1.01          |
| (1,428) | 1:5:A:VAL:HB    | 1:6:A:ARG:H    | 6        | 1.01          |
| (1,428) | 1:5:A:VAL:HB    | 1:6:A:ARG:H    | 8        | 1.01          |
| (3,87)  | 1:8:A:TYR:HB3   | 1:11:A:TRP:HE3 | 6        | 1.0           |
| (3,72)  | 1:12:A:LEU:HD11 | 1:16:A:GLY:HA2 | 2        | 1.0           |
| (3,72)  | 1:12:A:LEU:HD12 | 1:16:A:GLY:HA2 | 2        | 1.0           |
| (3,72)  | 1:12:A:LEU:HD13 | 1:16:A:GLY:HA2 | 2        | 1.0           |
| (3,72)  | 1:12:A:LEU:HD11 | 1:16:A:GLY:HA2 | 10       | 1.0           |
| (3,72)  | 1:12:A:LEU:HD12 | 1:16:A:GLY:HA2 | 10       | 1.0           |
| (3,72)  | 1:12:A:LEU:HD13 | 1:16:A:GLY:HA2 | 10       | 1.0           |
| (3,54)  | 1:5:A:VAL:HB    | 1:6:A:ARG:H    | 5        | 1.0           |
| (2,437) | 1:16:A:GLY:HA2  | 1:17:A:PRO:HG2 | 3        | 1.0           |
| (2,437) | 1:16:A:GLY:HA2  | 1:17:A:PRO:HG3 | 3        | 1.0           |
| (1,575) | 1:8:A:TYR:HB3   | 1:11:A:TRP:HE3 | 6        | 1.0           |
| (1,536) | 1:12:A:LEU:HD11 | 1:16:A:GLY:HA2 | 2        | 1.0           |
| (1,536) | 1:12:A:LEU:HD12 | 1:16:A:GLY:HA2 | 2        | 1.0           |
| (1,536) | 1:12:A:LEU:HD13 | 1:16:A:GLY:HA2 | 2        | 1.0           |
| (1,536) | 1:12:A:LEU:HD11 | 1:16:A:GLY:HA2 | 10       | 1.0           |
| (1,536) | 1:12:A:LEU:HD12 | 1:16:A:GLY:HA2 | 10       | 1.0           |
| (1,536) | 1:12:A:LEU:HD13 | 1:16:A:GLY:HA2 | 10       | 1.0           |
| (1,504) | 1:16:A:GLY:HA2  | 1:17:A:PRO:HG2 | 3        | 1.0           |
| (1,504) | 1:16:A:GLY:HA2  | 1:17:A:PRO:HG3 | 3        | 1.0           |
| (1,428) | 1:5:A:VAL:HB    | 1:6:A:ARG:H    | 5        | 1.0           |
| (2,496) | 1:1:A:GLU:HB3   | 1:2:A:GLU:HG2  | 10       | 0.99          |
| (2,479) | 1:9:A:ILE:HG21  | 1:13:A:LYS:HG2 | 9        | 0.99          |
| (2,479) | 1:9:A:ILE:HG22  | 1:13:A:LYS:HG2 | 9        | 0.99          |
| (2,479) | 1:9:A:ILE:HG23  | 1:13:A:LYS:HG2 | 9        | 0.99          |
| (2,424) | 1:21:A:ARG:HB2  | 1:22:A:PRO:HD3 | 9        | 0.99          |
| (1,585) | 1:1:A:GLU:HB3   | 1:2:A:GLU:HG2  | 10       | 0.99          |
| (1,561) | 1:9:A:ILE:HG21  | 1:13:A:LYS:HG2 | 9        | 0.99          |
| (1,561) | 1:9:A:ILE:HG22  | 1:13:A:LYS:HG2 | 9        | 0.99          |
| (1,561) | 1:9:A:ILE:HG23  | 1:13:A:LYS:HG2 | 9        | 0.99          |
| (1,489) | 1:21:A:ARG:HB2  | 1:22:A:PRO:HD3 | 9        | 0.99          |
| (3,87)  | 1:8:A:TYR:HB3   | 1:11:A:TRP:HE3 | 2        | 0.98          |
| (3,87)  | 1:8:A:TYR:HB3   | 1:11:A:TRP:HE3 | 7        | 0.98          |
| (3,78)  | 1:7:A:LEU:HD21  | 1:24:A:PRO:HB2 | 8        | 0.98          |
| (3,78)  | 1:7:A:LEU:HD22  | 1:24:A:PRO:HB2 | 8        | 0.98          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (3,78)  | 1:7:A:LEU:HD23  | 1:24:A:PRO:HB2 | 8        | 0.98          |
| (2,479) | 1:9:A:ILE:HG21  | 1:13:A:LYS:HG2 | 7        | 0.98          |
| (2,479) | 1:9:A:ILE:HG22  | 1:13:A:LYS:HG2 | 7        | 0.98          |
| (2,479) | 1:9:A:ILE:HG23  | 1:13:A:LYS:HG2 | 7        | 0.98          |
| (1,575) | 1:8:A:TYR:HB3   | 1:11:A:TRP:HE3 | 2        | 0.98          |
| (1,575) | 1:8:A:TYR:HB3   | 1:11:A:TRP:HE3 | 7        | 0.98          |
| (1,561) | 1:9:A:ILE:HG21  | 1:13:A:LYS:HG2 | 7        | 0.98          |
| (1,561) | 1:9:A:ILE:HG22  | 1:13:A:LYS:HG2 | 7        | 0.98          |
| (1,561) | 1:9:A:ILE:HG23  | 1:13:A:LYS:HG2 | 7        | 0.98          |
| (1,554) | 1:7:A:LEU:HD21  | 1:24:A:PRO:HB2 | 8        | 0.98          |
| (1,554) | 1:7:A:LEU:HD22  | 1:24:A:PRO:HB2 | 8        | 0.98          |
| (1,554) | 1:7:A:LEU:HD23  | 1:24:A:PRO:HB2 | 8        | 0.98          |
| (3,87)  | 1:8:A:TYR:HB3   | 1:11:A:TRP:HE3 | 5        | 0.97          |
| (3,81)  | 1:4:A:ALA:HB1   | 1:7:A:LEU:HD21 | 9        | 0.97          |
| (3,81)  | 1:4:A:ALA:HB1   | 1:7:A:LEU:HD22 | 9        | 0.97          |
| (3,81)  | 1:4:A:ALA:HB1   | 1:7:A:LEU:HD23 | 9        | 0.97          |
| (3,81)  | 1:4:A:ALA:HB2   | 1:7:A:LEU:HD21 | 9        | 0.97          |
| (3,81)  | 1:4:A:ALA:HB2   | 1:7:A:LEU:HD22 | 9        | 0.97          |
| (3,81)  | 1:4:A:ALA:HB2   | 1:7:A:LEU:HD23 | 9        | 0.97          |
| (3,81)  | 1:4:A:ALA:HB3   | 1:7:A:LEU:HD21 | 9        | 0.97          |
| (3,81)  | 1:4:A:ALA:HB3   | 1:7:A:LEU:HD22 | 9        | 0.97          |
| (3,81)  | 1:4:A:ALA:HB3   | 1:7:A:LEU:HD23 | 9        | 0.97          |
| (3,72)  | 1:12:A:LEU:HD11 | 1:16:A:GLY:HA2 | 3        | 0.97          |
| (3,72)  | 1:12:A:LEU:HD12 | 1:16:A:GLY:HA2 | 3        | 0.97          |
| (3,72)  | 1:12:A:LEU:HD13 | 1:16:A:GLY:HA2 | 3        | 0.97          |
| (3,57)  | 1:7:A:LEU:HB2   | 1:10:A:GLN:H   | 1        | 0.97          |
| (2,437) | 1:16:A:GLY:HA2  | 1:17:A:PRO:HG2 | 2        | 0.97          |
| (2,437) | 1:16:A:GLY:HA2  | 1:17:A:PRO:HG3 | 2        | 0.97          |
| (2,437) | 1:16:A:GLY:HA2  | 1:17:A:PRO:HG2 | 5        | 0.97          |
| (2,437) | 1:16:A:GLY:HA2  | 1:17:A:PRO:HG3 | 5        | 0.97          |
| (2,437) | 1:16:A:GLY:HA2  | 1:17:A:PRO:HG2 | 9        | 0.97          |
| (2,437) | 1:16:A:GLY:HA2  | 1:17:A:PRO:HG3 | 9        | 0.97          |
| (2,305) | 1:11:A:TRP:HH2  | 1:17:A:PRO:HB2 | 3        | 0.97          |
| (2,261) | 1:11:A:TRP:HE1  | 1:24:A:PRO:HD2 | 6        | 0.97          |
| (1,575) | 1:8:A:TYR:HB3   | 1:11:A:TRP:HE3 | 5        | 0.97          |
| (1,559) | 1:4:A:ALA:HB1   | 1:7:A:LEU:HD21 | 9        | 0.97          |
| (1,559) | 1:4:A:ALA:HB1   | 1:7:A:LEU:HD22 | 9        | 0.97          |
| (1,559) | 1:4:A:ALA:HB1   | 1:7:A:LEU:HD23 | 9        | 0.97          |
| (1,559) | 1:4:A:ALA:HB2   | 1:7:A:LEU:HD21 | 9        | 0.97          |
| (1,559) | 1:4:A:ALA:HB2   | 1:7:A:LEU:HD22 | 9        | 0.97          |
| (1,559) | 1:4:A:ALA:HB2   | 1:7:A:LEU:HD23 | 9        | 0.97          |
| (1,559) | 1:4:A:ALA:HB3   | 1:7:A:LEU:HD21 | 9        | 0.97          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,559) | 1:4:A:ALA:HB3   | 1:7:A:LEU:HD22 | 9        | 0.97          |
| (1,559) | 1:4:A:ALA:HB3   | 1:7:A:LEU:HD23 | 9        | 0.97          |
| (1,536) | 1:12:A:LEU:HD11 | 1:16:A:GLY:HA2 | 3        | 0.97          |
| (1,536) | 1:12:A:LEU:HD12 | 1:16:A:GLY:HA2 | 3        | 0.97          |
| (1,536) | 1:12:A:LEU:HD13 | 1:16:A:GLY:HA2 | 3        | 0.97          |
| (1,504) | 1:16:A:GLY:HA2  | 1:17:A:PRO:HG2 | 2        | 0.97          |
| (1,504) | 1:16:A:GLY:HA2  | 1:17:A:PRO:HG3 | 2        | 0.97          |
| (1,504) | 1:16:A:GLY:HA2  | 1:17:A:PRO:HG2 | 5        | 0.97          |
| (1,504) | 1:16:A:GLY:HA2  | 1:17:A:PRO:HG3 | 5        | 0.97          |
| (1,504) | 1:16:A:GLY:HA2  | 1:17:A:PRO:HG2 | 9        | 0.97          |
| (1,504) | 1:16:A:GLY:HA2  | 1:17:A:PRO:HG3 | 9        | 0.97          |
| (1,435) | 1:7:A:LEU:HB2   | 1:10:A:GLN:H   | 1        | 0.97          |
| (1,341) | 1:11:A:TRP:HH2  | 1:17:A:PRO:HB2 | 3        | 0.97          |
| (1,280) | 1:11:A:TRP:HE1  | 1:24:A:PRO:HD2 | 6        | 0.97          |
| (3,87)  | 1:8:A:TYR:HB3   | 1:11:A:TRP:HE3 | 3        | 0.96          |
| (2,479) | 1:9:A:ILE:HG21  | 1:13:A:LYS:HG2 | 10       | 0.96          |
| (2,479) | 1:9:A:ILE:HG22  | 1:13:A:LYS:HG2 | 10       | 0.96          |
| (2,479) | 1:9:A:ILE:HG23  | 1:13:A:LYS:HG2 | 10       | 0.96          |
| (2,437) | 1:16:A:GLY:HA2  | 1:17:A:PRO:HG2 | 1        | 0.96          |
| (2,437) | 1:16:A:GLY:HA2  | 1:17:A:PRO:HG3 | 1        | 0.96          |
| (2,437) | 1:16:A:GLY:HA2  | 1:17:A:PRO:HG2 | 4        | 0.96          |
| (2,437) | 1:16:A:GLY:HA2  | 1:17:A:PRO:HG3 | 4        | 0.96          |
| (2,437) | 1:16:A:GLY:HA2  | 1:17:A:PRO:HG2 | 7        | 0.96          |
| (2,437) | 1:16:A:GLY:HA2  | 1:17:A:PRO:HG3 | 7        | 0.96          |
| (2,261) | 1:11:A:TRP:HE1  | 1:24:A:PRO:HD2 | 10       | 0.96          |
| (1,575) | 1:8:A:TYR:HB3   | 1:11:A:TRP:HE3 | 3        | 0.96          |
| (1,561) | 1:9:A:ILE:HG21  | 1:13:A:LYS:HG2 | 10       | 0.96          |
| (1,561) | 1:9:A:ILE:HG22  | 1:13:A:LYS:HG2 | 10       | 0.96          |
| (1,561) | 1:9:A:ILE:HG23  | 1:13:A:LYS:HG2 | 10       | 0.96          |
| (1,504) | 1:16:A:GLY:HA2  | 1:17:A:PRO:HG2 | 1        | 0.96          |
| (1,504) | 1:16:A:GLY:HA2  | 1:17:A:PRO:HG3 | 1        | 0.96          |
| (1,504) | 1:16:A:GLY:HA2  | 1:17:A:PRO:HG2 | 4        | 0.96          |
| (1,504) | 1:16:A:GLY:HA2  | 1:17:A:PRO:HG3 | 4        | 0.96          |
| (1,504) | 1:16:A:GLY:HA2  | 1:17:A:PRO:HG2 | 7        | 0.96          |
| (1,504) | 1:16:A:GLY:HA2  | 1:17:A:PRO:HG3 | 7        | 0.96          |
| (1,280) | 1:11:A:TRP:HE1  | 1:24:A:PRO:HD2 | 10       | 0.96          |
| (2,305) | 1:11:A:TRP:HH2  | 1:17:A:PRO:HB2 | 2        | 0.95          |
| (1,341) | 1:11:A:TRP:HH2  | 1:17:A:PRO:HB2 | 2        | 0.95          |
| (3,81)  | 1:4:A:ALA:HB1   | 1:7:A:LEU:HD21 | 10       | 0.94          |
| (3,81)  | 1:4:A:ALA:HB1   | 1:7:A:LEU:HD22 | 10       | 0.94          |
| (3,81)  | 1:4:A:ALA:HB1   | 1:7:A:LEU:HD23 | 10       | 0.94          |
| (3,81)  | 1:4:A:ALA:HB2   | 1:7:A:LEU:HD21 | 10       | 0.94          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (3,81)  | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD22 | 10       | 0.94          |
| (3,81)  | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD23 | 10       | 0.94          |
| (3,81)  | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD21 | 10       | 0.94          |
| (3,81)  | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD22 | 10       | 0.94          |
| (3,81)  | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD23 | 10       | 0.94          |
| (3,59)  | 1:7:A:LEU:HB3  | 1:10:A:GLN:H   | 10       | 0.94          |
| (3,56)  | 1:3:A:GLU:HB3  | 1:6:A:ARG:H    | 8        | 0.94          |
| (3,52)  | 1:21:A:ARG:H   | 1:22:A:PRO:HD2 | 4        | 0.94          |
| (3,52)  | 1:21:A:ARG:H   | 1:22:A:PRO:HD2 | 9        | 0.94          |
| (2,479) | 1:9:A:ILE:HG21 | 1:13:A:LYS:HG2 | 1        | 0.94          |
| (2,479) | 1:9:A:ILE:HG22 | 1:13:A:LYS:HG2 | 1        | 0.94          |
| (2,479) | 1:9:A:ILE:HG23 | 1:13:A:LYS:HG2 | 1        | 0.94          |
| (2,437) | 1:16:A:GLY:HA2 | 1:17:A:PRO:HG2 | 8        | 0.94          |
| (2,437) | 1:16:A:GLY:HA2 | 1:17:A:PRO:HG3 | 8        | 0.94          |
| (2,281) | 1:8:A:TYR:HE1  | 1:24:A:PRO:HB3 | 1        | 0.94          |
| (2,281) | 1:8:A:TYR:HE2  | 1:24:A:PRO:HB3 | 1        | 0.94          |
| (2,276) | 1:8:A:TYR:HD1  | 1:24:A:PRO:HD3 | 6        | 0.94          |
| (2,276) | 1:8:A:TYR:HD2  | 1:24:A:PRO:HD3 | 6        | 0.94          |
| (1,561) | 1:9:A:ILE:HG21 | 1:13:A:LYS:HG2 | 1        | 0.94          |
| (1,561) | 1:9:A:ILE:HG22 | 1:13:A:LYS:HG2 | 1        | 0.94          |
| (1,561) | 1:9:A:ILE:HG23 | 1:13:A:LYS:HG2 | 1        | 0.94          |
| (1,559) | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD21 | 10       | 0.94          |
| (1,559) | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD22 | 10       | 0.94          |
| (1,559) | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD23 | 10       | 0.94          |
| (1,559) | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD21 | 10       | 0.94          |
| (1,559) | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD22 | 10       | 0.94          |
| (1,559) | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD23 | 10       | 0.94          |
| (1,559) | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD21 | 10       | 0.94          |
| (1,559) | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD22 | 10       | 0.94          |
| (1,559) | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD23 | 10       | 0.94          |
| (1,504) | 1:16:A:GLY:HA2 | 1:17:A:PRO:HG2 | 8        | 0.94          |
| (1,504) | 1:16:A:GLY:HA2 | 1:17:A:PRO:HG3 | 8        | 0.94          |
| (1,441) | 1:7:A:LEU:HB3  | 1:10:A:GLN:H   | 10       | 0.94          |
| (1,432) | 1:3:A:GLU:HB3  | 1:6:A:ARG:H    | 8        | 0.94          |
| (1,418) | 1:21:A:ARG:H   | 1:22:A:PRO:HD2 | 4        | 0.94          |
| (1,418) | 1:21:A:ARG:H   | 1:22:A:PRO:HD2 | 9        | 0.94          |
| (1,304) | 1:8:A:TYR:HE1  | 1:24:A:PRO:HB3 | 1        | 0.94          |
| (1,304) | 1:8:A:TYR:HE2  | 1:24:A:PRO:HB3 | 1        | 0.94          |
| (1,299) | 1:8:A:TYR:HD1  | 1:24:A:PRO:HD3 | 6        | 0.94          |
| (1,299) | 1:8:A:TYR:HD2  | 1:24:A:PRO:HD3 | 6        | 0.94          |
| (3,88)  | 1:1:A:GLU:HB2  | 1:3:A:GLU:HA   | 2        | 0.93          |
| (3,87)  | 1:8:A:TYR:HB3  | 1:11:A:TRP:HE3 | 8        | 0.93          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (3,76)  | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG21 | 1        | 0.93          |
| (3,76)  | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG22 | 1        | 0.93          |
| (3,76)  | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG23 | 1        | 0.93          |
| (3,76)  | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG21 | 1        | 0.93          |
| (3,76)  | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG22 | 1        | 0.93          |
| (3,76)  | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG23 | 1        | 0.93          |
| (3,76)  | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG21 | 1        | 0.93          |
| (3,76)  | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG22 | 1        | 0.93          |
| (3,76)  | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG23 | 1        | 0.93          |
| (2,479) | 1:9:A:ILE:HG21 | 1:13:A:LYS:HG2 | 2        | 0.93          |
| (2,479) | 1:9:A:ILE:HG22 | 1:13:A:LYS:HG2 | 2        | 0.93          |
| (2,479) | 1:9:A:ILE:HG23 | 1:13:A:LYS:HG2 | 2        | 0.93          |
| (2,479) | 1:9:A:ILE:HG21 | 1:13:A:LYS:HG2 | 3        | 0.93          |
| (2,479) | 1:9:A:ILE:HG22 | 1:13:A:LYS:HG2 | 3        | 0.93          |
| (2,479) | 1:9:A:ILE:HG23 | 1:13:A:LYS:HG2 | 3        | 0.93          |
| (2,479) | 1:9:A:ILE:HG21 | 1:13:A:LYS:HG2 | 5        | 0.93          |
| (2,479) | 1:9:A:ILE:HG22 | 1:13:A:LYS:HG2 | 5        | 0.93          |
| (2,479) | 1:9:A:ILE:HG23 | 1:13:A:LYS:HG2 | 5        | 0.93          |
| (2,479) | 1:9:A:ILE:HG21 | 1:13:A:LYS:HG2 | 6        | 0.93          |
| (2,479) | 1:9:A:ILE:HG22 | 1:13:A:LYS:HG2 | 6        | 0.93          |
| (2,479) | 1:9:A:ILE:HG23 | 1:13:A:LYS:HG2 | 6        | 0.93          |
| (2,305) | 1:11:A:TRP:HH2 | 1:17:A:PRO:HB2 | 8        | 0.93          |
| (2,138) | 1:13:A:LYS:H   | 1:13:A:LYS:HG2 | 6        | 0.93          |
| (2,138) | 1:13:A:LYS:H   | 1:13:A:LYS:HG2 | 7        | 0.93          |
| (1,578) | 1:1:A:GLU:HB2  | 1:3:A:GLU:HA   | 2        | 0.93          |
| (1,575) | 1:8:A:TYR:HB3  | 1:11:A:TRP:HE3 | 8        | 0.93          |
| (1,561) | 1:9:A:ILE:HG21 | 1:13:A:LYS:HG2 | 2        | 0.93          |
| (1,561) | 1:9:A:ILE:HG22 | 1:13:A:LYS:HG2 | 2        | 0.93          |
| (1,561) | 1:9:A:ILE:HG23 | 1:13:A:LYS:HG2 | 2        | 0.93          |
| (1,561) | 1:9:A:ILE:HG21 | 1:13:A:LYS:HG2 | 3        | 0.93          |
| (1,561) | 1:9:A:ILE:HG22 | 1:13:A:LYS:HG2 | 3        | 0.93          |
| (1,561) | 1:9:A:ILE:HG23 | 1:13:A:LYS:HG2 | 3        | 0.93          |
| (1,561) | 1:9:A:ILE:HG21 | 1:13:A:LYS:HG2 | 5        | 0.93          |
| (1,561) | 1:9:A:ILE:HG22 | 1:13:A:LYS:HG2 | 5        | 0.93          |
| (1,561) | 1:9:A:ILE:HG23 | 1:13:A:LYS:HG2 | 5        | 0.93          |
| (1,561) | 1:9:A:ILE:HG21 | 1:13:A:LYS:HG2 | 6        | 0.93          |
| (1,561) | 1:9:A:ILE:HG22 | 1:13:A:LYS:HG2 | 6        | 0.93          |
| (1,561) | 1:9:A:ILE:HG23 | 1:13:A:LYS:HG2 | 6        | 0.93          |
| (1,546) | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG21 | 1        | 0.93          |
| (1,546) | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG22 | 1        | 0.93          |
| (1,546) | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG23 | 1        | 0.93          |
| (1,546) | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG21 | 1        | 0.93          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,546) | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG22 | 1        | 0.93          |
| (1,546) | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG23 | 1        | 0.93          |
| (1,546) | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG21 | 1        | 0.93          |
| (1,546) | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG22 | 1        | 0.93          |
| (1,546) | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG23 | 1        | 0.93          |
| (1,341) | 1:11:A:TRP:HH2 | 1:17:A:PRO:HB2 | 8        | 0.93          |
| (1,152) | 1:13:A:LYS:H   | 1:13:A:LYS:HG2 | 6        | 0.93          |
| (1,152) | 1:13:A:LYS:H   | 1:13:A:LYS:HG2 | 7        | 0.93          |
| (3,57)  | 1:7:A:LEU:HB2  | 1:10:A:GLN:H   | 4        | 0.92          |
| (3,52)  | 1:21:A:ARG:H   | 1:22:A:PRO:HD2 | 3        | 0.92          |
| (3,52)  | 1:21:A:ARG:H   | 1:22:A:PRO:HD2 | 8        | 0.92          |
| (3,29)  | 1:5:A:VAL:HG21 | 1:8:A:TYR:HE1  | 1        | 0.92          |
| (3,29)  | 1:5:A:VAL:HG21 | 1:8:A:TYR:HE2  | 1        | 0.92          |
| (3,29)  | 1:5:A:VAL:HG22 | 1:8:A:TYR:HE1  | 1        | 0.92          |
| (3,29)  | 1:5:A:VAL:HG22 | 1:8:A:TYR:HE2  | 1        | 0.92          |
| (3,29)  | 1:5:A:VAL:HG23 | 1:8:A:TYR:HE1  | 1        | 0.92          |
| (3,29)  | 1:5:A:VAL:HG23 | 1:8:A:TYR:HE2  | 1        | 0.92          |
| (2,479) | 1:9:A:ILE:HG21 | 1:13:A:LYS:HG2 | 4        | 0.92          |
| (2,479) | 1:9:A:ILE:HG22 | 1:13:A:LYS:HG2 | 4        | 0.92          |
| (2,479) | 1:9:A:ILE:HG23 | 1:13:A:LYS:HG2 | 4        | 0.92          |
| (2,305) | 1:11:A:TRP:HH2 | 1:17:A:PRO:HB2 | 4        | 0.92          |
| (2,138) | 1:13:A:LYS:H   | 1:13:A:LYS:HG2 | 9        | 0.92          |
| (1,561) | 1:9:A:ILE:HG21 | 1:13:A:LYS:HG2 | 4        | 0.92          |
| (1,561) | 1:9:A:ILE:HG22 | 1:13:A:LYS:HG2 | 4        | 0.92          |
| (1,561) | 1:9:A:ILE:HG23 | 1:13:A:LYS:HG2 | 4        | 0.92          |
| (1,435) | 1:7:A:LEU:HB2  | 1:10:A:GLN:H   | 4        | 0.92          |
| (1,418) | 1:21:A:ARG:H   | 1:22:A:PRO:HD2 | 3        | 0.92          |
| (1,418) | 1:21:A:ARG:H   | 1:22:A:PRO:HD2 | 8        | 0.92          |
| (1,341) | 1:11:A:TRP:HH2 | 1:17:A:PRO:HB2 | 4        | 0.92          |
| (1,317) | 1:5:A:VAL:HG21 | 1:8:A:TYR:HE1  | 1        | 0.92          |
| (1,317) | 1:5:A:VAL:HG21 | 1:8:A:TYR:HE2  | 1        | 0.92          |
| (1,317) | 1:5:A:VAL:HG22 | 1:8:A:TYR:HE1  | 1        | 0.92          |
| (1,317) | 1:5:A:VAL:HG22 | 1:8:A:TYR:HE2  | 1        | 0.92          |
| (1,317) | 1:5:A:VAL:HG23 | 1:8:A:TYR:HE1  | 1        | 0.92          |
| (1,317) | 1:5:A:VAL:HG23 | 1:8:A:TYR:HE2  | 1        | 0.92          |
| (1,152) | 1:13:A:LYS:H   | 1:13:A:LYS:HG2 | 9        | 0.92          |
| (3,89)  | 1:8:A:TYR:HB3  | 1:24:A:PRO:HG3 | 10       | 0.91          |
| (3,56)  | 1:3:A:GLU:HB3  | 1:6:A:ARG:H    | 5        | 0.91          |
| (2,495) | 1:11:A:TRP:HB2 | 1:24:A:PRO:HD2 | 3        | 0.91          |
| (2,495) | 1:11:A:TRP:HB2 | 1:24:A:PRO:HD2 | 4        | 0.91          |
| (2,485) | 1:16:A:GLY:H   | 1:19:A:SER:HB3 | 5        | 0.91          |
| (2,479) | 1:9:A:ILE:HG21 | 1:13:A:LYS:HG2 | 8        | 0.91          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (2,479) | 1:9:A:ILE:HG22 | 1:13:A:LYS:HG2 | 8        | 0.91          |
| (2,479) | 1:9:A:ILE:HG23 | 1:13:A:LYS:HG2 | 8        | 0.91          |
| (2,276) | 1:8:A:TYR:HD1  | 1:24:A:PRO:HD3 | 5        | 0.91          |
| (2,276) | 1:8:A:TYR:HD2  | 1:24:A:PRO:HD3 | 5        | 0.91          |
| (2,276) | 1:8:A:TYR:HD1  | 1:24:A:PRO:HD3 | 8        | 0.91          |
| (2,276) | 1:8:A:TYR:HD2  | 1:24:A:PRO:HD3 | 8        | 0.91          |
| (1,584) | 1:8:A:TYR:HB3  | 1:24:A:PRO:HG3 | 10       | 0.91          |
| (1,583) | 1:11:A:TRP:HB2 | 1:24:A:PRO:HD2 | 3        | 0.91          |
| (1,583) | 1:11:A:TRP:HB2 | 1:24:A:PRO:HD2 | 4        | 0.91          |
| (1,568) | 1:16:A:GLY:H   | 1:19:A:SER:HB3 | 5        | 0.91          |
| (1,561) | 1:9:A:ILE:HG21 | 1:13:A:LYS:HG2 | 8        | 0.91          |
| (1,561) | 1:9:A:ILE:HG22 | 1:13:A:LYS:HG2 | 8        | 0.91          |
| (1,561) | 1:9:A:ILE:HG23 | 1:13:A:LYS:HG2 | 8        | 0.91          |
| (1,432) | 1:3:A:GLU:HB3  | 1:6:A:ARG:H    | 5        | 0.91          |
| (1,299) | 1:8:A:TYR:HD1  | 1:24:A:PRO:HD3 | 5        | 0.91          |
| (1,299) | 1:8:A:TYR:HD2  | 1:24:A:PRO:HD3 | 5        | 0.91          |
| (1,299) | 1:8:A:TYR:HD1  | 1:24:A:PRO:HD3 | 8        | 0.91          |
| (1,299) | 1:8:A:TYR:HD2  | 1:24:A:PRO:HD3 | 8        | 0.91          |
| (3,89)  | 1:8:A:TYR:HB3  | 1:24:A:PRO:HG3 | 9        | 0.9           |
| (3,76)  | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG21 | 9        | 0.9           |
| (3,76)  | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG22 | 9        | 0.9           |
| (3,76)  | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG23 | 9        | 0.9           |
| (3,76)  | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG21 | 9        | 0.9           |
| (3,76)  | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG22 | 9        | 0.9           |
| (3,76)  | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG23 | 9        | 0.9           |
| (3,76)  | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG21 | 9        | 0.9           |
| (3,76)  | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG22 | 9        | 0.9           |
| (3,76)  | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG23 | 9        | 0.9           |
| (3,59)  | 1:7:A:LEU:HB3  | 1:10:A:GLN:H   | 9        | 0.9           |
| (3,52)  | 1:21:A:ARG:H   | 1:22:A:PRO:HD2 | 7        | 0.9           |
| (2,276) | 1:8:A:TYR:HD1  | 1:24:A:PRO:HD3 | 9        | 0.9           |
| (2,276) | 1:8:A:TYR:HD2  | 1:24:A:PRO:HD3 | 9        | 0.9           |
| (2,138) | 1:13:A:LYS:H   | 1:13:A:LYS:HG2 | 5        | 0.9           |
| (1,584) | 1:8:A:TYR:HB3  | 1:24:A:PRO:HG3 | 9        | 0.9           |
| (1,546) | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG21 | 9        | 0.9           |
| (1,546) | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG22 | 9        | 0.9           |
| (1,546) | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG23 | 9        | 0.9           |
| (1,546) | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG21 | 9        | 0.9           |
| (1,546) | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG22 | 9        | 0.9           |
| (1,546) | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG23 | 9        | 0.9           |
| (1,546) | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG21 | 9        | 0.9           |
| (1,546) | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG22 | 9        | 0.9           |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,546) | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG23 | 9        | 0.9           |
| (1,441) | 1:7:A:LEU:HB3  | 1:10:A:GLN:H   | 9        | 0.9           |
| (1,418) | 1:21:A:ARG:H   | 1:22:A:PRO:HD2 | 7        | 0.9           |
| (1,299) | 1:8:A:TYR:HD1  | 1:24:A:PRO:HD3 | 9        | 0.9           |
| (1,299) | 1:8:A:TYR:HD2  | 1:24:A:PRO:HD3 | 9        | 0.9           |
| (1,152) | 1:13:A:LYS:H   | 1:13:A:LYS:HG2 | 5        | 0.9           |
| (3,89)  | 1:8:A:TYR:HB3  | 1:24:A:PRO:HG3 | 3        | 0.89          |
| (3,56)  | 1:3:A:GLU:HB3  | 1:6:A:ARG:H    | 10       | 0.89          |
| (3,42)  | 1:11:A:TRP:H   | 1:11:A:TRP:HD1 | 5        | 0.89          |
| (2,495) | 1:11:A:TRP:HB2 | 1:24:A:PRO:HD2 | 2        | 0.89          |
| (2,305) | 1:11:A:TRP:HH2 | 1:17:A:PRO:HB2 | 10       | 0.89          |
| (2,276) | 1:8:A:TYR:HD1  | 1:24:A:PRO:HD3 | 1        | 0.89          |
| (2,276) | 1:8:A:TYR:HD2  | 1:24:A:PRO:HD3 | 1        | 0.89          |
| (2,138) | 1:13:A:LYS:H   | 1:13:A:LYS:HG2 | 2        | 0.89          |
| (2,138) | 1:13:A:LYS:H   | 1:13:A:LYS:HG2 | 3        | 0.89          |
| (2,138) | 1:13:A:LYS:H   | 1:13:A:LYS:HG2 | 4        | 0.89          |
| (2,138) | 1:13:A:LYS:H   | 1:13:A:LYS:HG2 | 10       | 0.89          |
| (1,584) | 1:8:A:TYR:HB3  | 1:24:A:PRO:HG3 | 3        | 0.89          |
| (1,583) | 1:11:A:TRP:HB2 | 1:24:A:PRO:HD2 | 2        | 0.89          |
| (1,432) | 1:3:A:GLU:HB3  | 1:6:A:ARG:H    | 10       | 0.89          |
| (1,371) | 1:11:A:TRP:H   | 1:11:A:TRP:HD1 | 5        | 0.89          |
| (1,341) | 1:11:A:TRP:HH2 | 1:17:A:PRO:HB2 | 10       | 0.89          |
| (1,299) | 1:8:A:TYR:HD1  | 1:24:A:PRO:HD3 | 1        | 0.89          |
| (1,299) | 1:8:A:TYR:HD2  | 1:24:A:PRO:HD3 | 1        | 0.89          |
| (1,152) | 1:13:A:LYS:H   | 1:13:A:LYS:HG2 | 2        | 0.89          |
| (1,152) | 1:13:A:LYS:H   | 1:13:A:LYS:HG2 | 3        | 0.89          |
| (1,152) | 1:13:A:LYS:H   | 1:13:A:LYS:HG2 | 4        | 0.89          |
| (1,152) | 1:13:A:LYS:H   | 1:13:A:LYS:HG2 | 10       | 0.89          |
| (3,89)  | 1:8:A:TYR:HB3  | 1:24:A:PRO:HG3 | 5        | 0.88          |
| (3,78)  | 1:7:A:LEU:HD21 | 1:24:A:PRO:HB2 | 4        | 0.88          |
| (3,78)  | 1:7:A:LEU:HD22 | 1:24:A:PRO:HB2 | 4        | 0.88          |
| (3,78)  | 1:7:A:LEU:HD23 | 1:24:A:PRO:HB2 | 4        | 0.88          |
| (3,76)  | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG21 | 3        | 0.88          |
| (3,76)  | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG22 | 3        | 0.88          |
| (3,76)  | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG23 | 3        | 0.88          |
| (3,76)  | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG21 | 3        | 0.88          |
| (3,76)  | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG22 | 3        | 0.88          |
| (3,76)  | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG23 | 3        | 0.88          |
| (3,76)  | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG21 | 3        | 0.88          |
| (3,76)  | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG22 | 3        | 0.88          |
| (3,76)  | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG23 | 3        | 0.88          |
| (3,76)  | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG21 | 10       | 0.88          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (3,76)  | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG22 | 10       | 0.88          |
| (3,76)  | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG23 | 10       | 0.88          |
| (3,76)  | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG21 | 10       | 0.88          |
| (3,76)  | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG22 | 10       | 0.88          |
| (3,76)  | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG23 | 10       | 0.88          |
| (3,76)  | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG21 | 10       | 0.88          |
| (3,76)  | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG22 | 10       | 0.88          |
| (3,76)  | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG23 | 10       | 0.88          |
| (3,56)  | 1:3:A:GLU:HB3  | 1:6:A:ARG:H    | 6        | 0.88          |
| (3,56)  | 1:3:A:GLU:HB3  | 1:6:A:ARG:H    | 7        | 0.88          |
| (3,42)  | 1:11:A:TRP:H   | 1:11:A:TRP:HD1 | 2        | 0.88          |
| (3,42)  | 1:11:A:TRP:H   | 1:11:A:TRP:HD1 | 7        | 0.88          |
| (2,495) | 1:11:A:TRP:HB2 | 1:24:A:PRO:HD2 | 10       | 0.88          |
| (2,485) | 1:16:A:GLY:H   | 1:19:A:SER:HB3 | 7        | 0.88          |
| (2,420) | 1:21:A:ARG:HB2 | 1:22:A:PRO:HD2 | 6        | 0.88          |
| (2,138) | 1:13:A:LYS:H   | 1:13:A:LYS:HG2 | 1        | 0.88          |
| (2,138) | 1:13:A:LYS:H   | 1:13:A:LYS:HG2 | 8        | 0.88          |
| (1,584) | 1:8:A:TYR:HB3  | 1:24:A:PRO:HG3 | 5        | 0.88          |
| (1,583) | 1:11:A:TRP:HB2 | 1:24:A:PRO:HD2 | 10       | 0.88          |
| (1,568) | 1:16:A:GLY:H   | 1:19:A:SER:HB3 | 7        | 0.88          |
| (1,554) | 1:7:A:LEU:HD21 | 1:24:A:PRO:HB2 | 4        | 0.88          |
| (1,554) | 1:7:A:LEU:HD22 | 1:24:A:PRO:HB2 | 4        | 0.88          |
| (1,554) | 1:7:A:LEU:HD23 | 1:24:A:PRO:HB2 | 4        | 0.88          |
| (1,546) | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG21 | 3        | 0.88          |
| (1,546) | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG22 | 3        | 0.88          |
| (1,546) | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG23 | 3        | 0.88          |
| (1,546) | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG21 | 3        | 0.88          |
| (1,546) | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG22 | 3        | 0.88          |
| (1,546) | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG23 | 3        | 0.88          |
| (1,546) | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG21 | 3        | 0.88          |
| (1,546) | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG22 | 3        | 0.88          |
| (1,546) | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG23 | 3        | 0.88          |
| (1,546) | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG21 | 10       | 0.88          |
| (1,546) | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG22 | 10       | 0.88          |
| (1,546) | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG23 | 10       | 0.88          |
| (1,546) | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG21 | 10       | 0.88          |
| (1,546) | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG22 | 10       | 0.88          |
| (1,546) | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG23 | 10       | 0.88          |
| (1,546) | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG21 | 10       | 0.88          |
| (1,546) | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG22 | 10       | 0.88          |
| (1,546) | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG23 | 10       | 0.88          |
| (1,485) | 1:21:A:ARG:HB2 | 1:22:A:PRO:HD2 | 6        | 0.88          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,432) | 1:3:A:GLU:HB3  | 1:6:A:ARG:H    | 6        | 0.88          |
| (1,432) | 1:3:A:GLU:HB3  | 1:6:A:ARG:H    | 7        | 0.88          |
| (1,371) | 1:11:A:TRP:H   | 1:11:A:TRP:HD1 | 2        | 0.88          |
| (1,371) | 1:11:A:TRP:H   | 1:11:A:TRP:HD1 | 7        | 0.88          |
| (1,152) | 1:13:A:LYS:H   | 1:13:A:LYS:HG2 | 1        | 0.88          |
| (1,152) | 1:13:A:LYS:H   | 1:13:A:LYS:HG2 | 8        | 0.88          |
| (3,78)  | 1:7:A:LEU:HD21 | 1:24:A:PRO:HB2 | 6        | 0.87          |
| (3,78)  | 1:7:A:LEU:HD22 | 1:24:A:PRO:HB2 | 6        | 0.87          |
| (3,78)  | 1:7:A:LEU:HD23 | 1:24:A:PRO:HB2 | 6        | 0.87          |
| (3,76)  | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG21 | 4        | 0.87          |
| (3,76)  | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG22 | 4        | 0.87          |
| (3,76)  | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG23 | 4        | 0.87          |
| (3,76)  | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG21 | 4        | 0.87          |
| (3,76)  | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG22 | 4        | 0.87          |
| (3,76)  | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG23 | 4        | 0.87          |
| (3,76)  | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG21 | 4        | 0.87          |
| (3,76)  | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG22 | 4        | 0.87          |
| (3,76)  | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG23 | 4        | 0.87          |
| (3,57)  | 1:7:A:LEU:HB2  | 1:10:A:GLN:H   | 2        | 0.87          |
| (3,57)  | 1:7:A:LEU:HB2  | 1:10:A:GLN:H   | 3        | 0.87          |
| (3,57)  | 1:7:A:LEU:HB2  | 1:10:A:GLN:H   | 5        | 0.87          |
| (3,52)  | 1:21:A:ARG:H   | 1:22:A:PRO:HD2 | 10       | 0.87          |
| (2,420) | 1:21:A:ARG:HB2 | 1:22:A:PRO:HD2 | 1        | 0.87          |
| (2,305) | 1:11:A:TRP:HH2 | 1:17:A:PRO:HB2 | 9        | 0.87          |
| (2,276) | 1:8:A:TYR:HD1  | 1:24:A:PRO:HD3 | 4        | 0.87          |
| (2,276) | 1:8:A:TYR:HD2  | 1:24:A:PRO:HD3 | 4        | 0.87          |
| (1,554) | 1:7:A:LEU:HD21 | 1:24:A:PRO:HB2 | 6        | 0.87          |
| (1,554) | 1:7:A:LEU:HD22 | 1:24:A:PRO:HB2 | 6        | 0.87          |
| (1,554) | 1:7:A:LEU:HD23 | 1:24:A:PRO:HB2 | 6        | 0.87          |
| (1,546) | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG21 | 4        | 0.87          |
| (1,546) | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG22 | 4        | 0.87          |
| (1,546) | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG23 | 4        | 0.87          |
| (1,546) | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG21 | 4        | 0.87          |
| (1,546) | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG22 | 4        | 0.87          |
| (1,546) | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG23 | 4        | 0.87          |
| (1,546) | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG21 | 4        | 0.87          |
| (1,546) | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG22 | 4        | 0.87          |
| (1,546) | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG23 | 4        | 0.87          |
| (1,485) | 1:21:A:ARG:HB2 | 1:22:A:PRO:HD2 | 1        | 0.87          |
| (1,435) | 1:7:A:LEU:HB2  | 1:10:A:GLN:H   | 2        | 0.87          |
| (1,435) | 1:7:A:LEU:HB2  | 1:10:A:GLN:H   | 3        | 0.87          |
| (1,435) | 1:7:A:LEU:HB2  | 1:10:A:GLN:H   | 5        | 0.87          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,418) | 1:21:A:ARG:H   | 1:22:A:PRO:HD2 | 10       | 0.87          |
| (1,341) | 1:11:A:TRP:HH2 | 1:17:A:PRO:HB2 | 9        | 0.87          |
| (1,299) | 1:8:A:TYR:HD1  | 1:24:A:PRO:HD3 | 4        | 0.87          |
| (1,299) | 1:8:A:TYR:HD2  | 1:24:A:PRO:HD3 | 4        | 0.87          |
| (3,87)  | 1:8:A:TYR:HB3  | 1:11:A:TRP:HE3 | 9        | 0.86          |
| (3,78)  | 1:7:A:LEU:HD21 | 1:24:A:PRO:HB2 | 2        | 0.86          |
| (3,78)  | 1:7:A:LEU:HD22 | 1:24:A:PRO:HB2 | 2        | 0.86          |
| (3,78)  | 1:7:A:LEU:HD23 | 1:24:A:PRO:HB2 | 2        | 0.86          |
| (3,57)  | 1:7:A:LEU:HB2  | 1:10:A:GLN:H   | 6        | 0.86          |
| (3,57)  | 1:7:A:LEU:HB2  | 1:10:A:GLN:H   | 7        | 0.86          |
| (3,56)  | 1:3:A:GLU:HB3  | 1:6:A:ARG:H    | 9        | 0.86          |
| (3,42)  | 1:11:A:TRP:H   | 1:11:A:TRP:HD1 | 9        | 0.86          |
| (3,16)  | 1:24:A:PRO:HA  | 1:25:A:SER:H   | 7        | 0.86          |
| (2,495) | 1:11:A:TRP:HB2 | 1:24:A:PRO:HD2 | 1        | 0.86          |
| (2,386) | 1:23:A:PRO:HB3 | 1:25:A:SER:H   | 8        | 0.86          |
| (2,276) | 1:8:A:TYR:HD1  | 1:24:A:PRO:HD3 | 2        | 0.86          |
| (2,276) | 1:8:A:TYR:HD2  | 1:24:A:PRO:HD3 | 2        | 0.86          |
| (2,276) | 1:8:A:TYR:HD1  | 1:24:A:PRO:HD3 | 7        | 0.86          |
| (2,276) | 1:8:A:TYR:HD2  | 1:24:A:PRO:HD3 | 7        | 0.86          |
| (1,583) | 1:11:A:TRP:HB2 | 1:24:A:PRO:HD2 | 1        | 0.86          |
| (1,575) | 1:8:A:TYR:HB3  | 1:11:A:TRP:HE3 | 9        | 0.86          |
| (1,554) | 1:7:A:LEU:HD21 | 1:24:A:PRO:HB2 | 2        | 0.86          |
| (1,554) | 1:7:A:LEU:HD22 | 1:24:A:PRO:HB2 | 2        | 0.86          |
| (1,554) | 1:7:A:LEU:HD23 | 1:24:A:PRO:HB2 | 2        | 0.86          |
| (1,448) | 1:23:A:PRO:HB3 | 1:25:A:SER:H   | 8        | 0.86          |
| (1,435) | 1:7:A:LEU:HB2  | 1:10:A:GLN:H   | 6        | 0.86          |
| (1,435) | 1:7:A:LEU:HB2  | 1:10:A:GLN:H   | 7        | 0.86          |
| (1,432) | 1:3:A:GLU:HB3  | 1:6:A:ARG:H    | 9        | 0.86          |
| (1,371) | 1:11:A:TRP:H   | 1:11:A:TRP:HD1 | 9        | 0.86          |
| (1,299) | 1:8:A:TYR:HD1  | 1:24:A:PRO:HD3 | 2        | 0.86          |
| (1,299) | 1:8:A:TYR:HD2  | 1:24:A:PRO:HD3 | 2        | 0.86          |
| (1,299) | 1:8:A:TYR:HD1  | 1:24:A:PRO:HD3 | 7        | 0.86          |
| (1,299) | 1:8:A:TYR:HD2  | 1:24:A:PRO:HD3 | 7        | 0.86          |
| (1,184) | 1:24:A:PRO:HA  | 1:25:A:SER:H   | 7        | 0.86          |
| (3,89)  | 1:8:A:TYR:HB3  | 1:24:A:PRO:HG3 | 1        | 0.85          |
| (3,89)  | 1:8:A:TYR:HB3  | 1:24:A:PRO:HG3 | 2        | 0.85          |
| (3,89)  | 1:8:A:TYR:HB3  | 1:24:A:PRO:HG3 | 4        | 0.85          |
| (3,87)  | 1:8:A:TYR:HB3  | 1:11:A:TRP:HE3 | 10       | 0.85          |
| (3,78)  | 1:7:A:LEU:HD21 | 1:24:A:PRO:HB2 | 7        | 0.85          |
| (3,78)  | 1:7:A:LEU:HD22 | 1:24:A:PRO:HB2 | 7        | 0.85          |
| (3,78)  | 1:7:A:LEU:HD23 | 1:24:A:PRO:HB2 | 7        | 0.85          |
| (3,76)  | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG21 | 2        | 0.85          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (3,76)  | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG22 | 2        | 0.85          |
| (3,76)  | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG23 | 2        | 0.85          |
| (3,76)  | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG21 | 2        | 0.85          |
| (3,76)  | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG22 | 2        | 0.85          |
| (3,76)  | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG23 | 2        | 0.85          |
| (3,76)  | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG21 | 2        | 0.85          |
| (3,76)  | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG22 | 2        | 0.85          |
| (3,76)  | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG23 | 2        | 0.85          |
| (3,57)  | 1:7:A:LEU:HB2  | 1:10:A:GLN:H   | 8        | 0.85          |
| (3,42)  | 1:11:A:TRP:H   | 1:11:A:TRP:HD1 | 4        | 0.85          |
| (3,42)  | 1:11:A:TRP:H   | 1:11:A:TRP:HD1 | 8        | 0.85          |
| (3,16)  | 1:24:A:PRO:HA  | 1:25:A:SER:H   | 10       | 0.85          |
| (2,305) | 1:11:A:TRP:HH2 | 1:17:A:PRO:HB2 | 1        | 0.85          |
| (2,276) | 1:8:A:TYR:HD1  | 1:24:A:PRO:HD3 | 3        | 0.85          |
| (2,276) | 1:8:A:TYR:HD2  | 1:24:A:PRO:HD3 | 3        | 0.85          |
| (2,276) | 1:8:A:TYR:HD1  | 1:24:A:PRO:HD3 | 10       | 0.85          |
| (2,276) | 1:8:A:TYR:HD2  | 1:24:A:PRO:HD3 | 10       | 0.85          |
| (1,584) | 1:8:A:TYR:HB3  | 1:24:A:PRO:HG3 | 1        | 0.85          |
| (1,584) | 1:8:A:TYR:HB3  | 1:24:A:PRO:HG3 | 2        | 0.85          |
| (1,584) | 1:8:A:TYR:HB3  | 1:24:A:PRO:HG3 | 4        | 0.85          |
| (1,575) | 1:8:A:TYR:HB3  | 1:11:A:TRP:HE3 | 10       | 0.85          |
| (1,554) | 1:7:A:LEU:HD21 | 1:24:A:PRO:HB2 | 7        | 0.85          |
| (1,554) | 1:7:A:LEU:HD22 | 1:24:A:PRO:HB2 | 7        | 0.85          |
| (1,554) | 1:7:A:LEU:HD23 | 1:24:A:PRO:HB2 | 7        | 0.85          |
| (1,546) | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG21 | 2        | 0.85          |
| (1,546) | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG22 | 2        | 0.85          |
| (1,546) | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG23 | 2        | 0.85          |
| (1,546) | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG21 | 2        | 0.85          |
| (1,546) | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG22 | 2        | 0.85          |
| (1,546) | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG23 | 2        | 0.85          |
| (1,546) | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG21 | 2        | 0.85          |
| (1,546) | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG22 | 2        | 0.85          |
| (1,546) | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG23 | 2        | 0.85          |
| (1,435) | 1:7:A:LEU:HB2  | 1:10:A:GLN:H   | 8        | 0.85          |
| (1,371) | 1:11:A:TRP:H   | 1:11:A:TRP:HD1 | 4        | 0.85          |
| (1,371) | 1:11:A:TRP:H   | 1:11:A:TRP:HD1 | 8        | 0.85          |
| (1,341) | 1:11:A:TRP:HH2 | 1:17:A:PRO:HB2 | 1        | 0.85          |
| (1,299) | 1:8:A:TYR:HD1  | 1:24:A:PRO:HD3 | 3        | 0.85          |
| (1,299) | 1:8:A:TYR:HD2  | 1:24:A:PRO:HD3 | 3        | 0.85          |
| (1,299) | 1:8:A:TYR:HD1  | 1:24:A:PRO:HD3 | 10       | 0.85          |
| (1,299) | 1:8:A:TYR:HD2  | 1:24:A:PRO:HD3 | 10       | 0.85          |
| (1,184) | 1:24:A:PRO:HA  | 1:25:A:SER:H   | 10       | 0.85          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (3,89)  | 1:8:A:TYR:HB3  | 1:24:A:PRO:HG3 | 7        | 0.84          |
| (3,42)  | 1:11:A:TRP:H   | 1:11:A:TRP:HD1 | 3        | 0.84          |
| (3,27)  | 1:8:A:TYR:HD1  | 1:9:A:ILE:HG13 | 10       | 0.84          |
| (3,27)  | 1:8:A:TYR:HD2  | 1:9:A:ILE:HG13 | 10       | 0.84          |
| (3,16)  | 1:24:A:PRO:HA  | 1:25:A:SER:H   | 6        | 0.84          |
| (3,16)  | 1:24:A:PRO:HA  | 1:25:A:SER:H   | 8        | 0.84          |
| (2,495) | 1:11:A:TRP:HB2 | 1:24:A:PRO:HD2 | 5        | 0.84          |
| (2,305) | 1:11:A:TRP:HH2 | 1:17:A:PRO:HB2 | 5        | 0.84          |
| (1,584) | 1:8:A:TYR:HB3  | 1:24:A:PRO:HG3 | 7        | 0.84          |
| (1,583) | 1:11:A:TRP:HB2 | 1:24:A:PRO:HD2 | 5        | 0.84          |
| (1,371) | 1:11:A:TRP:H   | 1:11:A:TRP:HD1 | 3        | 0.84          |
| (1,341) | 1:11:A:TRP:HH2 | 1:17:A:PRO:HB2 | 5        | 0.84          |
| (1,313) | 1:8:A:TYR:HD1  | 1:9:A:ILE:HG13 | 10       | 0.84          |
| (1,313) | 1:8:A:TYR:HD2  | 1:9:A:ILE:HG13 | 10       | 0.84          |
| (1,184) | 1:24:A:PRO:HA  | 1:25:A:SER:H   | 6        | 0.84          |
| (1,184) | 1:24:A:PRO:HA  | 1:25:A:SER:H   | 8        | 0.84          |
| (3,89)  | 1:8:A:TYR:HB3  | 1:24:A:PRO:HG3 | 6        | 0.83          |
| (2,305) | 1:11:A:TRP:HH2 | 1:17:A:PRO:HB2 | 6        | 0.83          |
| (2,305) | 1:11:A:TRP:HH2 | 1:17:A:PRO:HB2 | 7        | 0.83          |
| (1,584) | 1:8:A:TYR:HB3  | 1:24:A:PRO:HG3 | 6        | 0.83          |
| (1,341) | 1:11:A:TRP:HH2 | 1:17:A:PRO:HB2 | 6        | 0.83          |
| (1,341) | 1:11:A:TRP:HH2 | 1:17:A:PRO:HB2 | 7        | 0.83          |
| (3,78)  | 1:7:A:LEU:HD21 | 1:24:A:PRO:HB2 | 1        | 0.82          |
| (3,78)  | 1:7:A:LEU:HD22 | 1:24:A:PRO:HB2 | 1        | 0.82          |
| (3,78)  | 1:7:A:LEU:HD23 | 1:24:A:PRO:HB2 | 1        | 0.82          |
| (3,42)  | 1:11:A:TRP:H   | 1:11:A:TRP:HD1 | 6        | 0.82          |
| (2,495) | 1:11:A:TRP:HB2 | 1:24:A:PRO:HD2 | 7        | 0.82          |
| (2,447) | 1:7:A:LEU:HB3  | 1:24:A:PRO:HB2 | 10       | 0.82          |
| (1,583) | 1:11:A:TRP:HB2 | 1:24:A:PRO:HD2 | 7        | 0.82          |
| (1,554) | 1:7:A:LEU:HD21 | 1:24:A:PRO:HB2 | 1        | 0.82          |
| (1,554) | 1:7:A:LEU:HD22 | 1:24:A:PRO:HB2 | 1        | 0.82          |
| (1,554) | 1:7:A:LEU:HD23 | 1:24:A:PRO:HB2 | 1        | 0.82          |
| (1,514) | 1:7:A:LEU:HB3  | 1:24:A:PRO:HB2 | 10       | 0.82          |
| (1,371) | 1:11:A:TRP:H   | 1:11:A:TRP:HD1 | 6        | 0.82          |
| (3,78)  | 1:7:A:LEU:HD21 | 1:24:A:PRO:HB2 | 5        | 0.81          |
| (3,78)  | 1:7:A:LEU:HD22 | 1:24:A:PRO:HB2 | 5        | 0.81          |
| (3,78)  | 1:7:A:LEU:HD23 | 1:24:A:PRO:HB2 | 5        | 0.81          |
| (3,56)  | 1:3:A:GLU:HB3  | 1:6:A:ARG:H    | 2        | 0.81          |
| (3,27)  | 1:8:A:TYR:HD1  | 1:9:A:ILE:HG13 | 9        | 0.81          |
| (3,27)  | 1:8:A:TYR:HD2  | 1:9:A:ILE:HG13 | 9        | 0.81          |
| (1,554) | 1:7:A:LEU:HD21 | 1:24:A:PRO:HB2 | 5        | 0.81          |
| (1,554) | 1:7:A:LEU:HD22 | 1:24:A:PRO:HB2 | 5        | 0.81          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,554) | 1:7:A:LEU:HD23 | 1:24:A:PRO:HB2 | 5        | 0.81          |
| (1,432) | 1:3:A:GLU:HB3  | 1:6:A:ARG:H    | 2        | 0.81          |
| (1,313) | 1:8:A:TYR:HD1  | 1:9:A:ILE:HG13 | 9        | 0.81          |
| (1,313) | 1:8:A:TYR:HD2  | 1:9:A:ILE:HG13 | 9        | 0.81          |
| (3,61)  | 1:9:A:ILE:HD11 | 1:10:A:GLN:H   | 6        | 0.8           |
| (3,61)  | 1:9:A:ILE:HD12 | 1:10:A:GLN:H   | 6        | 0.8           |
| (3,61)  | 1:9:A:ILE:HD13 | 1:10:A:GLN:H   | 6        | 0.8           |
| (3,29)  | 1:5:A:VAL:HG21 | 1:8:A:TYR:HE1  | 5        | 0.8           |
| (3,29)  | 1:5:A:VAL:HG21 | 1:8:A:TYR:HE2  | 5        | 0.8           |
| (3,29)  | 1:5:A:VAL:HG22 | 1:8:A:TYR:HE1  | 5        | 0.8           |
| (3,29)  | 1:5:A:VAL:HG22 | 1:8:A:TYR:HE2  | 5        | 0.8           |
| (3,29)  | 1:5:A:VAL:HG23 | 1:8:A:TYR:HE1  | 5        | 0.8           |
| (3,29)  | 1:5:A:VAL:HG23 | 1:8:A:TYR:HE2  | 5        | 0.8           |
| (2,495) | 1:11:A:TRP:HB2 | 1:24:A:PRO:HD2 | 6        | 0.8           |
| (1,583) | 1:11:A:TRP:HB2 | 1:24:A:PRO:HD2 | 6        | 0.8           |
| (1,446) | 1:9:A:ILE:HD11 | 1:10:A:GLN:H   | 6        | 0.8           |
| (1,446) | 1:9:A:ILE:HD12 | 1:10:A:GLN:H   | 6        | 0.8           |
| (1,446) | 1:9:A:ILE:HD13 | 1:10:A:GLN:H   | 6        | 0.8           |
| (1,317) | 1:5:A:VAL:HG21 | 1:8:A:TYR:HE1  | 5        | 0.8           |
| (1,317) | 1:5:A:VAL:HG21 | 1:8:A:TYR:HE2  | 5        | 0.8           |
| (1,317) | 1:5:A:VAL:HG22 | 1:8:A:TYR:HE1  | 5        | 0.8           |
| (1,317) | 1:5:A:VAL:HG22 | 1:8:A:TYR:HE2  | 5        | 0.8           |
| (1,317) | 1:5:A:VAL:HG23 | 1:8:A:TYR:HE1  | 5        | 0.8           |
| (1,317) | 1:5:A:VAL:HG23 | 1:8:A:TYR:HE2  | 5        | 0.8           |
| (3,61)  | 1:9:A:ILE:HD11 | 1:10:A:GLN:H   | 5        | 0.79          |
| (3,61)  | 1:9:A:ILE:HD12 | 1:10:A:GLN:H   | 5        | 0.79          |
| (3,61)  | 1:9:A:ILE:HD13 | 1:10:A:GLN:H   | 5        | 0.79          |
| (3,55)  | 1:10:A:GLN:HB2 | 1:11:A:TRP:H   | 10       | 0.79          |
| (3,42)  | 1:11:A:TRP:H   | 1:11:A:TRP:HD1 | 10       | 0.79          |
| (3,16)  | 1:24:A:PRO:HA  | 1:25:A:SER:H   | 2        | 0.79          |
| (3,16)  | 1:24:A:PRO:HA  | 1:25:A:SER:H   | 3        | 0.79          |
| (3,16)  | 1:24:A:PRO:HA  | 1:25:A:SER:H   | 4        | 0.79          |
| (1,446) | 1:9:A:ILE:HD11 | 1:10:A:GLN:H   | 5        | 0.79          |
| (1,446) | 1:9:A:ILE:HD12 | 1:10:A:GLN:H   | 5        | 0.79          |
| (1,446) | 1:9:A:ILE:HD13 | 1:10:A:GLN:H   | 5        | 0.79          |
| (1,429) | 1:10:A:GLN:HB2 | 1:11:A:TRP:H   | 10       | 0.79          |
| (1,371) | 1:11:A:TRP:H   | 1:11:A:TRP:HD1 | 10       | 0.79          |
| (1,184) | 1:24:A:PRO:HA  | 1:25:A:SER:H   | 2        | 0.79          |
| (1,184) | 1:24:A:PRO:HA  | 1:25:A:SER:H   | 3        | 0.79          |
| (1,184) | 1:24:A:PRO:HA  | 1:25:A:SER:H   | 4        | 0.79          |
| (3,78)  | 1:7:A:LEU:HD21 | 1:24:A:PRO:HB2 | 3        | 0.78          |
| (3,78)  | 1:7:A:LEU:HD22 | 1:24:A:PRO:HB2 | 3        | 0.78          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (3,78)  | 1:7:A:LEU:HD23 | 1:24:A:PRO:HB2 | 3        | 0.78          |
| (3,42)  | 1:11:A:TRP:H   | 1:11:A:TRP:HD1 | 1        | 0.78          |
| (2,281) | 1:8:A:TYR:HE1  | 1:24:A:PRO:HB3 | 9        | 0.78          |
| (2,281) | 1:8:A:TYR:HE2  | 1:24:A:PRO:HB3 | 9        | 0.78          |
| (1,554) | 1:7:A:LEU:HD21 | 1:24:A:PRO:HB2 | 3        | 0.78          |
| (1,554) | 1:7:A:LEU:HD22 | 1:24:A:PRO:HB2 | 3        | 0.78          |
| (1,554) | 1:7:A:LEU:HD23 | 1:24:A:PRO:HB2 | 3        | 0.78          |
| (1,371) | 1:11:A:TRP:H   | 1:11:A:TRP:HD1 | 1        | 0.78          |
| (1,304) | 1:8:A:TYR:HE1  | 1:24:A:PRO:HB3 | 9        | 0.78          |
| (1,304) | 1:8:A:TYR:HE2  | 1:24:A:PRO:HB3 | 9        | 0.78          |
| (3,61)  | 1:9:A:ILE:HD11 | 1:10:A:GLN:H   | 4        | 0.77          |
| (3,61)  | 1:9:A:ILE:HD12 | 1:10:A:GLN:H   | 4        | 0.77          |
| (3,61)  | 1:9:A:ILE:HD13 | 1:10:A:GLN:H   | 4        | 0.77          |
| (3,29)  | 1:5:A:VAL:HG21 | 1:8:A:TYR:HE1  | 3        | 0.77          |
| (3,29)  | 1:5:A:VAL:HG21 | 1:8:A:TYR:HE2  | 3        | 0.77          |
| (3,29)  | 1:5:A:VAL:HG22 | 1:8:A:TYR:HE1  | 3        | 0.77          |
| (3,29)  | 1:5:A:VAL:HG22 | 1:8:A:TYR:HE2  | 3        | 0.77          |
| (3,29)  | 1:5:A:VAL:HG23 | 1:8:A:TYR:HE1  | 3        | 0.77          |
| (3,29)  | 1:5:A:VAL:HG23 | 1:8:A:TYR:HE2  | 3        | 0.77          |
| (3,29)  | 1:5:A:VAL:HG21 | 1:8:A:TYR:HE1  | 8        | 0.77          |
| (3,29)  | 1:5:A:VAL:HG21 | 1:8:A:TYR:HE2  | 8        | 0.77          |
| (3,29)  | 1:5:A:VAL:HG22 | 1:8:A:TYR:HE1  | 8        | 0.77          |
| (3,29)  | 1:5:A:VAL:HG22 | 1:8:A:TYR:HE2  | 8        | 0.77          |
| (3,29)  | 1:5:A:VAL:HG23 | 1:8:A:TYR:HE1  | 8        | 0.77          |
| (3,29)  | 1:5:A:VAL:HG23 | 1:8:A:TYR:HE2  | 8        | 0.77          |
| (2,495) | 1:11:A:TRP:HB2 | 1:24:A:PRO:HD2 | 9        | 0.77          |
| (2,404) | 1:11:A:TRP:HA  | 1:14:A:ASP:HB3 | 2        | 0.77          |
| (2,404) | 1:11:A:TRP:HA  | 1:14:A:ASP:HB3 | 7        | 0.77          |
| (2,293) | 1:11:A:TRP:HZ2 | 1:23:A:PRO:HB2 | 8        | 0.77          |
| (1,583) | 1:11:A:TRP:HB2 | 1:24:A:PRO:HD2 | 9        | 0.77          |
| (1,466) | 1:11:A:TRP:HA  | 1:14:A:ASP:HB3 | 2        | 0.77          |
| (1,466) | 1:11:A:TRP:HA  | 1:14:A:ASP:HB3 | 7        | 0.77          |
| (1,446) | 1:9:A:ILE:HD11 | 1:10:A:GLN:H   | 4        | 0.77          |
| (1,446) | 1:9:A:ILE:HD12 | 1:10:A:GLN:H   | 4        | 0.77          |
| (1,446) | 1:9:A:ILE:HD13 | 1:10:A:GLN:H   | 4        | 0.77          |
| (1,324) | 1:11:A:TRP:HZ2 | 1:23:A:PRO:HB2 | 8        | 0.77          |
| (1,317) | 1:5:A:VAL:HG21 | 1:8:A:TYR:HE1  | 3        | 0.77          |
| (1,317) | 1:5:A:VAL:HG21 | 1:8:A:TYR:HE2  | 3        | 0.77          |
| (1,317) | 1:5:A:VAL:HG22 | 1:8:A:TYR:HE1  | 3        | 0.77          |
| (1,317) | 1:5:A:VAL:HG22 | 1:8:A:TYR:HE2  | 3        | 0.77          |
| (1,317) | 1:5:A:VAL:HG23 | 1:8:A:TYR:HE1  | 3        | 0.77          |
| (1,317) | 1:5:A:VAL:HG23 | 1:8:A:TYR:HE2  | 3        | 0.77          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,317) | 1:5:A:VAL:HG21 | 1:8:A:TYR:HE1  | 8        | 0.77          |
| (1,317) | 1:5:A:VAL:HG21 | 1:8:A:TYR:HE2  | 8        | 0.77          |
| (1,317) | 1:5:A:VAL:HG22 | 1:8:A:TYR:HE1  | 8        | 0.77          |
| (1,317) | 1:5:A:VAL:HG22 | 1:8:A:TYR:HE2  | 8        | 0.77          |
| (1,317) | 1:5:A:VAL:HG23 | 1:8:A:TYR:HE1  | 8        | 0.77          |
| (1,317) | 1:5:A:VAL:HG23 | 1:8:A:TYR:HE2  | 8        | 0.77          |
| (3,76)  | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG21 | 5        | 0.76          |
| (3,76)  | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG22 | 5        | 0.76          |
| (3,76)  | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG23 | 5        | 0.76          |
| (3,76)  | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG21 | 5        | 0.76          |
| (3,76)  | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG22 | 5        | 0.76          |
| (3,76)  | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG23 | 5        | 0.76          |
| (3,76)  | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG21 | 5        | 0.76          |
| (3,76)  | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG22 | 5        | 0.76          |
| (3,76)  | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG23 | 5        | 0.76          |
| (3,65)  | 1:6:A:ARG:HA   | 1:10:A:GLN:HB3 | 9        | 0.76          |
| (3,61)  | 1:9:A:ILE:HD11 | 1:10:A:GLN:H   | 2        | 0.76          |
| (3,61)  | 1:9:A:ILE:HD12 | 1:10:A:GLN:H   | 2        | 0.76          |
| (3,61)  | 1:9:A:ILE:HD13 | 1:10:A:GLN:H   | 2        | 0.76          |
| (3,16)  | 1:24:A:PRO:HA  | 1:25:A:SER:H   | 5        | 0.76          |
| (2,496) | 1:1:A:GLU:HB3  | 1:2:A:GLU:HG2  | 4        | 0.76          |
| (2,275) | 1:11:A:TRP:HD1 | 1:21:A:ARG:HD2 | 1        | 0.76          |
| (1,585) | 1:1:A:GLU:HB3  | 1:2:A:GLU:HG2  | 4        | 0.76          |
| (1,546) | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG21 | 5        | 0.76          |
| (1,546) | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG22 | 5        | 0.76          |
| (1,546) | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG23 | 5        | 0.76          |
| (1,546) | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG21 | 5        | 0.76          |
| (1,546) | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG22 | 5        | 0.76          |
| (1,546) | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG23 | 5        | 0.76          |
| (1,546) | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG21 | 5        | 0.76          |
| (1,546) | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG22 | 5        | 0.76          |
| (1,546) | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG23 | 5        | 0.76          |
| (1,482) | 1:6:A:ARG:HA   | 1:10:A:GLN:HB3 | 9        | 0.76          |
| (1,446) | 1:9:A:ILE:HD11 | 1:10:A:GLN:H   | 2        | 0.76          |
| (1,446) | 1:9:A:ILE:HD12 | 1:10:A:GLN:H   | 2        | 0.76          |
| (1,446) | 1:9:A:ILE:HD13 | 1:10:A:GLN:H   | 2        | 0.76          |
| (1,298) | 1:11:A:TRP:HD1 | 1:21:A:ARG:HD2 | 1        | 0.76          |
| (1,184) | 1:24:A:PRO:HA  | 1:25:A:SER:H   | 5        | 0.76          |
| (3,76)  | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG21 | 7        | 0.75          |
| (3,76)  | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG22 | 7        | 0.75          |
| (3,76)  | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG23 | 7        | 0.75          |
| (3,76)  | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG21 | 7        | 0.75          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (3,76)  | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG22  | 7        | 0.75          |
| (3,76)  | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG23  | 7        | 0.75          |
| (3,76)  | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG21  | 7        | 0.75          |
| (3,76)  | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG22  | 7        | 0.75          |
| (3,76)  | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG23  | 7        | 0.75          |
| (3,76)  | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG21  | 8        | 0.75          |
| (3,76)  | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG22  | 8        | 0.75          |
| (3,76)  | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG23  | 8        | 0.75          |
| (3,76)  | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG21  | 8        | 0.75          |
| (3,76)  | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG22  | 8        | 0.75          |
| (3,76)  | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG23  | 8        | 0.75          |
| (3,76)  | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG21  | 8        | 0.75          |
| (3,76)  | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG22  | 8        | 0.75          |
| (3,76)  | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG23  | 8        | 0.75          |
| (3,61)  | 1:9:A:ILE:HD11 | 1:10:A:GLN:H    | 7        | 0.75          |
| (3,61)  | 1:9:A:ILE:HD12 | 1:10:A:GLN:H    | 7        | 0.75          |
| (3,61)  | 1:9:A:ILE:HD13 | 1:10:A:GLN:H    | 7        | 0.75          |
| (3,32)  | 1:11:A:TRP:HH2 | 1:12:A:LEU:HD11 | 1        | 0.75          |
| (3,32)  | 1:11:A:TRP:HH2 | 1:12:A:LEU:HD12 | 1        | 0.75          |
| (3,32)  | 1:11:A:TRP:HH2 | 1:12:A:LEU:HD13 | 1        | 0.75          |
| (3,29)  | 1:5:A:VAL:HG21 | 1:8:A:TYR:HE1   | 7        | 0.75          |
| (3,29)  | 1:5:A:VAL:HG21 | 1:8:A:TYR:HE2   | 7        | 0.75          |
| (3,29)  | 1:5:A:VAL:HG22 | 1:8:A:TYR:HE1   | 7        | 0.75          |
| (3,29)  | 1:5:A:VAL:HG22 | 1:8:A:TYR:HE2   | 7        | 0.75          |
| (3,29)  | 1:5:A:VAL:HG23 | 1:8:A:TYR:HE1   | 7        | 0.75          |
| (3,29)  | 1:5:A:VAL:HG23 | 1:8:A:TYR:HE2   | 7        | 0.75          |
| (3,16)  | 1:24:A:PRO:HA  | 1:25:A:SER:H    | 9        | 0.75          |
| (2,293) | 1:11:A:TRP:HZ2 | 1:23:A:PRO:HB2  | 4        | 0.75          |
| (1,546) | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG21  | 7        | 0.75          |
| (1,546) | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG22  | 7        | 0.75          |
| (1,546) | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG23  | 7        | 0.75          |
| (1,546) | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG21  | 7        | 0.75          |
| (1,546) | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG22  | 7        | 0.75          |
| (1,546) | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG23  | 7        | 0.75          |
| (1,546) | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG21  | 7        | 0.75          |
| (1,546) | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG22  | 7        | 0.75          |
| (1,546) | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG23  | 7        | 0.75          |
| (1,546) | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG21  | 8        | 0.75          |
| (1,546) | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG22  | 8        | 0.75          |
| (1,546) | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG23  | 8        | 0.75          |
| (1,546) | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG21  | 8        | 0.75          |
| (1,546) | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG22  | 8        | 0.75          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,546) | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG23  | 8        | 0.75          |
| (1,546) | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG21  | 8        | 0.75          |
| (1,546) | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG22  | 8        | 0.75          |
| (1,546) | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG23  | 8        | 0.75          |
| (1,446) | 1:9:A:ILE:HD11 | 1:10:A:GLN:H    | 7        | 0.75          |
| (1,446) | 1:9:A:ILE:HD12 | 1:10:A:GLN:H    | 7        | 0.75          |
| (1,446) | 1:9:A:ILE:HD13 | 1:10:A:GLN:H    | 7        | 0.75          |
| (1,326) | 1:11:A:TRP:HH2 | 1:12:A:LEU:HD11 | 1        | 0.75          |
| (1,326) | 1:11:A:TRP:HH2 | 1:12:A:LEU:HD12 | 1        | 0.75          |
| (1,326) | 1:11:A:TRP:HH2 | 1:12:A:LEU:HD13 | 1        | 0.75          |
| (1,324) | 1:11:A:TRP:HZ2 | 1:23:A:PRO:HB2  | 4        | 0.75          |
| (1,317) | 1:5:A:VAL:HG21 | 1:8:A:TYR:HE1   | 7        | 0.75          |
| (1,317) | 1:5:A:VAL:HG21 | 1:8:A:TYR:HE2   | 7        | 0.75          |
| (1,317) | 1:5:A:VAL:HG22 | 1:8:A:TYR:HE1   | 7        | 0.75          |
| (1,317) | 1:5:A:VAL:HG22 | 1:8:A:TYR:HE2   | 7        | 0.75          |
| (1,317) | 1:5:A:VAL:HG23 | 1:8:A:TYR:HE1   | 7        | 0.75          |
| (1,317) | 1:5:A:VAL:HG23 | 1:8:A:TYR:HE2   | 7        | 0.75          |
| (1,184) | 1:24:A:PRO:HA  | 1:25:A:SER:H    | 9        | 0.75          |
| (3,61)  | 1:9:A:ILE:HD11 | 1:10:A:GLN:H    | 3        | 0.74          |
| (3,61)  | 1:9:A:ILE:HD12 | 1:10:A:GLN:H    | 3        | 0.74          |
| (3,61)  | 1:9:A:ILE:HD13 | 1:10:A:GLN:H    | 3        | 0.74          |
| (3,61)  | 1:9:A:ILE:HD11 | 1:10:A:GLN:H    | 8        | 0.74          |
| (3,61)  | 1:9:A:ILE:HD12 | 1:10:A:GLN:H    | 8        | 0.74          |
| (3,61)  | 1:9:A:ILE:HD13 | 1:10:A:GLN:H    | 8        | 0.74          |
| (3,55)  | 1:10:A:GLN:HB2 | 1:11:A:TRP:H    | 9        | 0.74          |
| (2,496) | 1:1:A:GLU:HB3  | 1:2:A:GLU:HG2   | 8        | 0.74          |
| (2,404) | 1:11:A:TRP:HA  | 1:14:A:ASP:HB3  | 10       | 0.74          |
| (2,293) | 1:11:A:TRP:HZ2 | 1:23:A:PRO:HB2  | 3        | 0.74          |
| (2,293) | 1:11:A:TRP:HZ2 | 1:23:A:PRO:HB2  | 5        | 0.74          |
| (1,585) | 1:1:A:GLU:HB3  | 1:2:A:GLU:HG2   | 8        | 0.74          |
| (1,466) | 1:11:A:TRP:HA  | 1:14:A:ASP:HB3  | 10       | 0.74          |
| (1,446) | 1:9:A:ILE:HD11 | 1:10:A:GLN:H    | 3        | 0.74          |
| (1,446) | 1:9:A:ILE:HD12 | 1:10:A:GLN:H    | 3        | 0.74          |
| (1,446) | 1:9:A:ILE:HD13 | 1:10:A:GLN:H    | 3        | 0.74          |
| (1,446) | 1:9:A:ILE:HD11 | 1:10:A:GLN:H    | 8        | 0.74          |
| (1,446) | 1:9:A:ILE:HD12 | 1:10:A:GLN:H    | 8        | 0.74          |
| (1,446) | 1:9:A:ILE:HD13 | 1:10:A:GLN:H    | 8        | 0.74          |
| (1,429) | 1:10:A:GLN:HB2 | 1:11:A:TRP:H    | 9        | 0.74          |
| (1,324) | 1:11:A:TRP:HZ2 | 1:23:A:PRO:HB2  | 3        | 0.74          |
| (1,324) | 1:11:A:TRP:HZ2 | 1:23:A:PRO:HB2  | 5        | 0.74          |
| (3,76)  | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG21  | 6        | 0.73          |
| (3,76)  | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG22  | 6        | 0.73          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (3,76)  | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG23 | 6        | 0.73          |
| (3,76)  | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG21 | 6        | 0.73          |
| (3,76)  | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG22 | 6        | 0.73          |
| (3,76)  | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG23 | 6        | 0.73          |
| (3,76)  | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG21 | 6        | 0.73          |
| (3,76)  | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG22 | 6        | 0.73          |
| (3,76)  | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG23 | 6        | 0.73          |
| (3,29)  | 1:5:A:VAL:HG21 | 1:8:A:TYR:HE1  | 6        | 0.73          |
| (3,29)  | 1:5:A:VAL:HG21 | 1:8:A:TYR:HE2  | 6        | 0.73          |
| (3,29)  | 1:5:A:VAL:HG22 | 1:8:A:TYR:HE1  | 6        | 0.73          |
| (3,29)  | 1:5:A:VAL:HG22 | 1:8:A:TYR:HE2  | 6        | 0.73          |
| (3,29)  | 1:5:A:VAL:HG23 | 1:8:A:TYR:HE1  | 6        | 0.73          |
| (3,29)  | 1:5:A:VAL:HG23 | 1:8:A:TYR:HE2  | 6        | 0.73          |
| (2,298) | 1:11:A:TRP:HZ2 | 1:23:A:PRO:HG2 | 6        | 0.73          |
| (2,293) | 1:11:A:TRP:HZ2 | 1:23:A:PRO:HB2 | 1        | 0.73          |
| (1,546) | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG21 | 6        | 0.73          |
| (1,546) | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG22 | 6        | 0.73          |
| (1,546) | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG23 | 6        | 0.73          |
| (1,546) | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG21 | 6        | 0.73          |
| (1,546) | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG22 | 6        | 0.73          |
| (1,546) | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG23 | 6        | 0.73          |
| (1,546) | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG21 | 6        | 0.73          |
| (1,546) | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG22 | 6        | 0.73          |
| (1,546) | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG23 | 6        | 0.73          |
| (1,332) | 1:11:A:TRP:HZ2 | 1:23:A:PRO:HG2 | 6        | 0.73          |
| (1,324) | 1:11:A:TRP:HZ2 | 1:23:A:PRO:HB2 | 1        | 0.73          |
| (1,317) | 1:5:A:VAL:HG21 | 1:8:A:TYR:HE1  | 6        | 0.73          |
| (1,317) | 1:5:A:VAL:HG21 | 1:8:A:TYR:HE2  | 6        | 0.73          |
| (1,317) | 1:5:A:VAL:HG22 | 1:8:A:TYR:HE1  | 6        | 0.73          |
| (1,317) | 1:5:A:VAL:HG22 | 1:8:A:TYR:HE2  | 6        | 0.73          |
| (1,317) | 1:5:A:VAL:HG23 | 1:8:A:TYR:HE1  | 6        | 0.73          |
| (1,317) | 1:5:A:VAL:HG23 | 1:8:A:TYR:HE2  | 6        | 0.73          |
| (3,56)  | 1:3:A:GLU:HB3  | 1:6:A:ARG:H    | 3        | 0.72          |
| (2,485) | 1:16:A:GLY:H   | 1:19:A:SER:HB3 | 2        | 0.72          |
| (2,298) | 1:11:A:TRP:HZ2 | 1:23:A:PRO:HG2 | 1        | 0.72          |
| (2,298) | 1:11:A:TRP:HZ2 | 1:23:A:PRO:HG2 | 5        | 0.72          |
| (2,298) | 1:11:A:TRP:HZ2 | 1:23:A:PRO:HG2 | 9        | 0.72          |
| (2,298) | 1:11:A:TRP:HZ2 | 1:23:A:PRO:HG2 | 10       | 0.72          |
| (2,293) | 1:11:A:TRP:HZ2 | 1:23:A:PRO:HB2 | 2        | 0.72          |
| (2,293) | 1:11:A:TRP:HZ2 | 1:23:A:PRO:HB2 | 7        | 0.72          |
| (1,568) | 1:16:A:GLY:H   | 1:19:A:SER:HB3 | 2        | 0.72          |
| (1,432) | 1:3:A:GLU:HB3  | 1:6:A:ARG:H    | 3        | 0.72          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,332) | 1:11:A:TRP:HZ2 | 1:23:A:PRO:HG2  | 1        | 0.72          |
| (1,332) | 1:11:A:TRP:HZ2 | 1:23:A:PRO:HG2  | 5        | 0.72          |
| (1,332) | 1:11:A:TRP:HZ2 | 1:23:A:PRO:HG2  | 9        | 0.72          |
| (1,332) | 1:11:A:TRP:HZ2 | 1:23:A:PRO:HG2  | 10       | 0.72          |
| (1,324) | 1:11:A:TRP:HZ2 | 1:23:A:PRO:HB2  | 2        | 0.72          |
| (1,324) | 1:11:A:TRP:HZ2 | 1:23:A:PRO:HB2  | 7        | 0.72          |
| (3,32)  | 1:11:A:TRP:HH2 | 1:12:A:LEU:HD11 | 9        | 0.71          |
| (3,32)  | 1:11:A:TRP:HH2 | 1:12:A:LEU:HD12 | 9        | 0.71          |
| (3,32)  | 1:11:A:TRP:HH2 | 1:12:A:LEU:HD13 | 9        | 0.71          |
| (2,496) | 1:1:A:GLU:HB3  | 1:2:A:GLU:HG2   | 7        | 0.71          |
| (2,298) | 1:11:A:TRP:HZ2 | 1:23:A:PRO:HG2  | 7        | 0.71          |
| (2,298) | 1:11:A:TRP:HZ2 | 1:23:A:PRO:HG2  | 8        | 0.71          |
| (2,293) | 1:11:A:TRP:HZ2 | 1:23:A:PRO:HB2  | 6        | 0.71          |
| (2,293) | 1:11:A:TRP:HZ2 | 1:23:A:PRO:HB2  | 10       | 0.71          |
| (2,219) | 1:22:A:PRO:HB3 | 1:22:A:PRO:HD3  | 1        | 0.71          |
| (1,585) | 1:1:A:GLU:HB3  | 1:2:A:GLU:HG2   | 7        | 0.71          |
| (1,332) | 1:11:A:TRP:HZ2 | 1:23:A:PRO:HG2  | 7        | 0.71          |
| (1,332) | 1:11:A:TRP:HZ2 | 1:23:A:PRO:HG2  | 8        | 0.71          |
| (1,326) | 1:11:A:TRP:HH2 | 1:12:A:LEU:HD11 | 9        | 0.71          |
| (1,326) | 1:11:A:TRP:HH2 | 1:12:A:LEU:HD12 | 9        | 0.71          |
| (1,326) | 1:11:A:TRP:HH2 | 1:12:A:LEU:HD13 | 9        | 0.71          |
| (1,324) | 1:11:A:TRP:HZ2 | 1:23:A:PRO:HB2  | 6        | 0.71          |
| (1,324) | 1:11:A:TRP:HZ2 | 1:23:A:PRO:HB2  | 10       | 0.71          |
| (1,238) | 1:22:A:PRO:HB3 | 1:22:A:PRO:HD3  | 1        | 0.71          |
| (3,29)  | 1:5:A:VAL:HG21 | 1:8:A:TYR:HE1   | 2        | 0.7           |
| (3,29)  | 1:5:A:VAL:HG21 | 1:8:A:TYR:HE2   | 2        | 0.7           |
| (3,29)  | 1:5:A:VAL:HG22 | 1:8:A:TYR:HE1   | 2        | 0.7           |
| (3,29)  | 1:5:A:VAL:HG22 | 1:8:A:TYR:HE2   | 2        | 0.7           |
| (3,29)  | 1:5:A:VAL:HG23 | 1:8:A:TYR:HE1   | 2        | 0.7           |
| (3,29)  | 1:5:A:VAL:HG23 | 1:8:A:TYR:HE2   | 2        | 0.7           |
| (3,29)  | 1:5:A:VAL:HG21 | 1:8:A:TYR:HE1   | 4        | 0.7           |
| (3,29)  | 1:5:A:VAL:HG21 | 1:8:A:TYR:HE2   | 4        | 0.7           |
| (3,29)  | 1:5:A:VAL:HG22 | 1:8:A:TYR:HE1   | 4        | 0.7           |
| (3,29)  | 1:5:A:VAL:HG22 | 1:8:A:TYR:HE2   | 4        | 0.7           |
| (3,29)  | 1:5:A:VAL:HG23 | 1:8:A:TYR:HE1   | 4        | 0.7           |
| (3,29)  | 1:5:A:VAL:HG23 | 1:8:A:TYR:HE2   | 4        | 0.7           |
| (3,2)   | 1:5:A:VAL:H    | 1:5:A:VAL:HG21  | 4        | 0.7           |
| (3,2)   | 1:5:A:VAL:H    | 1:5:A:VAL:HG22  | 4        | 0.7           |
| (3,2)   | 1:5:A:VAL:H    | 1:5:A:VAL:HG23  | 4        | 0.7           |
| (3,2)   | 1:5:A:VAL:H    | 1:5:A:VAL:HG21  | 6        | 0.7           |
| (3,2)   | 1:5:A:VAL:H    | 1:5:A:VAL:HG22  | 6        | 0.7           |
| (3,2)   | 1:5:A:VAL:H    | 1:5:A:VAL:HG23  | 6        | 0.7           |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (3,2)   | 1:5:A:VAL:H    | 1:5:A:VAL:HG21 | 7        | 0.7           |
| (3,2)   | 1:5:A:VAL:H    | 1:5:A:VAL:HG22 | 7        | 0.7           |
| (3,2)   | 1:5:A:VAL:H    | 1:5:A:VAL:HG23 | 7        | 0.7           |
| (3,2)   | 1:5:A:VAL:H    | 1:5:A:VAL:HG21 | 8        | 0.7           |
| (3,2)   | 1:5:A:VAL:H    | 1:5:A:VAL:HG22 | 8        | 0.7           |
| (3,2)   | 1:5:A:VAL:H    | 1:5:A:VAL:HG23 | 8        | 0.7           |
| (2,219) | 1:22:A:PRO:HB3 | 1:22:A:PRO:HD3 | 2        | 0.7           |
| (2,219) | 1:22:A:PRO:HB3 | 1:22:A:PRO:HD3 | 6        | 0.7           |
| (1,317) | 1:5:A:VAL:HG21 | 1:8:A:TYR:HE1  | 2        | 0.7           |
| (1,317) | 1:5:A:VAL:HG21 | 1:8:A:TYR:HE2  | 2        | 0.7           |
| (1,317) | 1:5:A:VAL:HG22 | 1:8:A:TYR:HE1  | 2        | 0.7           |
| (1,317) | 1:5:A:VAL:HG22 | 1:8:A:TYR:HE2  | 2        | 0.7           |
| (1,317) | 1:5:A:VAL:HG23 | 1:8:A:TYR:HE1  | 2        | 0.7           |
| (1,317) | 1:5:A:VAL:HG23 | 1:8:A:TYR:HE2  | 2        | 0.7           |
| (1,317) | 1:5:A:VAL:HG21 | 1:8:A:TYR:HE1  | 4        | 0.7           |
| (1,317) | 1:5:A:VAL:HG21 | 1:8:A:TYR:HE2  | 4        | 0.7           |
| (1,317) | 1:5:A:VAL:HG22 | 1:8:A:TYR:HE1  | 4        | 0.7           |
| (1,317) | 1:5:A:VAL:HG22 | 1:8:A:TYR:HE2  | 4        | 0.7           |
| (1,317) | 1:5:A:VAL:HG23 | 1:8:A:TYR:HE1  | 4        | 0.7           |
| (1,317) | 1:5:A:VAL:HG23 | 1:8:A:TYR:HE2  | 4        | 0.7           |
| (1,238) | 1:22:A:PRO:HB3 | 1:22:A:PRO:HD3 | 2        | 0.7           |
| (1,238) | 1:22:A:PRO:HB3 | 1:22:A:PRO:HD3 | 6        | 0.7           |
| (1,28)  | 1:5:A:VAL:H    | 1:5:A:VAL:HG21 | 4        | 0.7           |
| (1,28)  | 1:5:A:VAL:H    | 1:5:A:VAL:HG22 | 4        | 0.7           |
| (1,28)  | 1:5:A:VAL:H    | 1:5:A:VAL:HG23 | 4        | 0.7           |
| (1,28)  | 1:5:A:VAL:H    | 1:5:A:VAL:HG21 | 6        | 0.7           |
| (1,28)  | 1:5:A:VAL:H    | 1:5:A:VAL:HG22 | 6        | 0.7           |
| (1,28)  | 1:5:A:VAL:H    | 1:5:A:VAL:HG23 | 6        | 0.7           |
| (1,28)  | 1:5:A:VAL:H    | 1:5:A:VAL:HG21 | 7        | 0.7           |
| (1,28)  | 1:5:A:VAL:H    | 1:5:A:VAL:HG22 | 7        | 0.7           |
| (1,28)  | 1:5:A:VAL:H    | 1:5:A:VAL:HG23 | 7        | 0.7           |
| (1,28)  | 1:5:A:VAL:H    | 1:5:A:VAL:HG21 | 8        | 0.7           |
| (1,28)  | 1:5:A:VAL:H    | 1:5:A:VAL:HG22 | 8        | 0.7           |
| (1,28)  | 1:5:A:VAL:H    | 1:5:A:VAL:HG23 | 8        | 0.7           |
| (3,16)  | 1:24:A:PRO:HA  | 1:25:A:SER:H   | 1        | 0.69          |
| (3,2)   | 1:5:A:VAL:H    | 1:5:A:VAL:HG21 | 5        | 0.69          |
| (3,2)   | 1:5:A:VAL:H    | 1:5:A:VAL:HG22 | 5        | 0.69          |
| (3,2)   | 1:5:A:VAL:H    | 1:5:A:VAL:HG23 | 5        | 0.69          |
| (2,293) | 1:11:A:TRP:HZ2 | 1:23:A:PRO:HB2 | 9        | 0.69          |
| (2,219) | 1:22:A:PRO:HB3 | 1:22:A:PRO:HD3 | 5        | 0.69          |
| (1,324) | 1:11:A:TRP:HZ2 | 1:23:A:PRO:HB2 | 9        | 0.69          |
| (1,238) | 1:22:A:PRO:HB3 | 1:22:A:PRO:HD3 | 5        | 0.69          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,184) | 1:24:A:PRO:HA  | 1:25:A:SER:H   | 1        | 0.69          |
| (1,28)  | 1:5:A:VAL:H    | 1:5:A:VAL:HG21 | 5        | 0.69          |
| (1,28)  | 1:5:A:VAL:H    | 1:5:A:VAL:HG22 | 5        | 0.69          |
| (1,28)  | 1:5:A:VAL:H    | 1:5:A:VAL:HG23 | 5        | 0.69          |
| (3,61)  | 1:9:A:ILE:HD11 | 1:10:A:GLN:H   | 1        | 0.68          |
| (3,61)  | 1:9:A:ILE:HD12 | 1:10:A:GLN:H   | 1        | 0.68          |
| (3,61)  | 1:9:A:ILE:HD13 | 1:10:A:GLN:H   | 1        | 0.68          |
| (3,23)  | 1:8:A:TYR:HB3  | 1:8:A:TYR:HE1  | 1        | 0.68          |
| (3,23)  | 1:8:A:TYR:HB3  | 1:8:A:TYR:HE2  | 1        | 0.68          |
| (3,23)  | 1:8:A:TYR:HB3  | 1:8:A:TYR:HE1  | 10       | 0.68          |
| (3,23)  | 1:8:A:TYR:HB3  | 1:8:A:TYR:HE2  | 10       | 0.68          |
| (3,2)   | 1:5:A:VAL:H    | 1:5:A:VAL:HG21 | 2        | 0.68          |
| (3,2)   | 1:5:A:VAL:H    | 1:5:A:VAL:HG22 | 2        | 0.68          |
| (3,2)   | 1:5:A:VAL:H    | 1:5:A:VAL:HG23 | 2        | 0.68          |
| (3,2)   | 1:5:A:VAL:H    | 1:5:A:VAL:HG21 | 9        | 0.68          |
| (3,2)   | 1:5:A:VAL:H    | 1:5:A:VAL:HG22 | 9        | 0.68          |
| (3,2)   | 1:5:A:VAL:H    | 1:5:A:VAL:HG23 | 9        | 0.68          |
| (2,298) | 1:11:A:TRP:HZ2 | 1:23:A:PRO:HG2 | 2        | 0.68          |
| (2,48)  | 1:6:A:ARG:H    | 1:6:A:ARG:HB3  | 3        | 0.68          |
| (1,446) | 1:9:A:ILE:HD11 | 1:10:A:GLN:H   | 1        | 0.68          |
| (1,446) | 1:9:A:ILE:HD12 | 1:10:A:GLN:H   | 1        | 0.68          |
| (1,446) | 1:9:A:ILE:HD13 | 1:10:A:GLN:H   | 1        | 0.68          |
| (1,332) | 1:11:A:TRP:HZ2 | 1:23:A:PRO:HG2 | 2        | 0.68          |
| (1,297) | 1:8:A:TYR:HB3  | 1:8:A:TYR:HE1  | 1        | 0.68          |
| (1,297) | 1:8:A:TYR:HB3  | 1:8:A:TYR:HE2  | 1        | 0.68          |
| (1,297) | 1:8:A:TYR:HB3  | 1:8:A:TYR:HE1  | 10       | 0.68          |
| (1,297) | 1:8:A:TYR:HB3  | 1:8:A:TYR:HE2  | 10       | 0.68          |
| (1,51)  | 1:6:A:ARG:H    | 1:6:A:ARG:HB3  | 3        | 0.68          |
| (1,28)  | 1:5:A:VAL:H    | 1:5:A:VAL:HG21 | 2        | 0.68          |
| (1,28)  | 1:5:A:VAL:H    | 1:5:A:VAL:HG22 | 2        | 0.68          |
| (1,28)  | 1:5:A:VAL:H    | 1:5:A:VAL:HG23 | 2        | 0.68          |
| (1,28)  | 1:5:A:VAL:H    | 1:5:A:VAL:HG21 | 9        | 0.68          |
| (1,28)  | 1:5:A:VAL:H    | 1:5:A:VAL:HG22 | 9        | 0.68          |
| (1,28)  | 1:5:A:VAL:H    | 1:5:A:VAL:HG23 | 9        | 0.68          |
| (3,23)  | 1:8:A:TYR:HB3  | 1:8:A:TYR:HE1  | 2        | 0.67          |
| (3,23)  | 1:8:A:TYR:HB3  | 1:8:A:TYR:HE2  | 2        | 0.67          |
| (3,23)  | 1:8:A:TYR:HB3  | 1:8:A:TYR:HE1  | 4        | 0.67          |
| (3,23)  | 1:8:A:TYR:HB3  | 1:8:A:TYR:HE2  | 4        | 0.67          |
| (3,23)  | 1:8:A:TYR:HB3  | 1:8:A:TYR:HE1  | 6        | 0.67          |
| (3,23)  | 1:8:A:TYR:HB3  | 1:8:A:TYR:HE2  | 6        | 0.67          |
| (3,23)  | 1:8:A:TYR:HB3  | 1:8:A:TYR:HE1  | 7        | 0.67          |
| (3,23)  | 1:8:A:TYR:HB3  | 1:8:A:TYR:HE2  | 7        | 0.67          |

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| Key     | Atom-1        | Atom-2         | Model ID | Violation (Å) |
|---------|---------------|----------------|----------|---------------|
| (3,23)  | 1:8:A:TYR:HB3 | 1:8:A:TYR:HE1  | 9        | 0.67          |
| (3,23)  | 1:8:A:TYR:HB3 | 1:8:A:TYR:HE2  | 9        | 0.67          |
| (3,2)   | 1:5:A:VAL:H   | 1:5:A:VAL:HG21 | 3        | 0.67          |
| (3,2)   | 1:5:A:VAL:H   | 1:5:A:VAL:HG22 | 3        | 0.67          |
| (3,2)   | 1:5:A:VAL:H   | 1:5:A:VAL:HG23 | 3        | 0.67          |
| (3,2)   | 1:5:A:VAL:H   | 1:5:A:VAL:HG21 | 10       | 0.67          |
| (3,2)   | 1:5:A:VAL:H   | 1:5:A:VAL:HG22 | 10       | 0.67          |
| (3,2)   | 1:5:A:VAL:H   | 1:5:A:VAL:HG23 | 10       | 0.67          |
| (2,48)  | 1:6:A:ARG:H   | 1:6:A:ARG:HB3  | 1        | 0.67          |
| (2,48)  | 1:6:A:ARG:H   | 1:6:A:ARG:HB3  | 10       | 0.67          |
| (1,297) | 1:8:A:TYR:HB3 | 1:8:A:TYR:HE1  | 2        | 0.67          |
| (1,297) | 1:8:A:TYR:HB3 | 1:8:A:TYR:HE2  | 2        | 0.67          |
| (1,297) | 1:8:A:TYR:HB3 | 1:8:A:TYR:HE1  | 4        | 0.67          |
| (1,297) | 1:8:A:TYR:HB3 | 1:8:A:TYR:HE2  | 4        | 0.67          |
| (1,297) | 1:8:A:TYR:HB3 | 1:8:A:TYR:HE1  | 6        | 0.67          |
| (1,297) | 1:8:A:TYR:HB3 | 1:8:A:TYR:HE2  | 6        | 0.67          |
| (1,297) | 1:8:A:TYR:HB3 | 1:8:A:TYR:HE1  | 7        | 0.67          |
| (1,297) | 1:8:A:TYR:HB3 | 1:8:A:TYR:HE2  | 7        | 0.67          |
| (1,297) | 1:8:A:TYR:HB3 | 1:8:A:TYR:HE1  | 9        | 0.67          |
| (1,297) | 1:8:A:TYR:HB3 | 1:8:A:TYR:HE2  | 9        | 0.67          |
| (1,51)  | 1:6:A:ARG:H   | 1:6:A:ARG:HB3  | 1        | 0.67          |
| (1,51)  | 1:6:A:ARG:H   | 1:6:A:ARG:HB3  | 10       | 0.67          |
| (1,28)  | 1:5:A:VAL:H   | 1:5:A:VAL:HG21 | 3        | 0.67          |
| (1,28)  | 1:5:A:VAL:H   | 1:5:A:VAL:HG22 | 3        | 0.67          |
| (1,28)  | 1:5:A:VAL:H   | 1:5:A:VAL:HG23 | 3        | 0.67          |
| (1,28)  | 1:5:A:VAL:H   | 1:5:A:VAL:HG21 | 10       | 0.67          |
| (1,28)  | 1:5:A:VAL:H   | 1:5:A:VAL:HG22 | 10       | 0.67          |
| (1,28)  | 1:5:A:VAL:H   | 1:5:A:VAL:HG23 | 10       | 0.67          |
| (3,23)  | 1:8:A:TYR:HB3 | 1:8:A:TYR:HE1  | 5        | 0.66          |
| (3,23)  | 1:8:A:TYR:HB3 | 1:8:A:TYR:HE2  | 5        | 0.66          |
| (3,23)  | 1:8:A:TYR:HB3 | 1:8:A:TYR:HE1  | 8        | 0.66          |
| (3,23)  | 1:8:A:TYR:HB3 | 1:8:A:TYR:HE2  | 8        | 0.66          |
| (3,2)   | 1:5:A:VAL:H   | 1:5:A:VAL:HG21 | 1        | 0.66          |
| (3,2)   | 1:5:A:VAL:H   | 1:5:A:VAL:HG22 | 1        | 0.66          |
| (3,2)   | 1:5:A:VAL:H   | 1:5:A:VAL:HG23 | 1        | 0.66          |
| (2,48)  | 1:6:A:ARG:H   | 1:6:A:ARG:HB3  | 4        | 0.66          |
| (2,48)  | 1:6:A:ARG:H   | 1:6:A:ARG:HB3  | 9        | 0.66          |
| (1,297) | 1:8:A:TYR:HB3 | 1:8:A:TYR:HE1  | 5        | 0.66          |
| (1,297) | 1:8:A:TYR:HB3 | 1:8:A:TYR:HE2  | 5        | 0.66          |
| (1,297) | 1:8:A:TYR:HB3 | 1:8:A:TYR:HE1  | 8        | 0.66          |
| (1,297) | 1:8:A:TYR:HB3 | 1:8:A:TYR:HE2  | 8        | 0.66          |
| (1,51)  | 1:6:A:ARG:H   | 1:6:A:ARG:HB3  | 4        | 0.66          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,51)  | 1:6:A:ARG:H    | 1:6:A:ARG:HB3   | 9        | 0.66          |
| (1,28)  | 1:5:A:VAL:H    | 1:5:A:VAL:HG21  | 1        | 0.66          |
| (1,28)  | 1:5:A:VAL:H    | 1:5:A:VAL:HG22  | 1        | 0.66          |
| (1,28)  | 1:5:A:VAL:H    | 1:5:A:VAL:HG23  | 1        | 0.66          |
| (3,56)  | 1:3:A:GLU:HB3  | 1:6:A:ARG:H     | 1        | 0.65          |
| (3,32)  | 1:11:A:TRP:HH2 | 1:12:A:LEU:HD11 | 4        | 0.65          |
| (3,32)  | 1:11:A:TRP:HH2 | 1:12:A:LEU:HD12 | 4        | 0.65          |
| (3,32)  | 1:11:A:TRP:HH2 | 1:12:A:LEU:HD13 | 4        | 0.65          |
| (3,23)  | 1:8:A:TYR:HB3  | 1:8:A:TYR:HE1   | 3        | 0.65          |
| (3,23)  | 1:8:A:TYR:HB3  | 1:8:A:TYR:HE2   | 3        | 0.65          |
| (2,48)  | 1:6:A:ARG:H    | 1:6:A:ARG:HB3   | 2        | 0.65          |
| (1,432) | 1:3:A:GLU:HB3  | 1:6:A:ARG:H     | 1        | 0.65          |
| (1,326) | 1:11:A:TRP:HH2 | 1:12:A:LEU:HD11 | 4        | 0.65          |
| (1,326) | 1:11:A:TRP:HH2 | 1:12:A:LEU:HD12 | 4        | 0.65          |
| (1,326) | 1:11:A:TRP:HH2 | 1:12:A:LEU:HD13 | 4        | 0.65          |
| (1,297) | 1:8:A:TYR:HB3  | 1:8:A:TYR:HE1   | 3        | 0.65          |
| (1,297) | 1:8:A:TYR:HB3  | 1:8:A:TYR:HE2   | 3        | 0.65          |
| (1,51)  | 1:6:A:ARG:H    | 1:6:A:ARG:HB3   | 2        | 0.65          |
| (3,35)  | 1:11:A:TRP:HZ2 | 1:21:A:ARG:HB3  | 1        | 0.63          |
| (3,35)  | 1:11:A:TRP:HZ2 | 1:21:A:ARG:HB3  | 6        | 0.63          |
| (3,32)  | 1:11:A:TRP:HH2 | 1:12:A:LEU:HD11 | 8        | 0.63          |
| (3,32)  | 1:11:A:TRP:HH2 | 1:12:A:LEU:HD12 | 8        | 0.63          |
| (3,32)  | 1:11:A:TRP:HH2 | 1:12:A:LEU:HD13 | 8        | 0.63          |
| (2,404) | 1:11:A:TRP:HA  | 1:14:A:ASP:HB3  | 3        | 0.63          |
| (2,315) | 1:11:A:TRP:HB2 | 1:11:A:TRP:HE3  | 2        | 0.63          |
| (2,315) | 1:11:A:TRP:HB2 | 1:11:A:TRP:HE3  | 4        | 0.63          |
| (2,315) | 1:11:A:TRP:HB2 | 1:11:A:TRP:HE3  | 6        | 0.63          |
| (2,315) | 1:11:A:TRP:HB2 | 1:11:A:TRP:HE3  | 8        | 0.63          |
| (2,142) | 1:14:A:ASP:H   | 1:14:A:ASP:HB3  | 7        | 0.63          |
| (1,466) | 1:11:A:TRP:HA  | 1:14:A:ASP:HB3  | 3        | 0.63          |
| (1,353) | 1:11:A:TRP:HB2 | 1:11:A:TRP:HE3  | 2        | 0.63          |
| (1,353) | 1:11:A:TRP:HB2 | 1:11:A:TRP:HE3  | 4        | 0.63          |
| (1,353) | 1:11:A:TRP:HB2 | 1:11:A:TRP:HE3  | 6        | 0.63          |
| (1,353) | 1:11:A:TRP:HB2 | 1:11:A:TRP:HE3  | 8        | 0.63          |
| (1,336) | 1:11:A:TRP:HZ2 | 1:21:A:ARG:HB3  | 1        | 0.63          |
| (1,336) | 1:11:A:TRP:HZ2 | 1:21:A:ARG:HB3  | 6        | 0.63          |
| (1,326) | 1:11:A:TRP:HH2 | 1:12:A:LEU:HD11 | 8        | 0.63          |
| (1,326) | 1:11:A:TRP:HH2 | 1:12:A:LEU:HD12 | 8        | 0.63          |
| (1,326) | 1:11:A:TRP:HH2 | 1:12:A:LEU:HD13 | 8        | 0.63          |
| (1,157) | 1:14:A:ASP:H   | 1:14:A:ASP:HB3  | 7        | 0.63          |
| (2,315) | 1:11:A:TRP:HB2 | 1:11:A:TRP:HE3  | 1        | 0.62          |
| (2,315) | 1:11:A:TRP:HB2 | 1:11:A:TRP:HE3  | 3        | 0.62          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (2,315) | 1:11:A:TRP:HB2 | 1:11:A:TRP:HE3 | 5        | 0.62          |
| (2,315) | 1:11:A:TRP:HB2 | 1:11:A:TRP:HE3 | 7        | 0.62          |
| (1,353) | 1:11:A:TRP:HB2 | 1:11:A:TRP:HE3 | 1        | 0.62          |
| (1,353) | 1:11:A:TRP:HB2 | 1:11:A:TRP:HE3 | 3        | 0.62          |
| (1,353) | 1:11:A:TRP:HB2 | 1:11:A:TRP:HE3 | 5        | 0.62          |
| (1,353) | 1:11:A:TRP:HB2 | 1:11:A:TRP:HE3 | 7        | 0.62          |
| (2,483) | 1:6:A:ARG:HB3  | 1:7:A:LEU:H    | 5        | 0.61          |
| (2,413) | 1:16:A:GLY:HA2 | 1:17:A:PRO:HD2 | 10       | 0.61          |
| (2,402) | 1:3:A:GLU:HA   | 1:6:A:ARG:HB3  | 10       | 0.61          |
| (2,315) | 1:11:A:TRP:HB2 | 1:11:A:TRP:HE3 | 9        | 0.61          |
| (2,281) | 1:8:A:TYR:HE1  | 1:24:A:PRO:HB3 | 10       | 0.61          |
| (2,281) | 1:8:A:TYR:HE2  | 1:24:A:PRO:HB3 | 10       | 0.61          |
| (1,566) | 1:6:A:ARG:HB3  | 1:7:A:LEU:H    | 5        | 0.61          |
| (1,476) | 1:16:A:GLY:HA2 | 1:17:A:PRO:HD2 | 10       | 0.61          |
| (1,464) | 1:3:A:GLU:HA   | 1:6:A:ARG:HB3  | 10       | 0.61          |
| (1,353) | 1:11:A:TRP:HB2 | 1:11:A:TRP:HE3 | 9        | 0.61          |
| (1,304) | 1:8:A:TYR:HE1  | 1:24:A:PRO:HB3 | 10       | 0.61          |
| (1,304) | 1:8:A:TYR:HE2  | 1:24:A:PRO:HB3 | 10       | 0.61          |
| (2,413) | 1:16:A:GLY:HA2 | 1:17:A:PRO:HD2 | 3        | 0.6           |
| (2,344) | 1:11:A:TRP:HB2 | 1:12:A:LEU:H   | 2        | 0.6           |
| (2,344) | 1:11:A:TRP:HB2 | 1:12:A:LEU:H   | 5        | 0.6           |
| (2,315) | 1:11:A:TRP:HB2 | 1:11:A:TRP:HE3 | 10       | 0.6           |
| (2,298) | 1:11:A:TRP:HZ2 | 1:23:A:PRO:HG2 | 3        | 0.6           |
| (1,476) | 1:16:A:GLY:HA2 | 1:17:A:PRO:HD2 | 3        | 0.6           |
| (1,390) | 1:11:A:TRP:HB2 | 1:12:A:LEU:H   | 2        | 0.6           |
| (1,390) | 1:11:A:TRP:HB2 | 1:12:A:LEU:H   | 5        | 0.6           |
| (1,353) | 1:11:A:TRP:HB2 | 1:11:A:TRP:HE3 | 10       | 0.6           |
| (1,332) | 1:11:A:TRP:HZ2 | 1:23:A:PRO:HG2 | 3        | 0.6           |
| (2,483) | 1:6:A:ARG:HB3  | 1:7:A:LEU:H    | 7        | 0.59          |
| (2,402) | 1:3:A:GLU:HA   | 1:6:A:ARG:HB3  | 9        | 0.59          |
| (2,344) | 1:11:A:TRP:HB2 | 1:12:A:LEU:H   | 4        | 0.59          |
| (2,344) | 1:11:A:TRP:HB2 | 1:12:A:LEU:H   | 6        | 0.59          |
| (2,344) | 1:11:A:TRP:HB2 | 1:12:A:LEU:H   | 7        | 0.59          |
| (2,344) | 1:11:A:TRP:HB2 | 1:12:A:LEU:H   | 8        | 0.59          |
| (1,566) | 1:6:A:ARG:HB3  | 1:7:A:LEU:H    | 7        | 0.59          |
| (1,464) | 1:3:A:GLU:HA   | 1:6:A:ARG:HB3  | 9        | 0.59          |
| (1,390) | 1:11:A:TRP:HB2 | 1:12:A:LEU:H   | 4        | 0.59          |
| (1,390) | 1:11:A:TRP:HB2 | 1:12:A:LEU:H   | 6        | 0.59          |
| (1,390) | 1:11:A:TRP:HB2 | 1:12:A:LEU:H   | 7        | 0.59          |
| (1,390) | 1:11:A:TRP:HB2 | 1:12:A:LEU:H   | 8        | 0.59          |
| (2,413) | 1:16:A:GLY:HA2 | 1:17:A:PRO:HD2 | 7        | 0.58          |
| (2,351) | 1:3:A:GLU:HB2  | 1:4:A:ALA:H    | 3        | 0.58          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (2,344) | 1:11:A:TRP:HB2 | 1:12:A:LEU:H   | 1        | 0.58          |
| (2,48)  | 1:6:A:ARG:H    | 1:6:A:ARG:HB3  | 8        | 0.58          |
| (1,476) | 1:16:A:GLY:HA2 | 1:17:A:PRO:HD2 | 7        | 0.58          |
| (1,398) | 1:3:A:GLU:HB2  | 1:4:A:ALA:H    | 3        | 0.58          |
| (1,390) | 1:11:A:TRP:HB2 | 1:12:A:LEU:H   | 1        | 0.58          |
| (1,51)  | 1:6:A:ARG:H    | 1:6:A:ARG:HB3  | 8        | 0.58          |
| (2,483) | 1:6:A:ARG:HB3  | 1:7:A:LEU:H    | 6        | 0.57          |
| (2,483) | 1:6:A:ARG:HB3  | 1:7:A:LEU:H    | 8        | 0.57          |
| (2,413) | 1:16:A:GLY:HA2 | 1:17:A:PRO:HD2 | 5        | 0.57          |
| (2,351) | 1:3:A:GLU:HB2  | 1:4:A:ALA:H    | 1        | 0.57          |
| (2,344) | 1:11:A:TRP:HB2 | 1:12:A:LEU:H   | 3        | 0.57          |
| (2,344) | 1:11:A:TRP:HB2 | 1:12:A:LEU:H   | 10       | 0.57          |
| (2,48)  | 1:6:A:ARG:H    | 1:6:A:ARG:HB3  | 7        | 0.57          |
| (1,566) | 1:6:A:ARG:HB3  | 1:7:A:LEU:H    | 6        | 0.57          |
| (1,566) | 1:6:A:ARG:HB3  | 1:7:A:LEU:H    | 8        | 0.57          |
| (1,476) | 1:16:A:GLY:HA2 | 1:17:A:PRO:HD2 | 5        | 0.57          |
| (1,398) | 1:3:A:GLU:HB2  | 1:4:A:ALA:H    | 1        | 0.57          |
| (1,390) | 1:11:A:TRP:HB2 | 1:12:A:LEU:H   | 3        | 0.57          |
| (1,390) | 1:11:A:TRP:HB2 | 1:12:A:LEU:H   | 10       | 0.57          |
| (1,51)  | 1:6:A:ARG:H    | 1:6:A:ARG:HB3  | 7        | 0.57          |
| (2,483) | 1:6:A:ARG:HB3  | 1:7:A:LEU:H    | 4        | 0.56          |
| (2,413) | 1:16:A:GLY:HA2 | 1:17:A:PRO:HD2 | 4        | 0.56          |
| (2,344) | 1:11:A:TRP:HB2 | 1:12:A:LEU:H   | 9        | 0.56          |
| (2,298) | 1:11:A:TRP:HZ2 | 1:23:A:PRO:HG2 | 4        | 0.56          |
| (2,142) | 1:14:A:ASP:H   | 1:14:A:ASP:HB3 | 2        | 0.56          |
| (2,48)  | 1:6:A:ARG:H    | 1:6:A:ARG:HB3  | 5        | 0.56          |
| (1,566) | 1:6:A:ARG:HB3  | 1:7:A:LEU:H    | 4        | 0.56          |
| (1,476) | 1:16:A:GLY:HA2 | 1:17:A:PRO:HD2 | 4        | 0.56          |
| (1,390) | 1:11:A:TRP:HB2 | 1:12:A:LEU:H   | 9        | 0.56          |
| (1,332) | 1:11:A:TRP:HZ2 | 1:23:A:PRO:HG2 | 4        | 0.56          |
| (1,157) | 1:14:A:ASP:H   | 1:14:A:ASP:HB3 | 2        | 0.56          |
| (1,51)  | 1:6:A:ARG:H    | 1:6:A:ARG:HB3  | 5        | 0.56          |
| (3,59)  | 1:7:A:LEU:HB3  | 1:10:A:GLN:H   | 1        | 0.55          |
| (2,447) | 1:7:A:LEU:HB3  | 1:24:A:PRO:HB2 | 9        | 0.55          |
| (2,421) | 1:16:A:GLY:HA2 | 1:17:A:PRO:HD3 | 10       | 0.55          |
| (2,413) | 1:16:A:GLY:HA2 | 1:17:A:PRO:HD2 | 1        | 0.55          |
| (2,413) | 1:16:A:GLY:HA2 | 1:17:A:PRO:HD2 | 2        | 0.55          |
| (2,413) | 1:16:A:GLY:HA2 | 1:17:A:PRO:HD2 | 9        | 0.55          |
| (2,351) | 1:3:A:GLU:HB2  | 1:4:A:ALA:H    | 2        | 0.55          |
| (2,351) | 1:3:A:GLU:HB2  | 1:4:A:ALA:H    | 5        | 0.55          |
| (2,351) | 1:3:A:GLU:HB2  | 1:4:A:ALA:H    | 8        | 0.55          |
| (2,351) | 1:3:A:GLU:HB2  | 1:4:A:ALA:H    | 9        | 0.55          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (2,351) | 1:3:A:GLU:HB2  | 1:4:A:ALA:H     | 10       | 0.55          |
| (1,514) | 1:7:A:LEU:HB3  | 1:24:A:PRO:HB2  | 9        | 0.55          |
| (1,486) | 1:16:A:GLY:HA2 | 1:17:A:PRO:HD3  | 10       | 0.55          |
| (1,476) | 1:16:A:GLY:HA2 | 1:17:A:PRO:HD2  | 1        | 0.55          |
| (1,476) | 1:16:A:GLY:HA2 | 1:17:A:PRO:HD2  | 2        | 0.55          |
| (1,476) | 1:16:A:GLY:HA2 | 1:17:A:PRO:HD2  | 9        | 0.55          |
| (1,441) | 1:7:A:LEU:HB3  | 1:10:A:GLN:H    | 1        | 0.55          |
| (1,398) | 1:3:A:GLU:HB2  | 1:4:A:ALA:H     | 2        | 0.55          |
| (1,398) | 1:3:A:GLU:HB2  | 1:4:A:ALA:H     | 5        | 0.55          |
| (1,398) | 1:3:A:GLU:HB2  | 1:4:A:ALA:H     | 8        | 0.55          |
| (1,398) | 1:3:A:GLU:HB2  | 1:4:A:ALA:H     | 9        | 0.55          |
| (1,398) | 1:3:A:GLU:HB2  | 1:4:A:ALA:H     | 10       | 0.55          |
| (3,32)  | 1:11:A:TRP:HH2 | 1:12:A:LEU:HD11 | 10       | 0.54          |
| (3,32)  | 1:11:A:TRP:HH2 | 1:12:A:LEU:HD12 | 10       | 0.54          |
| (3,32)  | 1:11:A:TRP:HH2 | 1:12:A:LEU:HD13 | 10       | 0.54          |
| (2,421) | 1:16:A:GLY:HA2 | 1:17:A:PRO:HD3  | 3        | 0.54          |
| (2,351) | 1:3:A:GLU:HB2  | 1:4:A:ALA:H     | 6        | 0.54          |
| (2,351) | 1:3:A:GLU:HB2  | 1:4:A:ALA:H     | 7        | 0.54          |
| (2,277) | 1:8:A:TYR:HE1  | 1:24:A:PRO:HD3  | 6        | 0.54          |
| (2,277) | 1:8:A:TYR:HE2  | 1:24:A:PRO:HD3  | 6        | 0.54          |
| (2,48)  | 1:6:A:ARG:H    | 1:6:A:ARG:HB3   | 6        | 0.54          |
| (1,486) | 1:16:A:GLY:HA2 | 1:17:A:PRO:HD3  | 3        | 0.54          |
| (1,398) | 1:3:A:GLU:HB2  | 1:4:A:ALA:H     | 6        | 0.54          |
| (1,398) | 1:3:A:GLU:HB2  | 1:4:A:ALA:H     | 7        | 0.54          |
| (1,326) | 1:11:A:TRP:HH2 | 1:12:A:LEU:HD11 | 10       | 0.54          |
| (1,326) | 1:11:A:TRP:HH2 | 1:12:A:LEU:HD12 | 10       | 0.54          |
| (1,326) | 1:11:A:TRP:HH2 | 1:12:A:LEU:HD13 | 10       | 0.54          |
| (1,300) | 1:8:A:TYR:HE1  | 1:24:A:PRO:HD3  | 6        | 0.54          |
| (1,300) | 1:8:A:TYR:HE2  | 1:24:A:PRO:HD3  | 6        | 0.54          |
| (1,51)  | 1:6:A:ARG:H    | 1:6:A:ARG:HB3   | 6        | 0.54          |
| (3,56)  | 1:3:A:GLU:HB3  | 1:6:A:ARG:H     | 4        | 0.53          |
| (3,43)  | 1:8:A:TYR:HE1  | 1:11:A:TRP:HE3  | 3        | 0.53          |
| (3,43)  | 1:8:A:TYR:HE2  | 1:11:A:TRP:HE3  | 3        | 0.53          |
| (3,43)  | 1:8:A:TYR:HE1  | 1:11:A:TRP:HE3  | 6        | 0.53          |
| (3,43)  | 1:8:A:TYR:HE2  | 1:11:A:TRP:HE3  | 6        | 0.53          |
| (2,483) | 1:6:A:ARG:HB3  | 1:7:A:LEU:H     | 2        | 0.53          |
| (2,421) | 1:16:A:GLY:HA2 | 1:17:A:PRO:HD3  | 2        | 0.53          |
| (2,413) | 1:16:A:GLY:HA2 | 1:17:A:PRO:HD2  | 8        | 0.53          |
| (2,402) | 1:3:A:GLU:HA   | 1:6:A:ARG:HB3   | 8        | 0.53          |
| (2,292) | 1:8:A:TYR:HD1  | 1:23:A:PRO:HB2  | 9        | 0.53          |
| (2,292) | 1:8:A:TYR:HD2  | 1:23:A:PRO:HB2  | 9        | 0.53          |
| (2,292) | 1:8:A:TYR:HD1  | 1:23:A:PRO:HB2  | 10       | 0.53          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (2,292) | 1:8:A:TYR:HD2  | 1:23:A:PRO:HB2 | 10       | 0.53          |
| (2,142) | 1:14:A:ASP:H   | 1:14:A:ASP:HB3 | 10       | 0.53          |
| (1,566) | 1:6:A:ARG:HB3  | 1:7:A:LEU:H    | 2        | 0.53          |
| (1,486) | 1:16:A:GLY:HA2 | 1:17:A:PRO:HD3 | 2        | 0.53          |
| (1,476) | 1:16:A:GLY:HA2 | 1:17:A:PRO:HD2 | 8        | 0.53          |
| (1,464) | 1:3:A:GLU:HA   | 1:6:A:ARG:HB3  | 8        | 0.53          |
| (1,432) | 1:3:A:GLU:HB3  | 1:6:A:ARG:H    | 4        | 0.53          |
| (1,377) | 1:8:A:TYR:HE1  | 1:11:A:TRP:HE3 | 3        | 0.53          |
| (1,377) | 1:8:A:TYR:HE2  | 1:11:A:TRP:HE3 | 3        | 0.53          |
| (1,377) | 1:8:A:TYR:HE1  | 1:11:A:TRP:HE3 | 6        | 0.53          |
| (1,377) | 1:8:A:TYR:HE2  | 1:11:A:TRP:HE3 | 6        | 0.53          |
| (1,323) | 1:8:A:TYR:HD1  | 1:23:A:PRO:HB2 | 9        | 0.53          |
| (1,323) | 1:8:A:TYR:HD2  | 1:23:A:PRO:HB2 | 9        | 0.53          |
| (1,323) | 1:8:A:TYR:HD1  | 1:23:A:PRO:HB2 | 10       | 0.53          |
| (1,323) | 1:8:A:TYR:HD2  | 1:23:A:PRO:HB2 | 10       | 0.53          |
| (1,157) | 1:14:A:ASP:H   | 1:14:A:ASP:HB3 | 10       | 0.53          |
| (2,495) | 1:11:A:TRP:HB2 | 1:24:A:PRO:HD2 | 8        | 0.52          |
| (2,402) | 1:3:A:GLU:HA   | 1:6:A:ARG:HB3  | 2        | 0.52          |
| (2,402) | 1:3:A:GLU:HA   | 1:6:A:ARG:HB3  | 5        | 0.52          |
| (2,402) | 1:3:A:GLU:HA   | 1:6:A:ARG:HB3  | 7        | 0.52          |
| (1,583) | 1:11:A:TRP:HB2 | 1:24:A:PRO:HD2 | 8        | 0.52          |
| (1,464) | 1:3:A:GLU:HA   | 1:6:A:ARG:HB3  | 2        | 0.52          |
| (1,464) | 1:3:A:GLU:HA   | 1:6:A:ARG:HB3  | 5        | 0.52          |
| (1,464) | 1:3:A:GLU:HA   | 1:6:A:ARG:HB3  | 7        | 0.52          |
| (3,43)  | 1:8:A:TYR:HE1  | 1:11:A:TRP:HE3 | 2        | 0.51          |
| (3,43)  | 1:8:A:TYR:HE2  | 1:11:A:TRP:HE3 | 2        | 0.51          |
| (3,43)  | 1:8:A:TYR:HE1  | 1:11:A:TRP:HE3 | 5        | 0.51          |
| (3,43)  | 1:8:A:TYR:HE2  | 1:11:A:TRP:HE3 | 5        | 0.51          |
| (2,421) | 1:16:A:GLY:HA2 | 1:17:A:PRO:HD3 | 9        | 0.51          |
| (2,402) | 1:3:A:GLU:HA   | 1:6:A:ARG:HB3  | 3        | 0.51          |
| (2,402) | 1:3:A:GLU:HA   | 1:6:A:ARG:HB3  | 6        | 0.51          |
| (2,198) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD3 | 1        | 0.51          |
| (2,197) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD2 | 6        | 0.51          |
| (1,486) | 1:16:A:GLY:HA2 | 1:17:A:PRO:HD3 | 9        | 0.51          |
| (1,464) | 1:3:A:GLU:HA   | 1:6:A:ARG:HB3  | 3        | 0.51          |
| (1,464) | 1:3:A:GLU:HA   | 1:6:A:ARG:HB3  | 6        | 0.51          |
| (1,377) | 1:8:A:TYR:HE1  | 1:11:A:TRP:HE3 | 2        | 0.51          |
| (1,377) | 1:8:A:TYR:HE2  | 1:11:A:TRP:HE3 | 2        | 0.51          |
| (1,377) | 1:8:A:TYR:HE1  | 1:11:A:TRP:HE3 | 5        | 0.51          |
| (1,377) | 1:8:A:TYR:HE2  | 1:11:A:TRP:HE3 | 5        | 0.51          |
| (1,215) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD3 | 1        | 0.51          |
| (1,214) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD2 | 6        | 0.51          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (3,72)  | 1:12:A:LEU:HD11 | 1:16:A:GLY:HA2  | 6        | 0.5           |
| (3,72)  | 1:12:A:LEU:HD12 | 1:16:A:GLY:HA2  | 6        | 0.5           |
| (3,72)  | 1:12:A:LEU:HD13 | 1:16:A:GLY:HA2  | 6        | 0.5           |
| (2,483) | 1:6:A:ARG:HB3   | 1:7:A:LEU:H     | 1        | 0.5           |
| (2,483) | 1:6:A:ARG:HB3   | 1:7:A:LEU:H     | 3        | 0.5           |
| (2,483) | 1:6:A:ARG:HB3   | 1:7:A:LEU:H     | 9        | 0.5           |
| (2,402) | 1:3:A:GLU:HA    | 1:6:A:ARG:HB3   | 1        | 0.5           |
| (1,566) | 1:6:A:ARG:HB3   | 1:7:A:LEU:H     | 1        | 0.5           |
| (1,566) | 1:6:A:ARG:HB3   | 1:7:A:LEU:H     | 3        | 0.5           |
| (1,566) | 1:6:A:ARG:HB3   | 1:7:A:LEU:H     | 9        | 0.5           |
| (1,536) | 1:12:A:LEU:HD11 | 1:16:A:GLY:HA2  | 6        | 0.5           |
| (1,536) | 1:12:A:LEU:HD12 | 1:16:A:GLY:HA2  | 6        | 0.5           |
| (1,536) | 1:12:A:LEU:HD13 | 1:16:A:GLY:HA2  | 6        | 0.5           |
| (1,464) | 1:3:A:GLU:HA    | 1:6:A:ARG:HB3   | 1        | 0.5           |
| (3,59)  | 1:7:A:LEU:HB3   | 1:10:A:GLN:H    | 7        | 0.49          |
| (3,59)  | 1:7:A:LEU:HB3   | 1:10:A:GLN:H    | 8        | 0.49          |
| (3,32)  | 1:11:A:TRP:HH2  | 1:12:A:LEU:HD11 | 6        | 0.49          |
| (3,32)  | 1:11:A:TRP:HH2  | 1:12:A:LEU:HD12 | 6        | 0.49          |
| (3,32)  | 1:11:A:TRP:HH2  | 1:12:A:LEU:HD13 | 6        | 0.49          |
| (2,420) | 1:21:A:ARG:HB2  | 1:22:A:PRO:HD2  | 5        | 0.49          |
| (2,292) | 1:8:A:TYR:HD1   | 1:23:A:PRO:HB2  | 3        | 0.49          |
| (2,292) | 1:8:A:TYR:HD2   | 1:23:A:PRO:HB2  | 3        | 0.49          |
| (2,292) | 1:8:A:TYR:HD1   | 1:23:A:PRO:HB2  | 4        | 0.49          |
| (2,292) | 1:8:A:TYR:HD2   | 1:23:A:PRO:HB2  | 4        | 0.49          |
| (1,485) | 1:21:A:ARG:HB2  | 1:22:A:PRO:HD2  | 5        | 0.49          |
| (1,441) | 1:7:A:LEU:HB3   | 1:10:A:GLN:H    | 7        | 0.49          |
| (1,441) | 1:7:A:LEU:HB3   | 1:10:A:GLN:H    | 8        | 0.49          |
| (1,326) | 1:11:A:TRP:HH2  | 1:12:A:LEU:HD11 | 6        | 0.49          |
| (1,326) | 1:11:A:TRP:HH2  | 1:12:A:LEU:HD12 | 6        | 0.49          |
| (1,326) | 1:11:A:TRP:HH2  | 1:12:A:LEU:HD13 | 6        | 0.49          |
| (1,323) | 1:8:A:TYR:HD1   | 1:23:A:PRO:HB2  | 3        | 0.49          |
| (1,323) | 1:8:A:TYR:HD2   | 1:23:A:PRO:HB2  | 3        | 0.49          |
| (1,323) | 1:8:A:TYR:HD1   | 1:23:A:PRO:HB2  | 4        | 0.49          |
| (1,323) | 1:8:A:TYR:HD2   | 1:23:A:PRO:HB2  | 4        | 0.49          |
| (3,59)  | 1:7:A:LEU:HB3   | 1:10:A:GLN:H    | 4        | 0.48          |
| (3,59)  | 1:7:A:LEU:HB3   | 1:10:A:GLN:H    | 5        | 0.48          |
| (3,55)  | 1:10:A:GLN:HB2  | 1:11:A:TRP:H    | 5        | 0.48          |
| (3,32)  | 1:11:A:TRP:HH2  | 1:12:A:LEU:HD11 | 3        | 0.48          |
| (3,32)  | 1:11:A:TRP:HH2  | 1:12:A:LEU:HD12 | 3        | 0.48          |
| (3,32)  | 1:11:A:TRP:HH2  | 1:12:A:LEU:HD13 | 3        | 0.48          |
| (3,19)  | 1:22:A:PRO:HB3  | 1:22:A:PRO:HD2  | 2        | 0.48          |
| (3,19)  | 1:22:A:PRO:HB3  | 1:22:A:PRO:HD2  | 5        | 0.48          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (2,421) | 1:16:A:GLY:HA2 | 1:17:A:PRO:HD3  | 1        | 0.48          |
| (2,421) | 1:16:A:GLY:HA2 | 1:17:A:PRO:HD3  | 5        | 0.48          |
| (2,420) | 1:21:A:ARG:HB2 | 1:22:A:PRO:HD2  | 2        | 0.48          |
| (1,486) | 1:16:A:GLY:HA2 | 1:17:A:PRO:HD3  | 1        | 0.48          |
| (1,486) | 1:16:A:GLY:HA2 | 1:17:A:PRO:HD3  | 5        | 0.48          |
| (1,485) | 1:21:A:ARG:HB2 | 1:22:A:PRO:HD2  | 2        | 0.48          |
| (1,441) | 1:7:A:LEU:HB3  | 1:10:A:GLN:H    | 4        | 0.48          |
| (1,441) | 1:7:A:LEU:HB3  | 1:10:A:GLN:H    | 5        | 0.48          |
| (1,429) | 1:10:A:GLN:HB2 | 1:11:A:TRP:H    | 5        | 0.48          |
| (1,326) | 1:11:A:TRP:HH2 | 1:12:A:LEU:HD11 | 3        | 0.48          |
| (1,326) | 1:11:A:TRP:HH2 | 1:12:A:LEU:HD12 | 3        | 0.48          |
| (1,326) | 1:11:A:TRP:HH2 | 1:12:A:LEU:HD13 | 3        | 0.48          |
| (1,237) | 1:22:A:PRO:HB3 | 1:22:A:PRO:HD2  | 2        | 0.48          |
| (1,237) | 1:22:A:PRO:HB3 | 1:22:A:PRO:HD2  | 5        | 0.48          |
| (3,92)  | 1:9:A:ILE:H    | 1:9:A:ILE:HG21  | 9        | 0.47          |
| (3,92)  | 1:9:A:ILE:H    | 1:9:A:ILE:HG22  | 9        | 0.47          |
| (3,92)  | 1:9:A:ILE:H    | 1:9:A:ILE:HG23  | 9        | 0.47          |
| (3,92)  | 1:9:A:ILE:H    | 1:9:A:ILE:HG21  | 10       | 0.47          |
| (3,92)  | 1:9:A:ILE:H    | 1:9:A:ILE:HG22  | 10       | 0.47          |
| (3,92)  | 1:9:A:ILE:H    | 1:9:A:ILE:HG23  | 10       | 0.47          |
| (3,65)  | 1:6:A:ARG:HA   | 1:10:A:GLN:HB3  | 10       | 0.47          |
| (3,59)  | 1:7:A:LEU:HB3  | 1:10:A:GLN:H    | 3        | 0.47          |
| (3,59)  | 1:7:A:LEU:HB3  | 1:10:A:GLN:H    | 6        | 0.47          |
| (3,43)  | 1:8:A:TYR:HE1  | 1:11:A:TRP:HE3  | 4        | 0.47          |
| (3,43)  | 1:8:A:TYR:HE2  | 1:11:A:TRP:HE3  | 4        | 0.47          |
| (3,32)  | 1:11:A:TRP:HH2 | 1:12:A:LEU:HD11 | 5        | 0.47          |
| (3,32)  | 1:11:A:TRP:HH2 | 1:12:A:LEU:HD12 | 5        | 0.47          |
| (3,32)  | 1:11:A:TRP:HH2 | 1:12:A:LEU:HD13 | 5        | 0.47          |
| (3,32)  | 1:11:A:TRP:HH2 | 1:12:A:LEU:HD11 | 7        | 0.47          |
| (3,32)  | 1:11:A:TRP:HH2 | 1:12:A:LEU:HD12 | 7        | 0.47          |
| (3,32)  | 1:11:A:TRP:HH2 | 1:12:A:LEU:HD13 | 7        | 0.47          |
| (2,421) | 1:16:A:GLY:HA2 | 1:17:A:PRO:HD3  | 4        | 0.47          |
| (2,402) | 1:3:A:GLU:HA   | 1:6:A:ARG:HB3   | 4        | 0.47          |
| (2,277) | 1:8:A:TYR:HE1  | 1:24:A:PRO:HD3  | 5        | 0.47          |
| (2,277) | 1:8:A:TYR:HE2  | 1:24:A:PRO:HD3  | 5        | 0.47          |
| (1,600) | 1:9:A:ILE:H    | 1:9:A:ILE:HG21  | 9        | 0.47          |
| (1,600) | 1:9:A:ILE:H    | 1:9:A:ILE:HG22  | 9        | 0.47          |
| (1,600) | 1:9:A:ILE:H    | 1:9:A:ILE:HG23  | 9        | 0.47          |
| (1,600) | 1:9:A:ILE:H    | 1:9:A:ILE:HG21  | 10       | 0.47          |
| (1,600) | 1:9:A:ILE:H    | 1:9:A:ILE:HG22  | 10       | 0.47          |
| (1,600) | 1:9:A:ILE:H    | 1:9:A:ILE:HG23  | 10       | 0.47          |
| (1,486) | 1:16:A:GLY:HA2 | 1:17:A:PRO:HD3  | 4        | 0.47          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,482) | 1:6:A:ARG:HA   | 1:10:A:GLN:HB3  | 10       | 0.47          |
| (1,464) | 1:3:A:GLU:HA   | 1:6:A:ARG:HB3   | 4        | 0.47          |
| (1,441) | 1:7:A:LEU:HB3  | 1:10:A:GLN:H    | 3        | 0.47          |
| (1,441) | 1:7:A:LEU:HB3  | 1:10:A:GLN:H    | 6        | 0.47          |
| (1,377) | 1:8:A:TYR:HE1  | 1:11:A:TRP:HE3  | 4        | 0.47          |
| (1,377) | 1:8:A:TYR:HE2  | 1:11:A:TRP:HE3  | 4        | 0.47          |
| (1,326) | 1:11:A:TRP:HH2 | 1:12:A:LEU:HD11 | 5        | 0.47          |
| (1,326) | 1:11:A:TRP:HH2 | 1:12:A:LEU:HD12 | 5        | 0.47          |
| (1,326) | 1:11:A:TRP:HH2 | 1:12:A:LEU:HD13 | 5        | 0.47          |
| (1,326) | 1:11:A:TRP:HH2 | 1:12:A:LEU:HD11 | 7        | 0.47          |
| (1,326) | 1:11:A:TRP:HH2 | 1:12:A:LEU:HD12 | 7        | 0.47          |
| (1,326) | 1:11:A:TRP:HH2 | 1:12:A:LEU:HD13 | 7        | 0.47          |
| (1,300) | 1:8:A:TYR:HE1  | 1:24:A:PRO:HD3  | 5        | 0.47          |
| (1,300) | 1:8:A:TYR:HE2  | 1:24:A:PRO:HD3  | 5        | 0.47          |
| (3,69)  | 1:5:A:VAL:HG21 | 1:8:A:TYR:HA    | 10       | 0.46          |
| (3,69)  | 1:5:A:VAL:HG22 | 1:8:A:TYR:HA    | 10       | 0.46          |
| (3,69)  | 1:5:A:VAL:HG23 | 1:8:A:TYR:HA    | 10       | 0.46          |
| (3,59)  | 1:7:A:LEU:HB3  | 1:10:A:GLN:H    | 2        | 0.46          |
| (3,55)  | 1:10:A:GLN:HB2 | 1:11:A:TRP:H    | 7        | 0.46          |
| (3,55)  | 1:10:A:GLN:HB2 | 1:11:A:TRP:H    | 8        | 0.46          |
| (3,4)   | 1:7:A:LEU:HA   | 1:7:A:LEU:HG    | 9        | 0.46          |
| (2,421) | 1:16:A:GLY:HA2 | 1:17:A:PRO:HD3  | 7        | 0.46          |
| (1,520) | 1:5:A:VAL:HG21 | 1:8:A:TYR:HA    | 10       | 0.46          |
| (1,520) | 1:5:A:VAL:HG22 | 1:8:A:TYR:HA    | 10       | 0.46          |
| (1,520) | 1:5:A:VAL:HG23 | 1:8:A:TYR:HA    | 10       | 0.46          |
| (1,486) | 1:16:A:GLY:HA2 | 1:17:A:PRO:HD3  | 7        | 0.46          |
| (1,441) | 1:7:A:LEU:HB3  | 1:10:A:GLN:H    | 2        | 0.46          |
| (1,429) | 1:10:A:GLN:HB2 | 1:11:A:TRP:H    | 7        | 0.46          |
| (1,429) | 1:10:A:GLN:HB2 | 1:11:A:TRP:H    | 8        | 0.46          |
| (1,57)  | 1:7:A:LEU:HA   | 1:7:A:LEU:HG    | 9        | 0.46          |
| (3,92)  | 1:9:A:ILE:H    | 1:9:A:ILE:HG21  | 1        | 0.45          |
| (3,92)  | 1:9:A:ILE:H    | 1:9:A:ILE:HG22  | 1        | 0.45          |
| (3,92)  | 1:9:A:ILE:H    | 1:9:A:ILE:HG23  | 1        | 0.45          |
| (3,92)  | 1:9:A:ILE:H    | 1:9:A:ILE:HG21  | 2        | 0.45          |
| (3,92)  | 1:9:A:ILE:H    | 1:9:A:ILE:HG22  | 2        | 0.45          |
| (3,92)  | 1:9:A:ILE:H    | 1:9:A:ILE:HG23  | 2        | 0.45          |
| (3,92)  | 1:9:A:ILE:H    | 1:9:A:ILE:HG21  | 4        | 0.45          |
| (3,92)  | 1:9:A:ILE:H    | 1:9:A:ILE:HG22  | 4        | 0.45          |
| (3,92)  | 1:9:A:ILE:H    | 1:9:A:ILE:HG23  | 4        | 0.45          |
| (3,69)  | 1:5:A:VAL:HG21 | 1:8:A:TYR:HA    | 1        | 0.45          |
| (3,69)  | 1:5:A:VAL:HG22 | 1:8:A:TYR:HA    | 1        | 0.45          |
| (3,69)  | 1:5:A:VAL:HG23 | 1:8:A:TYR:HA    | 1        | 0.45          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (3,69)  | 1:5:A:VAL:HG21 | 1:8:A:TYR:HA    | 5        | 0.45          |
| (3,69)  | 1:5:A:VAL:HG22 | 1:8:A:TYR:HA    | 5        | 0.45          |
| (3,69)  | 1:5:A:VAL:HG23 | 1:8:A:TYR:HA    | 5        | 0.45          |
| (3,69)  | 1:5:A:VAL:HG21 | 1:8:A:TYR:HA    | 9        | 0.45          |
| (3,69)  | 1:5:A:VAL:HG22 | 1:8:A:TYR:HA    | 9        | 0.45          |
| (3,69)  | 1:5:A:VAL:HG23 | 1:8:A:TYR:HA    | 9        | 0.45          |
| (3,55)  | 1:10:A:GLN:HB2 | 1:11:A:TRP:H    | 4        | 0.45          |
| (3,55)  | 1:10:A:GLN:HB2 | 1:11:A:TRP:H    | 6        | 0.45          |
| (3,32)  | 1:11:A:TRP:HH2 | 1:12:A:LEU:HD11 | 2        | 0.45          |
| (3,32)  | 1:11:A:TRP:HH2 | 1:12:A:LEU:HD12 | 2        | 0.45          |
| (3,32)  | 1:11:A:TRP:HH2 | 1:12:A:LEU:HD13 | 2        | 0.45          |
| (3,19)  | 1:22:A:PRO:HB3 | 1:22:A:PRO:HD2  | 3        | 0.45          |
| (3,19)  | 1:22:A:PRO:HB3 | 1:22:A:PRO:HD2  | 4        | 0.45          |
| (3,19)  | 1:22:A:PRO:HB3 | 1:22:A:PRO:HD2  | 7        | 0.45          |
| (3,19)  | 1:22:A:PRO:HB3 | 1:22:A:PRO:HD2  | 9        | 0.45          |
| (3,4)   | 1:7:A:LEU:HA   | 1:7:A:LEU:HG    | 10       | 0.45          |
| (2,421) | 1:16:A:GLY:HA2 | 1:17:A:PRO:HD3  | 8        | 0.45          |
| (2,277) | 1:8:A:TYR:HE1  | 1:24:A:PRO:HD3  | 2        | 0.45          |
| (2,277) | 1:8:A:TYR:HE2  | 1:24:A:PRO:HD3  | 2        | 0.45          |
| (2,277) | 1:8:A:TYR:HE1  | 1:24:A:PRO:HD3  | 4        | 0.45          |
| (2,277) | 1:8:A:TYR:HE2  | 1:24:A:PRO:HD3  | 4        | 0.45          |
| (1,600) | 1:9:A:ILE:H    | 1:9:A:ILE:HG21  | 1        | 0.45          |
| (1,600) | 1:9:A:ILE:H    | 1:9:A:ILE:HG22  | 1        | 0.45          |
| (1,600) | 1:9:A:ILE:H    | 1:9:A:ILE:HG23  | 1        | 0.45          |
| (1,600) | 1:9:A:ILE:H    | 1:9:A:ILE:HG21  | 2        | 0.45          |
| (1,600) | 1:9:A:ILE:H    | 1:9:A:ILE:HG22  | 2        | 0.45          |
| (1,600) | 1:9:A:ILE:H    | 1:9:A:ILE:HG23  | 2        | 0.45          |
| (1,600) | 1:9:A:ILE:H    | 1:9:A:ILE:HG21  | 4        | 0.45          |
| (1,600) | 1:9:A:ILE:H    | 1:9:A:ILE:HG22  | 4        | 0.45          |
| (1,600) | 1:9:A:ILE:H    | 1:9:A:ILE:HG23  | 4        | 0.45          |
| (1,520) | 1:5:A:VAL:HG21 | 1:8:A:TYR:HA    | 1        | 0.45          |
| (1,520) | 1:5:A:VAL:HG22 | 1:8:A:TYR:HA    | 1        | 0.45          |
| (1,520) | 1:5:A:VAL:HG23 | 1:8:A:TYR:HA    | 1        | 0.45          |
| (1,520) | 1:5:A:VAL:HG21 | 1:8:A:TYR:HA    | 5        | 0.45          |
| (1,520) | 1:5:A:VAL:HG22 | 1:8:A:TYR:HA    | 5        | 0.45          |
| (1,520) | 1:5:A:VAL:HG23 | 1:8:A:TYR:HA    | 5        | 0.45          |
| (1,520) | 1:5:A:VAL:HG21 | 1:8:A:TYR:HA    | 9        | 0.45          |
| (1,520) | 1:5:A:VAL:HG22 | 1:8:A:TYR:HA    | 9        | 0.45          |
| (1,520) | 1:5:A:VAL:HG23 | 1:8:A:TYR:HA    | 9        | 0.45          |
| (1,486) | 1:16:A:GLY:HA2 | 1:17:A:PRO:HD3  | 8        | 0.45          |
| (1,429) | 1:10:A:GLN:HB2 | 1:11:A:TRP:H    | 4        | 0.45          |
| (1,429) | 1:10:A:GLN:HB2 | 1:11:A:TRP:H    | 6        | 0.45          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,326) | 1:11:A:TRP:HH2 | 1:12:A:LEU:HD11 | 2        | 0.45          |
| (1,326) | 1:11:A:TRP:HH2 | 1:12:A:LEU:HD12 | 2        | 0.45          |
| (1,326) | 1:11:A:TRP:HH2 | 1:12:A:LEU:HD13 | 2        | 0.45          |
| (1,300) | 1:8:A:TYR:HE1  | 1:24:A:PRO:HD3  | 2        | 0.45          |
| (1,300) | 1:8:A:TYR:HE2  | 1:24:A:PRO:HD3  | 2        | 0.45          |
| (1,300) | 1:8:A:TYR:HE1  | 1:24:A:PRO:HD3  | 4        | 0.45          |
| (1,300) | 1:8:A:TYR:HE2  | 1:24:A:PRO:HD3  | 4        | 0.45          |
| (1,237) | 1:22:A:PRO:HB3 | 1:22:A:PRO:HD2  | 3        | 0.45          |
| (1,237) | 1:22:A:PRO:HB3 | 1:22:A:PRO:HD2  | 4        | 0.45          |
| (1,237) | 1:22:A:PRO:HB3 | 1:22:A:PRO:HD2  | 7        | 0.45          |
| (1,237) | 1:22:A:PRO:HB3 | 1:22:A:PRO:HD2  | 9        | 0.45          |
| (1,57)  | 1:7:A:LEU:HA   | 1:7:A:LEU:HG    | 10       | 0.45          |
| (3,92)  | 1:9:A:ILE:H    | 1:9:A:ILE:HG21  | 3        | 0.44          |
| (3,92)  | 1:9:A:ILE:H    | 1:9:A:ILE:HG22  | 3        | 0.44          |
| (3,92)  | 1:9:A:ILE:H    | 1:9:A:ILE:HG23  | 3        | 0.44          |
| (3,92)  | 1:9:A:ILE:H    | 1:9:A:ILE:HG21  | 5        | 0.44          |
| (3,92)  | 1:9:A:ILE:H    | 1:9:A:ILE:HG22  | 5        | 0.44          |
| (3,92)  | 1:9:A:ILE:H    | 1:9:A:ILE:HG23  | 5        | 0.44          |
| (3,92)  | 1:9:A:ILE:H    | 1:9:A:ILE:HG21  | 6        | 0.44          |
| (3,92)  | 1:9:A:ILE:H    | 1:9:A:ILE:HG22  | 6        | 0.44          |
| (3,92)  | 1:9:A:ILE:H    | 1:9:A:ILE:HG23  | 6        | 0.44          |
| (3,92)  | 1:9:A:ILE:H    | 1:9:A:ILE:HG21  | 7        | 0.44          |
| (3,92)  | 1:9:A:ILE:H    | 1:9:A:ILE:HG22  | 7        | 0.44          |
| (3,92)  | 1:9:A:ILE:H    | 1:9:A:ILE:HG23  | 7        | 0.44          |
| (3,92)  | 1:9:A:ILE:H    | 1:9:A:ILE:HG21  | 8        | 0.44          |
| (3,92)  | 1:9:A:ILE:H    | 1:9:A:ILE:HG22  | 8        | 0.44          |
| (3,92)  | 1:9:A:ILE:H    | 1:9:A:ILE:HG23  | 8        | 0.44          |
| (3,61)  | 1:9:A:ILE:HD11 | 1:10:A:GLN:H    | 9        | 0.44          |
| (3,61)  | 1:9:A:ILE:HD12 | 1:10:A:GLN:H    | 9        | 0.44          |
| (3,61)  | 1:9:A:ILE:HD13 | 1:10:A:GLN:H    | 9        | 0.44          |
| (3,51)  | 1:4:A:ALA:H    | 1:5:A:VAL:HG21  | 1        | 0.44          |
| (3,51)  | 1:4:A:ALA:H    | 1:5:A:VAL:HG22  | 1        | 0.44          |
| (3,51)  | 1:4:A:ALA:H    | 1:5:A:VAL:HG23  | 1        | 0.44          |
| (3,51)  | 1:4:A:ALA:H    | 1:5:A:VAL:HG21  | 3        | 0.44          |
| (3,51)  | 1:4:A:ALA:H    | 1:5:A:VAL:HG22  | 3        | 0.44          |
| (3,51)  | 1:4:A:ALA:H    | 1:5:A:VAL:HG23  | 3        | 0.44          |
| (3,51)  | 1:4:A:ALA:H    | 1:5:A:VAL:HG21  | 7        | 0.44          |
| (3,51)  | 1:4:A:ALA:H    | 1:5:A:VAL:HG22  | 7        | 0.44          |
| (3,51)  | 1:4:A:ALA:H    | 1:5:A:VAL:HG23  | 7        | 0.44          |
| (3,27)  | 1:8:A:TYR:HD1  | 1:9:A:ILE:HG13  | 1        | 0.44          |
| (3,27)  | 1:8:A:TYR:HD2  | 1:9:A:ILE:HG13  | 1        | 0.44          |
| (3,19)  | 1:22:A:PRO:HB3 | 1:22:A:PRO:HD2  | 8        | 0.44          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (3,19)  | 1:22:A:PRO:HB3 | 1:22:A:PRO:HD2 | 10       | 0.44          |
| (2,206) | 1:21:A:ARG:H   | 1:21:A:ARG:HB3 | 6        | 0.44          |
| (1,600) | 1:9:A:ILE:H    | 1:9:A:ILE:HG21 | 3        | 0.44          |
| (1,600) | 1:9:A:ILE:H    | 1:9:A:ILE:HG22 | 3        | 0.44          |
| (1,600) | 1:9:A:ILE:H    | 1:9:A:ILE:HG23 | 3        | 0.44          |
| (1,600) | 1:9:A:ILE:H    | 1:9:A:ILE:HG21 | 5        | 0.44          |
| (1,600) | 1:9:A:ILE:H    | 1:9:A:ILE:HG22 | 5        | 0.44          |
| (1,600) | 1:9:A:ILE:H    | 1:9:A:ILE:HG23 | 5        | 0.44          |
| (1,600) | 1:9:A:ILE:H    | 1:9:A:ILE:HG21 | 6        | 0.44          |
| (1,600) | 1:9:A:ILE:H    | 1:9:A:ILE:HG22 | 6        | 0.44          |
| (1,600) | 1:9:A:ILE:H    | 1:9:A:ILE:HG23 | 6        | 0.44          |
| (1,600) | 1:9:A:ILE:H    | 1:9:A:ILE:HG21 | 7        | 0.44          |
| (1,600) | 1:9:A:ILE:H    | 1:9:A:ILE:HG22 | 7        | 0.44          |
| (1,600) | 1:9:A:ILE:H    | 1:9:A:ILE:HG23 | 7        | 0.44          |
| (1,600) | 1:9:A:ILE:H    | 1:9:A:ILE:HG21 | 8        | 0.44          |
| (1,600) | 1:9:A:ILE:H    | 1:9:A:ILE:HG22 | 8        | 0.44          |
| (1,600) | 1:9:A:ILE:H    | 1:9:A:ILE:HG23 | 8        | 0.44          |
| (1,446) | 1:9:A:ILE:HD11 | 1:10:A:GLN:H   | 9        | 0.44          |
| (1,446) | 1:9:A:ILE:HD12 | 1:10:A:GLN:H   | 9        | 0.44          |
| (1,446) | 1:9:A:ILE:HD13 | 1:10:A:GLN:H   | 9        | 0.44          |
| (1,408) | 1:4:A:ALA:H    | 1:5:A:VAL:HG21 | 1        | 0.44          |
| (1,408) | 1:4:A:ALA:H    | 1:5:A:VAL:HG22 | 1        | 0.44          |
| (1,408) | 1:4:A:ALA:H    | 1:5:A:VAL:HG23 | 1        | 0.44          |
| (1,408) | 1:4:A:ALA:H    | 1:5:A:VAL:HG21 | 3        | 0.44          |
| (1,408) | 1:4:A:ALA:H    | 1:5:A:VAL:HG22 | 3        | 0.44          |
| (1,408) | 1:4:A:ALA:H    | 1:5:A:VAL:HG23 | 3        | 0.44          |
| (1,408) | 1:4:A:ALA:H    | 1:5:A:VAL:HG21 | 7        | 0.44          |
| (1,408) | 1:4:A:ALA:H    | 1:5:A:VAL:HG22 | 7        | 0.44          |
| (1,408) | 1:4:A:ALA:H    | 1:5:A:VAL:HG23 | 7        | 0.44          |
| (1,313) | 1:8:A:TYR:HD1  | 1:9:A:ILE:HG13 | 1        | 0.44          |
| (1,313) | 1:8:A:TYR:HD2  | 1:9:A:ILE:HG13 | 1        | 0.44          |
| (1,237) | 1:22:A:PRO:HB3 | 1:22:A:PRO:HD2 | 8        | 0.44          |
| (1,237) | 1:22:A:PRO:HB3 | 1:22:A:PRO:HD2 | 10       | 0.44          |
| (1,224) | 1:21:A:ARG:H   | 1:21:A:ARG:HB3 | 6        | 0.44          |
| (3,27)  | 1:8:A:TYR:HD1  | 1:9:A:ILE:HG13 | 3        | 0.43          |
| (3,27)  | 1:8:A:TYR:HD2  | 1:9:A:ILE:HG13 | 3        | 0.43          |
| (3,19)  | 1:22:A:PRO:HB3 | 1:22:A:PRO:HD2 | 1        | 0.43          |
| (3,19)  | 1:22:A:PRO:HB3 | 1:22:A:PRO:HD2 | 6        | 0.43          |
| (2,404) | 1:11:A:TRP:HA  | 1:14:A:ASP:HB3 | 5        | 0.43          |
| (1,466) | 1:11:A:TRP:HA  | 1:14:A:ASP:HB3 | 5        | 0.43          |
| (1,313) | 1:8:A:TYR:HD1  | 1:9:A:ILE:HG13 | 3        | 0.43          |
| (1,313) | 1:8:A:TYR:HD2  | 1:9:A:ILE:HG13 | 3        | 0.43          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,237) | 1:22:A:PRO:HB3 | 1:22:A:PRO:HD2  | 1        | 0.43          |
| (1,237) | 1:22:A:PRO:HB3 | 1:22:A:PRO:HD2  | 6        | 0.43          |
| (3,61)  | 1:9:A:ILE:HD11 | 1:10:A:GLN:H    | 10       | 0.42          |
| (3,61)  | 1:9:A:ILE:HD12 | 1:10:A:GLN:H    | 10       | 0.42          |
| (3,61)  | 1:9:A:ILE:HD13 | 1:10:A:GLN:H    | 10       | 0.42          |
| (3,51)  | 1:4:A:ALA:H    | 1:5:A:VAL:HG21  | 2        | 0.42          |
| (3,51)  | 1:4:A:ALA:H    | 1:5:A:VAL:HG22  | 2        | 0.42          |
| (3,51)  | 1:4:A:ALA:H    | 1:5:A:VAL:HG23  | 2        | 0.42          |
| (3,51)  | 1:4:A:ALA:H    | 1:5:A:VAL:HG21  | 6        | 0.42          |
| (3,51)  | 1:4:A:ALA:H    | 1:5:A:VAL:HG22  | 6        | 0.42          |
| (3,51)  | 1:4:A:ALA:H    | 1:5:A:VAL:HG23  | 6        | 0.42          |
| (3,27)  | 1:8:A:TYR:HD1  | 1:9:A:ILE:HG13  | 6        | 0.42          |
| (3,27)  | 1:8:A:TYR:HD2  | 1:9:A:ILE:HG13  | 6        | 0.42          |
| (3,13)  | 1:12:A:LEU:H   | 1:12:A:LEU:HD21 | 3        | 0.42          |
| (3,13)  | 1:12:A:LEU:H   | 1:12:A:LEU:HD22 | 3        | 0.42          |
| (3,13)  | 1:12:A:LEU:H   | 1:12:A:LEU:HD23 | 3        | 0.42          |
| (3,13)  | 1:12:A:LEU:H   | 1:12:A:LEU:HD21 | 5        | 0.42          |
| (3,13)  | 1:12:A:LEU:H   | 1:12:A:LEU:HD22 | 5        | 0.42          |
| (3,13)  | 1:12:A:LEU:H   | 1:12:A:LEU:HD23 | 5        | 0.42          |
| (3,13)  | 1:12:A:LEU:H   | 1:12:A:LEU:HD21 | 6        | 0.42          |
| (3,13)  | 1:12:A:LEU:H   | 1:12:A:LEU:HD22 | 6        | 0.42          |
| (3,13)  | 1:12:A:LEU:H   | 1:12:A:LEU:HD23 | 6        | 0.42          |
| (3,13)  | 1:12:A:LEU:H   | 1:12:A:LEU:HD21 | 10       | 0.42          |
| (3,13)  | 1:12:A:LEU:H   | 1:12:A:LEU:HD22 | 10       | 0.42          |
| (3,13)  | 1:12:A:LEU:H   | 1:12:A:LEU:HD23 | 10       | 0.42          |
| (2,483) | 1:6:A:ARG:HB3  | 1:7:A:LEU:H     | 10       | 0.42          |
| (1,566) | 1:6:A:ARG:HB3  | 1:7:A:LEU:H     | 10       | 0.42          |
| (1,446) | 1:9:A:ILE:HD11 | 1:10:A:GLN:H    | 10       | 0.42          |
| (1,446) | 1:9:A:ILE:HD12 | 1:10:A:GLN:H    | 10       | 0.42          |
| (1,446) | 1:9:A:ILE:HD13 | 1:10:A:GLN:H    | 10       | 0.42          |
| (1,408) | 1:4:A:ALA:H    | 1:5:A:VAL:HG21  | 2        | 0.42          |
| (1,408) | 1:4:A:ALA:H    | 1:5:A:VAL:HG22  | 2        | 0.42          |
| (1,408) | 1:4:A:ALA:H    | 1:5:A:VAL:HG23  | 2        | 0.42          |
| (1,408) | 1:4:A:ALA:H    | 1:5:A:VAL:HG21  | 6        | 0.42          |
| (1,408) | 1:4:A:ALA:H    | 1:5:A:VAL:HG22  | 6        | 0.42          |
| (1,408) | 1:4:A:ALA:H    | 1:5:A:VAL:HG23  | 6        | 0.42          |
| (1,313) | 1:8:A:TYR:HD1  | 1:9:A:ILE:HG13  | 6        | 0.42          |
| (1,313) | 1:8:A:TYR:HD2  | 1:9:A:ILE:HG13  | 6        | 0.42          |
| (1,134) | 1:12:A:LEU:H   | 1:12:A:LEU:HD21 | 3        | 0.42          |
| (1,134) | 1:12:A:LEU:H   | 1:12:A:LEU:HD22 | 3        | 0.42          |
| (1,134) | 1:12:A:LEU:H   | 1:12:A:LEU:HD23 | 3        | 0.42          |
| (1,134) | 1:12:A:LEU:H   | 1:12:A:LEU:HD21 | 5        | 0.42          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,134) | 1:12:A:LEU:H   | 1:12:A:LEU:HD22 | 5        | 0.42          |
| (1,134) | 1:12:A:LEU:H   | 1:12:A:LEU:HD23 | 5        | 0.42          |
| (1,134) | 1:12:A:LEU:H   | 1:12:A:LEU:HD21 | 6        | 0.42          |
| (1,134) | 1:12:A:LEU:H   | 1:12:A:LEU:HD22 | 6        | 0.42          |
| (1,134) | 1:12:A:LEU:H   | 1:12:A:LEU:HD23 | 6        | 0.42          |
| (1,134) | 1:12:A:LEU:H   | 1:12:A:LEU:HD21 | 10       | 0.42          |
| (1,134) | 1:12:A:LEU:H   | 1:12:A:LEU:HD22 | 10       | 0.42          |
| (1,134) | 1:12:A:LEU:H   | 1:12:A:LEU:HD23 | 10       | 0.42          |
| (3,69)  | 1:5:A:VAL:HG21 | 1:8:A:TYR:HA    | 3        | 0.41          |
| (3,69)  | 1:5:A:VAL:HG22 | 1:8:A:TYR:HA    | 3        | 0.41          |
| (3,69)  | 1:5:A:VAL:HG23 | 1:8:A:TYR:HA    | 3        | 0.41          |
| (3,69)  | 1:5:A:VAL:HG21 | 1:8:A:TYR:HA    | 8        | 0.41          |
| (3,69)  | 1:5:A:VAL:HG22 | 1:8:A:TYR:HA    | 8        | 0.41          |
| (3,69)  | 1:5:A:VAL:HG23 | 1:8:A:TYR:HA    | 8        | 0.41          |
| (3,55)  | 1:10:A:GLN:HB2 | 1:11:A:TRP:H    | 1        | 0.41          |
| (3,51)  | 1:4:A:ALA:H    | 1:5:A:VAL:HG21  | 8        | 0.41          |
| (3,51)  | 1:4:A:ALA:H    | 1:5:A:VAL:HG22  | 8        | 0.41          |
| (3,51)  | 1:4:A:ALA:H    | 1:5:A:VAL:HG23  | 8        | 0.41          |
| (3,27)  | 1:8:A:TYR:HD1  | 1:9:A:ILE:HG13  | 5        | 0.41          |
| (3,27)  | 1:8:A:TYR:HD2  | 1:9:A:ILE:HG13  | 5        | 0.41          |
| (3,13)  | 1:12:A:LEU:H   | 1:12:A:LEU:HD21 | 2        | 0.41          |
| (3,13)  | 1:12:A:LEU:H   | 1:12:A:LEU:HD22 | 2        | 0.41          |
| (3,13)  | 1:12:A:LEU:H   | 1:12:A:LEU:HD23 | 2        | 0.41          |
| (3,10)  | 1:9:A:ILE:HG13 | 1:9:A:ILE:HG21  | 1        | 0.41          |
| (3,10)  | 1:9:A:ILE:HG13 | 1:9:A:ILE:HG22  | 1        | 0.41          |
| (3,10)  | 1:9:A:ILE:HG13 | 1:9:A:ILE:HG23  | 1        | 0.41          |
| (3,10)  | 1:9:A:ILE:HG13 | 1:9:A:ILE:HG21  | 2        | 0.41          |
| (3,10)  | 1:9:A:ILE:HG13 | 1:9:A:ILE:HG22  | 2        | 0.41          |
| (3,10)  | 1:9:A:ILE:HG13 | 1:9:A:ILE:HG23  | 2        | 0.41          |
| (3,10)  | 1:9:A:ILE:HG13 | 1:9:A:ILE:HG21  | 3        | 0.41          |
| (3,10)  | 1:9:A:ILE:HG13 | 1:9:A:ILE:HG22  | 3        | 0.41          |
| (3,10)  | 1:9:A:ILE:HG13 | 1:9:A:ILE:HG23  | 3        | 0.41          |
| (3,10)  | 1:9:A:ILE:HG13 | 1:9:A:ILE:HG21  | 5        | 0.41          |
| (3,10)  | 1:9:A:ILE:HG13 | 1:9:A:ILE:HG22  | 5        | 0.41          |
| (3,10)  | 1:9:A:ILE:HG13 | 1:9:A:ILE:HG23  | 5        | 0.41          |
| (3,10)  | 1:9:A:ILE:HG13 | 1:9:A:ILE:HG21  | 6        | 0.41          |
| (3,10)  | 1:9:A:ILE:HG13 | 1:9:A:ILE:HG22  | 6        | 0.41          |
| (3,10)  | 1:9:A:ILE:HG13 | 1:9:A:ILE:HG23  | 6        | 0.41          |
| (3,10)  | 1:9:A:ILE:HG13 | 1:9:A:ILE:HG21  | 7        | 0.41          |
| (3,10)  | 1:9:A:ILE:HG13 | 1:9:A:ILE:HG22  | 7        | 0.41          |
| (3,10)  | 1:9:A:ILE:HG13 | 1:9:A:ILE:HG23  | 7        | 0.41          |
| (3,10)  | 1:9:A:ILE:HG13 | 1:9:A:ILE:HG21  | 8        | 0.41          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (3,10)  | 1:9:A:ILE:HG13 | 1:9:A:ILE:HG22  | 8        | 0.41          |
| (3,10)  | 1:9:A:ILE:HG13 | 1:9:A:ILE:HG23  | 8        | 0.41          |
| (3,1)   | 1:5:A:VAL:HA   | 1:5:A:VAL:HG11  | 5        | 0.41          |
| (3,1)   | 1:5:A:VAL:HA   | 1:5:A:VAL:HG12  | 5        | 0.41          |
| (3,1)   | 1:5:A:VAL:HA   | 1:5:A:VAL:HG13  | 5        | 0.41          |
| (3,1)   | 1:5:A:VAL:HA   | 1:5:A:VAL:HG11  | 6        | 0.41          |
| (3,1)   | 1:5:A:VAL:HA   | 1:5:A:VAL:HG12  | 6        | 0.41          |
| (3,1)   | 1:5:A:VAL:HA   | 1:5:A:VAL:HG13  | 6        | 0.41          |
| (3,1)   | 1:5:A:VAL:HA   | 1:5:A:VAL:HG11  | 9        | 0.41          |
| (3,1)   | 1:5:A:VAL:HA   | 1:5:A:VAL:HG12  | 9        | 0.41          |
| (3,1)   | 1:5:A:VAL:HA   | 1:5:A:VAL:HG13  | 9        | 0.41          |
| (3,1)   | 1:5:A:VAL:HA   | 1:5:A:VAL:HG11  | 10       | 0.41          |
| (3,1)   | 1:5:A:VAL:HA   | 1:5:A:VAL:HG12  | 10       | 0.41          |
| (3,1)   | 1:5:A:VAL:HA   | 1:5:A:VAL:HG13  | 10       | 0.41          |
| (2,277) | 1:8:A:TYR:HE1  | 1:24:A:PRO:HD3  | 3        | 0.41          |
| (2,277) | 1:8:A:TYR:HE2  | 1:24:A:PRO:HD3  | 3        | 0.41          |
| (2,277) | 1:8:A:TYR:HE1  | 1:24:A:PRO:HD3  | 7        | 0.41          |
| (2,277) | 1:8:A:TYR:HE2  | 1:24:A:PRO:HD3  | 7        | 0.41          |
| (2,277) | 1:8:A:TYR:HE1  | 1:24:A:PRO:HD3  | 8        | 0.41          |
| (2,277) | 1:8:A:TYR:HE2  | 1:24:A:PRO:HD3  | 8        | 0.41          |
| (1,520) | 1:5:A:VAL:HG21 | 1:8:A:TYR:HA    | 3        | 0.41          |
| (1,520) | 1:5:A:VAL:HG22 | 1:8:A:TYR:HA    | 3        | 0.41          |
| (1,520) | 1:5:A:VAL:HG23 | 1:8:A:TYR:HA    | 3        | 0.41          |
| (1,520) | 1:5:A:VAL:HG21 | 1:8:A:TYR:HA    | 8        | 0.41          |
| (1,520) | 1:5:A:VAL:HG22 | 1:8:A:TYR:HA    | 8        | 0.41          |
| (1,520) | 1:5:A:VAL:HG23 | 1:8:A:TYR:HA    | 8        | 0.41          |
| (1,429) | 1:10:A:GLN:HB2 | 1:11:A:TRP:H    | 1        | 0.41          |
| (1,408) | 1:4:A:ALA:H    | 1:5:A:VAL:HG21  | 8        | 0.41          |
| (1,408) | 1:4:A:ALA:H    | 1:5:A:VAL:HG22  | 8        | 0.41          |
| (1,408) | 1:4:A:ALA:H    | 1:5:A:VAL:HG23  | 8        | 0.41          |
| (1,313) | 1:8:A:TYR:HD1  | 1:9:A:ILE:HG13  | 5        | 0.41          |
| (1,313) | 1:8:A:TYR:HD2  | 1:9:A:ILE:HG13  | 5        | 0.41          |
| (1,300) | 1:8:A:TYR:HE1  | 1:24:A:PRO:HD3  | 3        | 0.41          |
| (1,300) | 1:8:A:TYR:HE2  | 1:24:A:PRO:HD3  | 3        | 0.41          |
| (1,300) | 1:8:A:TYR:HE1  | 1:24:A:PRO:HD3  | 7        | 0.41          |
| (1,300) | 1:8:A:TYR:HE2  | 1:24:A:PRO:HD3  | 7        | 0.41          |
| (1,300) | 1:8:A:TYR:HE1  | 1:24:A:PRO:HD3  | 8        | 0.41          |
| (1,300) | 1:8:A:TYR:HE2  | 1:24:A:PRO:HD3  | 8        | 0.41          |
| (1,134) | 1:12:A:LEU:H   | 1:12:A:LEU:HD21 | 2        | 0.41          |
| (1,134) | 1:12:A:LEU:H   | 1:12:A:LEU:HD22 | 2        | 0.41          |
| (1,134) | 1:12:A:LEU:H   | 1:12:A:LEU:HD23 | 2        | 0.41          |
| (1,93)  | 1:9:A:ILE:HG13 | 1:9:A:ILE:HG21  | 1        | 0.41          |

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| Key    | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|--------|----------------|----------------|----------|---------------|
| (1,93) | 1:9:A:ILE:HG13 | 1:9:A:ILE:HG22 | 1        | 0.41          |
| (1,93) | 1:9:A:ILE:HG13 | 1:9:A:ILE:HG23 | 1        | 0.41          |
| (1,93) | 1:9:A:ILE:HG13 | 1:9:A:ILE:HG21 | 2        | 0.41          |
| (1,93) | 1:9:A:ILE:HG13 | 1:9:A:ILE:HG22 | 2        | 0.41          |
| (1,93) | 1:9:A:ILE:HG13 | 1:9:A:ILE:HG23 | 2        | 0.41          |
| (1,93) | 1:9:A:ILE:HG13 | 1:9:A:ILE:HG21 | 3        | 0.41          |
| (1,93) | 1:9:A:ILE:HG13 | 1:9:A:ILE:HG22 | 3        | 0.41          |
| (1,93) | 1:9:A:ILE:HG13 | 1:9:A:ILE:HG23 | 3        | 0.41          |
| (1,93) | 1:9:A:ILE:HG13 | 1:9:A:ILE:HG21 | 5        | 0.41          |
| (1,93) | 1:9:A:ILE:HG13 | 1:9:A:ILE:HG22 | 5        | 0.41          |
| (1,93) | 1:9:A:ILE:HG13 | 1:9:A:ILE:HG23 | 5        | 0.41          |
| (1,93) | 1:9:A:ILE:HG13 | 1:9:A:ILE:HG21 | 6        | 0.41          |
| (1,93) | 1:9:A:ILE:HG13 | 1:9:A:ILE:HG22 | 6        | 0.41          |
| (1,93) | 1:9:A:ILE:HG13 | 1:9:A:ILE:HG23 | 6        | 0.41          |
| (1,93) | 1:9:A:ILE:HG13 | 1:9:A:ILE:HG21 | 7        | 0.41          |
| (1,93) | 1:9:A:ILE:HG13 | 1:9:A:ILE:HG22 | 7        | 0.41          |
| (1,93) | 1:9:A:ILE:HG13 | 1:9:A:ILE:HG23 | 7        | 0.41          |
| (1,93) | 1:9:A:ILE:HG13 | 1:9:A:ILE:HG21 | 8        | 0.41          |
| (1,93) | 1:9:A:ILE:HG13 | 1:9:A:ILE:HG22 | 8        | 0.41          |
| (1,93) | 1:9:A:ILE:HG13 | 1:9:A:ILE:HG23 | 8        | 0.41          |
| (1,22) | 1:5:A:VAL:HA   | 1:5:A:VAL:HG11 | 5        | 0.41          |
| (1,22) | 1:5:A:VAL:HA   | 1:5:A:VAL:HG12 | 5        | 0.41          |
| (1,22) | 1:5:A:VAL:HA   | 1:5:A:VAL:HG13 | 5        | 0.41          |
| (1,22) | 1:5:A:VAL:HA   | 1:5:A:VAL:HG11 | 6        | 0.41          |
| (1,22) | 1:5:A:VAL:HA   | 1:5:A:VAL:HG12 | 6        | 0.41          |
| (1,22) | 1:5:A:VAL:HA   | 1:5:A:VAL:HG13 | 6        | 0.41          |
| (1,22) | 1:5:A:VAL:HA   | 1:5:A:VAL:HG11 | 9        | 0.41          |
| (1,22) | 1:5:A:VAL:HA   | 1:5:A:VAL:HG12 | 9        | 0.41          |
| (1,22) | 1:5:A:VAL:HA   | 1:5:A:VAL:HG13 | 9        | 0.41          |
| (1,22) | 1:5:A:VAL:HA   | 1:5:A:VAL:HG11 | 10       | 0.41          |
| (1,22) | 1:5:A:VAL:HA   | 1:5:A:VAL:HG12 | 10       | 0.41          |
| (1,22) | 1:5:A:VAL:HA   | 1:5:A:VAL:HG13 | 10       | 0.41          |
| (3,69) | 1:5:A:VAL:HG21 | 1:8:A:TYR:HA   | 4        | 0.4           |
| (3,69) | 1:5:A:VAL:HG22 | 1:8:A:TYR:HA   | 4        | 0.4           |
| (3,69) | 1:5:A:VAL:HG23 | 1:8:A:TYR:HA   | 4        | 0.4           |
| (3,69) | 1:5:A:VAL:HG21 | 1:8:A:TYR:HA   | 6        | 0.4           |
| (3,69) | 1:5:A:VAL:HG22 | 1:8:A:TYR:HA   | 6        | 0.4           |
| (3,69) | 1:5:A:VAL:HG23 | 1:8:A:TYR:HA   | 6        | 0.4           |
| (3,69) | 1:5:A:VAL:HG21 | 1:8:A:TYR:HA   | 7        | 0.4           |
| (3,69) | 1:5:A:VAL:HG22 | 1:8:A:TYR:HA   | 7        | 0.4           |
| (3,69) | 1:5:A:VAL:HG23 | 1:8:A:TYR:HA   | 7        | 0.4           |
| (3,55) | 1:10:A:GLN:HB2 | 1:11:A:TRP:H   | 2        | 0.4           |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (3,43)  | 1:8:A:TYR:HE1  | 1:11:A:TRP:HE3  | 7        | 0.4           |
| (3,43)  | 1:8:A:TYR:HE2  | 1:11:A:TRP:HE3  | 7        | 0.4           |
| (3,13)  | 1:12:A:LEU:H   | 1:12:A:LEU:HD21 | 7        | 0.4           |
| (3,13)  | 1:12:A:LEU:H   | 1:12:A:LEU:HD22 | 7        | 0.4           |
| (3,13)  | 1:12:A:LEU:H   | 1:12:A:LEU:HD23 | 7        | 0.4           |
| (3,13)  | 1:12:A:LEU:H   | 1:12:A:LEU:HD21 | 8        | 0.4           |
| (3,13)  | 1:12:A:LEU:H   | 1:12:A:LEU:HD22 | 8        | 0.4           |
| (3,13)  | 1:12:A:LEU:H   | 1:12:A:LEU:HD23 | 8        | 0.4           |
| (3,10)  | 1:9:A:ILE:HG13 | 1:9:A:ILE:HG21  | 4        | 0.4           |
| (3,10)  | 1:9:A:ILE:HG13 | 1:9:A:ILE:HG22  | 4        | 0.4           |
| (3,10)  | 1:9:A:ILE:HG13 | 1:9:A:ILE:HG23  | 4        | 0.4           |
| (3,6)   | 1:7:A:LEU:H    | 1:7:A:LEU:HB2   | 10       | 0.4           |
| (3,1)   | 1:5:A:VAL:HA   | 1:5:A:VAL:HG11  | 1        | 0.4           |
| (3,1)   | 1:5:A:VAL:HA   | 1:5:A:VAL:HG12  | 1        | 0.4           |
| (3,1)   | 1:5:A:VAL:HA   | 1:5:A:VAL:HG13  | 1        | 0.4           |
| (3,1)   | 1:5:A:VAL:HA   | 1:5:A:VAL:HG11  | 2        | 0.4           |
| (3,1)   | 1:5:A:VAL:HA   | 1:5:A:VAL:HG12  | 2        | 0.4           |
| (3,1)   | 1:5:A:VAL:HA   | 1:5:A:VAL:HG13  | 2        | 0.4           |
| (3,1)   | 1:5:A:VAL:HA   | 1:5:A:VAL:HG11  | 3        | 0.4           |
| (3,1)   | 1:5:A:VAL:HA   | 1:5:A:VAL:HG12  | 3        | 0.4           |
| (3,1)   | 1:5:A:VAL:HA   | 1:5:A:VAL:HG13  | 3        | 0.4           |
| (3,1)   | 1:5:A:VAL:HA   | 1:5:A:VAL:HG11  | 7        | 0.4           |
| (3,1)   | 1:5:A:VAL:HA   | 1:5:A:VAL:HG12  | 7        | 0.4           |
| (3,1)   | 1:5:A:VAL:HA   | 1:5:A:VAL:HG13  | 7        | 0.4           |
| (3,1)   | 1:5:A:VAL:HA   | 1:5:A:VAL:HG11  | 8        | 0.4           |
| (3,1)   | 1:5:A:VAL:HA   | 1:5:A:VAL:HG12  | 8        | 0.4           |
| (3,1)   | 1:5:A:VAL:HA   | 1:5:A:VAL:HG13  | 8        | 0.4           |
| (1,520) | 1:5:A:VAL:HG21 | 1:8:A:TYR:HA    | 4        | 0.4           |
| (1,520) | 1:5:A:VAL:HG22 | 1:8:A:TYR:HA    | 4        | 0.4           |
| (1,520) | 1:5:A:VAL:HG23 | 1:8:A:TYR:HA    | 4        | 0.4           |
| (1,520) | 1:5:A:VAL:HG21 | 1:8:A:TYR:HA    | 6        | 0.4           |
| (1,520) | 1:5:A:VAL:HG22 | 1:8:A:TYR:HA    | 6        | 0.4           |
| (1,520) | 1:5:A:VAL:HG23 | 1:8:A:TYR:HA    | 6        | 0.4           |
| (1,520) | 1:5:A:VAL:HG21 | 1:8:A:TYR:HA    | 7        | 0.4           |
| (1,520) | 1:5:A:VAL:HG22 | 1:8:A:TYR:HA    | 7        | 0.4           |
| (1,520) | 1:5:A:VAL:HG23 | 1:8:A:TYR:HA    | 7        | 0.4           |
| (1,429) | 1:10:A:GLN:HB2 | 1:11:A:TRP:H    | 2        | 0.4           |
| (1,377) | 1:8:A:TYR:HE1  | 1:11:A:TRP:HE3  | 7        | 0.4           |
| (1,377) | 1:8:A:TYR:HE2  | 1:11:A:TRP:HE3  | 7        | 0.4           |
| (1,134) | 1:12:A:LEU:H   | 1:12:A:LEU:HD21 | 7        | 0.4           |
| (1,134) | 1:12:A:LEU:H   | 1:12:A:LEU:HD22 | 7        | 0.4           |
| (1,134) | 1:12:A:LEU:H   | 1:12:A:LEU:HD23 | 7        | 0.4           |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,134) | 1:12:A:LEU:H   | 1:12:A:LEU:HD21 | 8        | 0.4           |
| (1,134) | 1:12:A:LEU:H   | 1:12:A:LEU:HD22 | 8        | 0.4           |
| (1,134) | 1:12:A:LEU:H   | 1:12:A:LEU:HD23 | 8        | 0.4           |
| (1,93)  | 1:9:A:ILE:HG13 | 1:9:A:ILE:HG21  | 4        | 0.4           |
| (1,93)  | 1:9:A:ILE:HG13 | 1:9:A:ILE:HG22  | 4        | 0.4           |
| (1,93)  | 1:9:A:ILE:HG13 | 1:9:A:ILE:HG23  | 4        | 0.4           |
| (1,69)  | 1:7:A:LEU:H    | 1:7:A:LEU:HB2   | 10       | 0.4           |
| (1,22)  | 1:5:A:VAL:HA   | 1:5:A:VAL:HG11  | 1        | 0.4           |
| (1,22)  | 1:5:A:VAL:HA   | 1:5:A:VAL:HG12  | 1        | 0.4           |
| (1,22)  | 1:5:A:VAL:HA   | 1:5:A:VAL:HG13  | 1        | 0.4           |
| (1,22)  | 1:5:A:VAL:HA   | 1:5:A:VAL:HG11  | 2        | 0.4           |
| (1,22)  | 1:5:A:VAL:HA   | 1:5:A:VAL:HG12  | 2        | 0.4           |
| (1,22)  | 1:5:A:VAL:HA   | 1:5:A:VAL:HG13  | 2        | 0.4           |
| (1,22)  | 1:5:A:VAL:HA   | 1:5:A:VAL:HG11  | 3        | 0.4           |
| (1,22)  | 1:5:A:VAL:HA   | 1:5:A:VAL:HG12  | 3        | 0.4           |
| (1,22)  | 1:5:A:VAL:HA   | 1:5:A:VAL:HG13  | 3        | 0.4           |
| (1,22)  | 1:5:A:VAL:HA   | 1:5:A:VAL:HG11  | 7        | 0.4           |
| (1,22)  | 1:5:A:VAL:HA   | 1:5:A:VAL:HG12  | 7        | 0.4           |
| (1,22)  | 1:5:A:VAL:HA   | 1:5:A:VAL:HG13  | 7        | 0.4           |
| (1,22)  | 1:5:A:VAL:HA   | 1:5:A:VAL:HG11  | 8        | 0.4           |
| (1,22)  | 1:5:A:VAL:HA   | 1:5:A:VAL:HG12  | 8        | 0.4           |
| (1,22)  | 1:5:A:VAL:HA   | 1:5:A:VAL:HG13  | 8        | 0.4           |
| (3,75)  | 1:5:A:VAL:HG21 | 1:6:A:ARG:HG3   | 10       | 0.39          |
| (3,75)  | 1:5:A:VAL:HG22 | 1:6:A:ARG:HG3   | 10       | 0.39          |
| (3,75)  | 1:5:A:VAL:HG23 | 1:6:A:ARG:HG3   | 10       | 0.39          |
| (3,69)  | 1:5:A:VAL:HG21 | 1:8:A:TYR:HA    | 2        | 0.39          |
| (3,69)  | 1:5:A:VAL:HG22 | 1:8:A:TYR:HA    | 2        | 0.39          |
| (3,69)  | 1:5:A:VAL:HG23 | 1:8:A:TYR:HA    | 2        | 0.39          |
| (3,55)  | 1:10:A:GLN:HB2 | 1:11:A:TRP:H    | 3        | 0.39          |
| (3,51)  | 1:4:A:ALA:H    | 1:5:A:VAL:HG21  | 5        | 0.39          |
| (3,51)  | 1:4:A:ALA:H    | 1:5:A:VAL:HG22  | 5        | 0.39          |
| (3,51)  | 1:4:A:ALA:H    | 1:5:A:VAL:HG23  | 5        | 0.39          |
| (3,27)  | 1:8:A:TYR:HD1  | 1:9:A:ILE:HG13  | 8        | 0.39          |
| (3,27)  | 1:8:A:TYR:HD2  | 1:9:A:ILE:HG13  | 8        | 0.39          |
| (3,25)  | 1:8:A:TYR:HE1  | 1:12:A:LEU:HG   | 3        | 0.39          |
| (3,25)  | 1:8:A:TYR:HE2  | 1:12:A:LEU:HG   | 3        | 0.39          |
| (3,13)  | 1:12:A:LEU:H   | 1:12:A:LEU:HD21 | 1        | 0.39          |
| (3,13)  | 1:12:A:LEU:H   | 1:12:A:LEU:HD22 | 1        | 0.39          |
| (3,13)  | 1:12:A:LEU:H   | 1:12:A:LEU:HD23 | 1        | 0.39          |
| (3,13)  | 1:12:A:LEU:H   | 1:12:A:LEU:HD21 | 4        | 0.39          |
| (3,13)  | 1:12:A:LEU:H   | 1:12:A:LEU:HD22 | 4        | 0.39          |
| (3,13)  | 1:12:A:LEU:H   | 1:12:A:LEU:HD23 | 4        | 0.39          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (3,13)  | 1:12:A:LEU:H   | 1:12:A:LEU:HD21 | 9        | 0.39          |
| (3,13)  | 1:12:A:LEU:H   | 1:12:A:LEU:HD22 | 9        | 0.39          |
| (3,13)  | 1:12:A:LEU:H   | 1:12:A:LEU:HD23 | 9        | 0.39          |
| (3,10)  | 1:9:A:ILE:HG13 | 1:9:A:ILE:HG21  | 10       | 0.39          |
| (3,10)  | 1:9:A:ILE:HG13 | 1:9:A:ILE:HG22  | 10       | 0.39          |
| (3,10)  | 1:9:A:ILE:HG13 | 1:9:A:ILE:HG23  | 10       | 0.39          |
| (3,6)   | 1:7:A:LEU:H    | 1:7:A:LEU:HB2   | 9        | 0.39          |
| (3,1)   | 1:5:A:VAL:HA   | 1:5:A:VAL:HG11  | 4        | 0.39          |
| (3,1)   | 1:5:A:VAL:HA   | 1:5:A:VAL:HG12  | 4        | 0.39          |
| (3,1)   | 1:5:A:VAL:HA   | 1:5:A:VAL:HG13  | 4        | 0.39          |
| (2,206) | 1:21:A:ARG:H   | 1:21:A:ARG:HB3  | 3        | 0.39          |
| (2,206) | 1:21:A:ARG:H   | 1:21:A:ARG:HB3  | 4        | 0.39          |
| (2,206) | 1:21:A:ARG:H   | 1:21:A:ARG:HB3  | 8        | 0.39          |
| (2,206) | 1:21:A:ARG:H   | 1:21:A:ARG:HB3  | 9        | 0.39          |
| (1,543) | 1:5:A:VAL:HG21 | 1:6:A:ARG:HG3   | 10       | 0.39          |
| (1,543) | 1:5:A:VAL:HG22 | 1:6:A:ARG:HG3   | 10       | 0.39          |
| (1,543) | 1:5:A:VAL:HG23 | 1:6:A:ARG:HG3   | 10       | 0.39          |
| (1,520) | 1:5:A:VAL:HG21 | 1:8:A:TYR:HA    | 2        | 0.39          |
| (1,520) | 1:5:A:VAL:HG22 | 1:8:A:TYR:HA    | 2        | 0.39          |
| (1,520) | 1:5:A:VAL:HG23 | 1:8:A:TYR:HA    | 2        | 0.39          |
| (1,429) | 1:10:A:GLN:HB2 | 1:11:A:TRP:H    | 3        | 0.39          |
| (1,408) | 1:4:A:ALA:H    | 1:5:A:VAL:HG21  | 5        | 0.39          |
| (1,408) | 1:4:A:ALA:H    | 1:5:A:VAL:HG22  | 5        | 0.39          |
| (1,408) | 1:4:A:ALA:H    | 1:5:A:VAL:HG23  | 5        | 0.39          |
| (1,313) | 1:8:A:TYR:HD1  | 1:9:A:ILE:HG13  | 8        | 0.39          |
| (1,313) | 1:8:A:TYR:HD2  | 1:9:A:ILE:HG13  | 8        | 0.39          |
| (1,310) | 1:8:A:TYR:HE1  | 1:12:A:LEU:HG   | 3        | 0.39          |
| (1,310) | 1:8:A:TYR:HE2  | 1:12:A:LEU:HG   | 3        | 0.39          |
| (1,224) | 1:21:A:ARG:H   | 1:21:A:ARG:HB3  | 3        | 0.39          |
| (1,224) | 1:21:A:ARG:H   | 1:21:A:ARG:HB3  | 4        | 0.39          |
| (1,224) | 1:21:A:ARG:H   | 1:21:A:ARG:HB3  | 8        | 0.39          |
| (1,224) | 1:21:A:ARG:H   | 1:21:A:ARG:HB3  | 9        | 0.39          |
| (1,134) | 1:12:A:LEU:H   | 1:12:A:LEU:HD21 | 1        | 0.39          |
| (1,134) | 1:12:A:LEU:H   | 1:12:A:LEU:HD22 | 1        | 0.39          |
| (1,134) | 1:12:A:LEU:H   | 1:12:A:LEU:HD23 | 1        | 0.39          |
| (1,134) | 1:12:A:LEU:H   | 1:12:A:LEU:HD21 | 4        | 0.39          |
| (1,134) | 1:12:A:LEU:H   | 1:12:A:LEU:HD22 | 4        | 0.39          |
| (1,134) | 1:12:A:LEU:H   | 1:12:A:LEU:HD23 | 4        | 0.39          |
| (1,134) | 1:12:A:LEU:H   | 1:12:A:LEU:HD21 | 9        | 0.39          |
| (1,134) | 1:12:A:LEU:H   | 1:12:A:LEU:HD22 | 9        | 0.39          |
| (1,134) | 1:12:A:LEU:H   | 1:12:A:LEU:HD23 | 9        | 0.39          |
| (1,93)  | 1:9:A:ILE:HG13 | 1:9:A:ILE:HG21  | 10       | 0.39          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,93)  | 1:9:A:ILE:HG13 | 1:9:A:ILE:HG22 | 10       | 0.39          |
| (1,93)  | 1:9:A:ILE:HG13 | 1:9:A:ILE:HG23 | 10       | 0.39          |
| (1,69)  | 1:7:A:LEU:H    | 1:7:A:LEU:HB2  | 9        | 0.39          |
| (1,22)  | 1:5:A:VAL:HA   | 1:5:A:VAL:HG11 | 4        | 0.39          |
| (1,22)  | 1:5:A:VAL:HA   | 1:5:A:VAL:HG12 | 4        | 0.39          |
| (1,22)  | 1:5:A:VAL:HA   | 1:5:A:VAL:HG13 | 4        | 0.39          |
| (3,43)  | 1:8:A:TYR:HE1  | 1:11:A:TRP:HE3 | 8        | 0.38          |
| (3,43)  | 1:8:A:TYR:HE2  | 1:11:A:TRP:HE3 | 8        | 0.38          |
| (3,27)  | 1:8:A:TYR:HD1  | 1:9:A:ILE:HG13 | 4        | 0.38          |
| (3,27)  | 1:8:A:TYR:HD2  | 1:9:A:ILE:HG13 | 4        | 0.38          |
| (3,27)  | 1:8:A:TYR:HD1  | 1:9:A:ILE:HG13 | 7        | 0.38          |
| (3,27)  | 1:8:A:TYR:HD2  | 1:9:A:ILE:HG13 | 7        | 0.38          |
| (3,10)  | 1:9:A:ILE:HG13 | 1:9:A:ILE:HG21 | 9        | 0.38          |
| (3,10)  | 1:9:A:ILE:HG13 | 1:9:A:ILE:HG22 | 9        | 0.38          |
| (3,10)  | 1:9:A:ILE:HG13 | 1:9:A:ILE:HG23 | 9        | 0.38          |
| (2,485) | 1:16:A:GLY:H   | 1:19:A:SER:HB3 | 6        | 0.38          |
| (2,206) | 1:21:A:ARG:H   | 1:21:A:ARG:HB3 | 7        | 0.38          |
| (1,568) | 1:16:A:GLY:H   | 1:19:A:SER:HB3 | 6        | 0.38          |
| (1,377) | 1:8:A:TYR:HE1  | 1:11:A:TRP:HE3 | 8        | 0.38          |
| (1,377) | 1:8:A:TYR:HE2  | 1:11:A:TRP:HE3 | 8        | 0.38          |
| (1,313) | 1:8:A:TYR:HD1  | 1:9:A:ILE:HG13 | 4        | 0.38          |
| (1,313) | 1:8:A:TYR:HD2  | 1:9:A:ILE:HG13 | 4        | 0.38          |
| (1,313) | 1:8:A:TYR:HD1  | 1:9:A:ILE:HG13 | 7        | 0.38          |
| (1,313) | 1:8:A:TYR:HD2  | 1:9:A:ILE:HG13 | 7        | 0.38          |
| (1,224) | 1:21:A:ARG:H   | 1:21:A:ARG:HB3 | 7        | 0.38          |
| (1,93)  | 1:9:A:ILE:HG13 | 1:9:A:ILE:HG21 | 9        | 0.38          |
| (1,93)  | 1:9:A:ILE:HG13 | 1:9:A:ILE:HG22 | 9        | 0.38          |
| (1,93)  | 1:9:A:ILE:HG13 | 1:9:A:ILE:HG23 | 9        | 0.38          |
| (3,30)  | 1:7:A:LEU:HD11 | 1:8:A:TYR:HD1  | 9        | 0.37          |
| (3,30)  | 1:7:A:LEU:HD11 | 1:8:A:TYR:HD2  | 9        | 0.37          |
| (3,30)  | 1:7:A:LEU:HD12 | 1:8:A:TYR:HD1  | 9        | 0.37          |
| (3,30)  | 1:7:A:LEU:HD12 | 1:8:A:TYR:HD2  | 9        | 0.37          |
| (3,30)  | 1:7:A:LEU:HD13 | 1:8:A:TYR:HD1  | 9        | 0.37          |
| (3,30)  | 1:7:A:LEU:HD13 | 1:8:A:TYR:HD2  | 9        | 0.37          |
| (3,27)  | 1:8:A:TYR:HD1  | 1:9:A:ILE:HG13 | 2        | 0.37          |
| (3,27)  | 1:8:A:TYR:HD2  | 1:9:A:ILE:HG13 | 2        | 0.37          |
| (3,12)  | 1:12:A:LEU:H   | 1:12:A:LEU:HB3 | 1        | 0.37          |
| (3,12)  | 1:12:A:LEU:H   | 1:12:A:LEU:HB3 | 2        | 0.37          |
| (3,12)  | 1:12:A:LEU:H   | 1:12:A:LEU:HB3 | 3        | 0.37          |
| (3,12)  | 1:12:A:LEU:H   | 1:12:A:LEU:HB3 | 4        | 0.37          |
| (3,12)  | 1:12:A:LEU:H   | 1:12:A:LEU:HB3 | 5        | 0.37          |
| (3,12)  | 1:12:A:LEU:H   | 1:12:A:LEU:HB3 | 7        | 0.37          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (3,12)  | 1:12:A:LEU:H   | 1:12:A:LEU:HB3 | 9        | 0.37          |
| (2,292) | 1:8:A:TYR:HD1  | 1:23:A:PRO:HB2 | 5        | 0.37          |
| (2,292) | 1:8:A:TYR:HD2  | 1:23:A:PRO:HB2 | 5        | 0.37          |
| (2,206) | 1:21:A:ARG:H   | 1:21:A:ARG:HB3 | 10       | 0.37          |
| (1,323) | 1:8:A:TYR:HD1  | 1:23:A:PRO:HB2 | 5        | 0.37          |
| (1,323) | 1:8:A:TYR:HD2  | 1:23:A:PRO:HB2 | 5        | 0.37          |
| (1,318) | 1:7:A:LEU:HD11 | 1:8:A:TYR:HD1  | 9        | 0.37          |
| (1,318) | 1:7:A:LEU:HD11 | 1:8:A:TYR:HD2  | 9        | 0.37          |
| (1,318) | 1:7:A:LEU:HD12 | 1:8:A:TYR:HD1  | 9        | 0.37          |
| (1,318) | 1:7:A:LEU:HD12 | 1:8:A:TYR:HD2  | 9        | 0.37          |
| (1,318) | 1:7:A:LEU:HD13 | 1:8:A:TYR:HD1  | 9        | 0.37          |
| (1,318) | 1:7:A:LEU:HD13 | 1:8:A:TYR:HD2  | 9        | 0.37          |
| (1,313) | 1:8:A:TYR:HD1  | 1:9:A:ILE:HG13 | 2        | 0.37          |
| (1,313) | 1:8:A:TYR:HD2  | 1:9:A:ILE:HG13 | 2        | 0.37          |
| (1,224) | 1:21:A:ARG:H   | 1:21:A:ARG:HB3 | 10       | 0.37          |
| (1,132) | 1:12:A:LEU:H   | 1:12:A:LEU:HB3 | 1        | 0.37          |
| (1,132) | 1:12:A:LEU:H   | 1:12:A:LEU:HB3 | 2        | 0.37          |
| (1,132) | 1:12:A:LEU:H   | 1:12:A:LEU:HB3 | 3        | 0.37          |
| (1,132) | 1:12:A:LEU:H   | 1:12:A:LEU:HB3 | 4        | 0.37          |
| (1,132) | 1:12:A:LEU:H   | 1:12:A:LEU:HB3 | 5        | 0.37          |
| (1,132) | 1:12:A:LEU:H   | 1:12:A:LEU:HB3 | 7        | 0.37          |
| (1,132) | 1:12:A:LEU:H   | 1:12:A:LEU:HB3 | 9        | 0.37          |
| (3,84)  | 1:3:A:GLU:HA   | 1:7:A:LEU:H    | 4        | 0.36          |
| (3,67)  | 1:22:A:PRO:HG2 | 1:23:A:PRO:HD2 | 7        | 0.36          |
| (3,67)  | 1:22:A:PRO:HG2 | 1:23:A:PRO:HD3 | 7        | 0.36          |
| (3,67)  | 1:22:A:PRO:HG3 | 1:23:A:PRO:HD2 | 7        | 0.36          |
| (3,67)  | 1:22:A:PRO:HG3 | 1:23:A:PRO:HD3 | 7        | 0.36          |
| (3,51)  | 1:4:A:ALA:H    | 1:5:A:VAL:HG21 | 9        | 0.36          |
| (3,51)  | 1:4:A:ALA:H    | 1:5:A:VAL:HG22 | 9        | 0.36          |
| (3,51)  | 1:4:A:ALA:H    | 1:5:A:VAL:HG23 | 9        | 0.36          |
| (3,17)  | 1:19:A:SER:HA  | 1:19:A:SER:HB3 | 3        | 0.36          |
| (3,17)  | 1:19:A:SER:HA  | 1:19:A:SER:HB3 | 10       | 0.36          |
| (3,12)  | 1:12:A:LEU:H   | 1:12:A:LEU:HB3 | 6        | 0.36          |
| (3,12)  | 1:12:A:LEU:H   | 1:12:A:LEU:HB3 | 8        | 0.36          |
| (3,12)  | 1:12:A:LEU:H   | 1:12:A:LEU:HB3 | 10       | 0.36          |
| (2,386) | 1:23:A:PRO:HB3 | 1:25:A:SER:H   | 6        | 0.36          |
| (2,292) | 1:8:A:TYR:HD1  | 1:23:A:PRO:HB2 | 6        | 0.36          |
| (2,292) | 1:8:A:TYR:HD2  | 1:23:A:PRO:HB2 | 6        | 0.36          |
| (2,277) | 1:8:A:TYR:HE1  | 1:24:A:PRO:HD3 | 1        | 0.36          |
| (2,277) | 1:8:A:TYR:HE2  | 1:24:A:PRO:HD3 | 1        | 0.36          |
| (2,142) | 1:14:A:ASP:H   | 1:14:A:ASP:HB3 | 3        | 0.36          |
| (1,569) | 1:3:A:GLU:HA   | 1:7:A:LEU:H    | 4        | 0.36          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,491) | 1:22:A:PRO:HG2 | 1:23:A:PRO:HD2  | 7        | 0.36          |
| (1,491) | 1:22:A:PRO:HG2 | 1:23:A:PRO:HD3  | 7        | 0.36          |
| (1,491) | 1:22:A:PRO:HG3 | 1:23:A:PRO:HD2  | 7        | 0.36          |
| (1,491) | 1:22:A:PRO:HG3 | 1:23:A:PRO:HD3  | 7        | 0.36          |
| (1,448) | 1:23:A:PRO:HB3 | 1:25:A:SER:H    | 6        | 0.36          |
| (1,408) | 1:4:A:ALA:H    | 1:5:A:VAL:HG21  | 9        | 0.36          |
| (1,408) | 1:4:A:ALA:H    | 1:5:A:VAL:HG22  | 9        | 0.36          |
| (1,408) | 1:4:A:ALA:H    | 1:5:A:VAL:HG23  | 9        | 0.36          |
| (1,323) | 1:8:A:TYR:HD1  | 1:23:A:PRO:HB2  | 6        | 0.36          |
| (1,323) | 1:8:A:TYR:HD2  | 1:23:A:PRO:HB2  | 6        | 0.36          |
| (1,300) | 1:8:A:TYR:HE1  | 1:24:A:PRO:HD3  | 1        | 0.36          |
| (1,300) | 1:8:A:TYR:HE2  | 1:24:A:PRO:HD3  | 1        | 0.36          |
| (1,197) | 1:19:A:SER:HA  | 1:19:A:SER:HB3  | 3        | 0.36          |
| (1,197) | 1:19:A:SER:HA  | 1:19:A:SER:HB3  | 10       | 0.36          |
| (1,157) | 1:14:A:ASP:H   | 1:14:A:ASP:HB3  | 3        | 0.36          |
| (1,132) | 1:12:A:LEU:H   | 1:12:A:LEU:HB3  | 6        | 0.36          |
| (1,132) | 1:12:A:LEU:H   | 1:12:A:LEU:HB3  | 8        | 0.36          |
| (1,132) | 1:12:A:LEU:H   | 1:12:A:LEU:HB3  | 10       | 0.36          |
| (3,77)  | 1:3:A:GLU:HG2  | 1:7:A:LEU:HD11  | 9        | 0.35          |
| (3,77)  | 1:3:A:GLU:HG2  | 1:7:A:LEU:HD12  | 9        | 0.35          |
| (3,77)  | 1:3:A:GLU:HG2  | 1:7:A:LEU:HD13  | 9        | 0.35          |
| (3,77)  | 1:3:A:GLU:HG3  | 1:7:A:LEU:HD11  | 9        | 0.35          |
| (3,77)  | 1:3:A:GLU:HG3  | 1:7:A:LEU:HD12  | 9        | 0.35          |
| (3,77)  | 1:3:A:GLU:HG3  | 1:7:A:LEU:HD13  | 9        | 0.35          |
| (3,67)  | 1:22:A:PRO:HG2 | 1:23:A:PRO:HD2  | 4        | 0.35          |
| (3,67)  | 1:22:A:PRO:HG2 | 1:23:A:PRO:HD3  | 4        | 0.35          |
| (3,67)  | 1:22:A:PRO:HG3 | 1:23:A:PRO:HD2  | 4        | 0.35          |
| (3,67)  | 1:22:A:PRO:HG3 | 1:23:A:PRO:HD3  | 4        | 0.35          |
| (3,67)  | 1:22:A:PRO:HG2 | 1:23:A:PRO:HD2  | 8        | 0.35          |
| (3,67)  | 1:22:A:PRO:HG2 | 1:23:A:PRO:HD3  | 8        | 0.35          |
| (3,67)  | 1:22:A:PRO:HG3 | 1:23:A:PRO:HD2  | 8        | 0.35          |
| (3,67)  | 1:22:A:PRO:HG3 | 1:23:A:PRO:HD3  | 8        | 0.35          |
| (3,60)  | 1:11:A:TRP:H   | 1:12:A:LEU:HD11 | 1        | 0.35          |
| (3,60)  | 1:11:A:TRP:H   | 1:12:A:LEU:HD12 | 1        | 0.35          |
| (3,60)  | 1:11:A:TRP:H   | 1:12:A:LEU:HD13 | 1        | 0.35          |
| (3,60)  | 1:11:A:TRP:H   | 1:12:A:LEU:HD11 | 4        | 0.35          |
| (3,60)  | 1:11:A:TRP:H   | 1:12:A:LEU:HD12 | 4        | 0.35          |
| (3,60)  | 1:11:A:TRP:H   | 1:12:A:LEU:HD13 | 4        | 0.35          |
| (3,51)  | 1:4:A:ALA:H    | 1:5:A:VAL:HG21  | 10       | 0.35          |
| (3,51)  | 1:4:A:ALA:H    | 1:5:A:VAL:HG22  | 10       | 0.35          |
| (3,51)  | 1:4:A:ALA:H    | 1:5:A:VAL:HG23  | 10       | 0.35          |
| (3,43)  | 1:8:A:TYR:HE1  | 1:11:A:TRP:HE3  | 1        | 0.35          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (3,43)  | 1:8:A:TYR:HE2  | 1:11:A:TRP:HE3  | 1        | 0.35          |
| (3,43)  | 1:8:A:TYR:HE1  | 1:11:A:TRP:HE3  | 10       | 0.35          |
| (3,43)  | 1:8:A:TYR:HE2  | 1:11:A:TRP:HE3  | 10       | 0.35          |
| (3,25)  | 1:8:A:TYR:HE1  | 1:12:A:LEU:HG   | 5        | 0.35          |
| (3,25)  | 1:8:A:TYR:HE2  | 1:12:A:LEU:HG   | 5        | 0.35          |
| (3,25)  | 1:8:A:TYR:HE1  | 1:12:A:LEU:HG   | 6        | 0.35          |
| (3,25)  | 1:8:A:TYR:HE2  | 1:12:A:LEU:HG   | 6        | 0.35          |
| (2,292) | 1:8:A:TYR:HD1  | 1:23:A:PRO:HB2  | 1        | 0.35          |
| (2,292) | 1:8:A:TYR:HD2  | 1:23:A:PRO:HB2  | 1        | 0.35          |
| (2,206) | 1:21:A:ARG:H   | 1:21:A:ARG:HB3  | 1        | 0.35          |
| (2,206) | 1:21:A:ARG:H   | 1:21:A:ARG:HB3  | 2        | 0.35          |
| (1,552) | 1:3:A:GLU:HG2  | 1:7:A:LEU:HD11  | 9        | 0.35          |
| (1,552) | 1:3:A:GLU:HG2  | 1:7:A:LEU:HD12  | 9        | 0.35          |
| (1,552) | 1:3:A:GLU:HG2  | 1:7:A:LEU:HD13  | 9        | 0.35          |
| (1,552) | 1:3:A:GLU:HG3  | 1:7:A:LEU:HD11  | 9        | 0.35          |
| (1,552) | 1:3:A:GLU:HG3  | 1:7:A:LEU:HD12  | 9        | 0.35          |
| (1,552) | 1:3:A:GLU:HG3  | 1:7:A:LEU:HD13  | 9        | 0.35          |
| (1,491) | 1:22:A:PRO:HG2 | 1:23:A:PRO:HD2  | 4        | 0.35          |
| (1,491) | 1:22:A:PRO:HG2 | 1:23:A:PRO:HD3  | 4        | 0.35          |
| (1,491) | 1:22:A:PRO:HG3 | 1:23:A:PRO:HD2  | 4        | 0.35          |
| (1,491) | 1:22:A:PRO:HG3 | 1:23:A:PRO:HD3  | 4        | 0.35          |
| (1,491) | 1:22:A:PRO:HG2 | 1:23:A:PRO:HD2  | 8        | 0.35          |
| (1,491) | 1:22:A:PRO:HG2 | 1:23:A:PRO:HD3  | 8        | 0.35          |
| (1,491) | 1:22:A:PRO:HG3 | 1:23:A:PRO:HD2  | 8        | 0.35          |
| (1,491) | 1:22:A:PRO:HG3 | 1:23:A:PRO:HD3  | 8        | 0.35          |
| (1,444) | 1:11:A:TRP:H   | 1:12:A:LEU:HD11 | 1        | 0.35          |
| (1,444) | 1:11:A:TRP:H   | 1:12:A:LEU:HD12 | 1        | 0.35          |
| (1,444) | 1:11:A:TRP:H   | 1:12:A:LEU:HD13 | 1        | 0.35          |
| (1,444) | 1:11:A:TRP:H   | 1:12:A:LEU:HD11 | 4        | 0.35          |
| (1,444) | 1:11:A:TRP:H   | 1:12:A:LEU:HD12 | 4        | 0.35          |
| (1,444) | 1:11:A:TRP:H   | 1:12:A:LEU:HD13 | 4        | 0.35          |
| (1,408) | 1:4:A:ALA:H    | 1:5:A:VAL:HG21  | 10       | 0.35          |
| (1,408) | 1:4:A:ALA:H    | 1:5:A:VAL:HG22  | 10       | 0.35          |
| (1,408) | 1:4:A:ALA:H    | 1:5:A:VAL:HG23  | 10       | 0.35          |
| (1,377) | 1:8:A:TYR:HE1  | 1:11:A:TRP:HE3  | 1        | 0.35          |
| (1,377) | 1:8:A:TYR:HE2  | 1:11:A:TRP:HE3  | 1        | 0.35          |
| (1,377) | 1:8:A:TYR:HE1  | 1:11:A:TRP:HE3  | 10       | 0.35          |
| (1,377) | 1:8:A:TYR:HE2  | 1:11:A:TRP:HE3  | 10       | 0.35          |
| (1,323) | 1:8:A:TYR:HD1  | 1:23:A:PRO:HB2  | 1        | 0.35          |
| (1,323) | 1:8:A:TYR:HD2  | 1:23:A:PRO:HB2  | 1        | 0.35          |
| (1,310) | 1:8:A:TYR:HE1  | 1:12:A:LEU:HG   | 5        | 0.35          |
| (1,310) | 1:8:A:TYR:HE2  | 1:12:A:LEU:HG   | 5        | 0.35          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,310) | 1:8:A:TYR:HE1  | 1:12:A:LEU:HG   | 6        | 0.35          |
| (1,310) | 1:8:A:TYR:HE2  | 1:12:A:LEU:HG   | 6        | 0.35          |
| (1,224) | 1:21:A:ARG:H   | 1:21:A:ARG:HB3  | 1        | 0.35          |
| (1,224) | 1:21:A:ARG:H   | 1:21:A:ARG:HB3  | 2        | 0.35          |
| (3,75)  | 1:5:A:VAL:HG21 | 1:6:A:ARG:HG3   | 3        | 0.34          |
| (3,75)  | 1:5:A:VAL:HG22 | 1:6:A:ARG:HG3   | 3        | 0.34          |
| (3,75)  | 1:5:A:VAL:HG23 | 1:6:A:ARG:HG3   | 3        | 0.34          |
| (3,64)  | 1:6:A:ARG:HA   | 1:10:A:GLN:HB2  | 10       | 0.34          |
| (3,60)  | 1:11:A:TRP:H   | 1:12:A:LEU:HD11 | 2        | 0.34          |
| (3,60)  | 1:11:A:TRP:H   | 1:12:A:LEU:HD12 | 2        | 0.34          |
| (3,60)  | 1:11:A:TRP:H   | 1:12:A:LEU:HD13 | 2        | 0.34          |
| (3,60)  | 1:11:A:TRP:H   | 1:12:A:LEU:HD11 | 5        | 0.34          |
| (3,60)  | 1:11:A:TRP:H   | 1:12:A:LEU:HD12 | 5        | 0.34          |
| (3,60)  | 1:11:A:TRP:H   | 1:12:A:LEU:HD13 | 5        | 0.34          |
| (3,60)  | 1:11:A:TRP:H   | 1:12:A:LEU:HD11 | 7        | 0.34          |
| (3,60)  | 1:11:A:TRP:H   | 1:12:A:LEU:HD12 | 7        | 0.34          |
| (3,60)  | 1:11:A:TRP:H   | 1:12:A:LEU:HD13 | 7        | 0.34          |
| (3,60)  | 1:11:A:TRP:H   | 1:12:A:LEU:HD11 | 8        | 0.34          |
| (3,60)  | 1:11:A:TRP:H   | 1:12:A:LEU:HD12 | 8        | 0.34          |
| (3,60)  | 1:11:A:TRP:H   | 1:12:A:LEU:HD13 | 8        | 0.34          |
| (3,31)  | 1:8:A:TYR:HE1  | 1:12:A:LEU:HD21 | 10       | 0.34          |
| (3,31)  | 1:8:A:TYR:HE1  | 1:12:A:LEU:HD22 | 10       | 0.34          |
| (3,31)  | 1:8:A:TYR:HE1  | 1:12:A:LEU:HD23 | 10       | 0.34          |
| (3,31)  | 1:8:A:TYR:HE2  | 1:12:A:LEU:HD21 | 10       | 0.34          |
| (3,31)  | 1:8:A:TYR:HE2  | 1:12:A:LEU:HD22 | 10       | 0.34          |
| (3,31)  | 1:8:A:TYR:HE2  | 1:12:A:LEU:HD23 | 10       | 0.34          |
| (2,445) | 1:1:A:GLU:HB2  | 1:2:A:GLU:HG2   | 2        | 0.34          |
| (2,206) | 1:21:A:ARG:H   | 1:21:A:ARG:HB3  | 5        | 0.34          |
| (1,543) | 1:5:A:VAL:HG21 | 1:6:A:ARG:HG3   | 3        | 0.34          |
| (1,543) | 1:5:A:VAL:HG22 | 1:6:A:ARG:HG3   | 3        | 0.34          |
| (1,543) | 1:5:A:VAL:HG23 | 1:6:A:ARG:HG3   | 3        | 0.34          |
| (1,512) | 1:1:A:GLU:HB2  | 1:2:A:GLU:HG2   | 2        | 0.34          |
| (1,480) | 1:6:A:ARG:HA   | 1:10:A:GLN:HB2  | 10       | 0.34          |
| (1,444) | 1:11:A:TRP:H   | 1:12:A:LEU:HD11 | 2        | 0.34          |
| (1,444) | 1:11:A:TRP:H   | 1:12:A:LEU:HD12 | 2        | 0.34          |
| (1,444) | 1:11:A:TRP:H   | 1:12:A:LEU:HD13 | 2        | 0.34          |
| (1,444) | 1:11:A:TRP:H   | 1:12:A:LEU:HD11 | 5        | 0.34          |
| (1,444) | 1:11:A:TRP:H   | 1:12:A:LEU:HD12 | 5        | 0.34          |
| (1,444) | 1:11:A:TRP:H   | 1:12:A:LEU:HD13 | 5        | 0.34          |
| (1,444) | 1:11:A:TRP:H   | 1:12:A:LEU:HD11 | 7        | 0.34          |
| (1,444) | 1:11:A:TRP:H   | 1:12:A:LEU:HD12 | 7        | 0.34          |
| (1,444) | 1:11:A:TRP:H   | 1:12:A:LEU:HD13 | 7        | 0.34          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,444) | 1:11:A:TRP:H   | 1:12:A:LEU:HD11 | 8        | 0.34          |
| (1,444) | 1:11:A:TRP:H   | 1:12:A:LEU:HD12 | 8        | 0.34          |
| (1,444) | 1:11:A:TRP:H   | 1:12:A:LEU:HD13 | 8        | 0.34          |
| (1,321) | 1:8:A:TYR:HE1  | 1:12:A:LEU:HD21 | 10       | 0.34          |
| (1,321) | 1:8:A:TYR:HE1  | 1:12:A:LEU:HD22 | 10       | 0.34          |
| (1,321) | 1:8:A:TYR:HE1  | 1:12:A:LEU:HD23 | 10       | 0.34          |
| (1,321) | 1:8:A:TYR:HE2  | 1:12:A:LEU:HD21 | 10       | 0.34          |
| (1,321) | 1:8:A:TYR:HE2  | 1:12:A:LEU:HD22 | 10       | 0.34          |
| (1,321) | 1:8:A:TYR:HE2  | 1:12:A:LEU:HD23 | 10       | 0.34          |
| (1,224) | 1:21:A:ARG:H   | 1:21:A:ARG:HB3  | 5        | 0.34          |
| (3,75)  | 1:5:A:VAL:HG21 | 1:6:A:ARG:HG3   | 9        | 0.33          |
| (3,75)  | 1:5:A:VAL:HG22 | 1:6:A:ARG:HG3   | 9        | 0.33          |
| (3,75)  | 1:5:A:VAL:HG23 | 1:6:A:ARG:HG3   | 9        | 0.33          |
| (3,60)  | 1:11:A:TRP:H   | 1:12:A:LEU:HD11 | 3        | 0.33          |
| (3,60)  | 1:11:A:TRP:H   | 1:12:A:LEU:HD12 | 3        | 0.33          |
| (3,60)  | 1:11:A:TRP:H   | 1:12:A:LEU:HD13 | 3        | 0.33          |
| (3,31)  | 1:8:A:TYR:HE1  | 1:12:A:LEU:HD21 | 3        | 0.33          |
| (3,31)  | 1:8:A:TYR:HE1  | 1:12:A:LEU:HD22 | 3        | 0.33          |
| (3,31)  | 1:8:A:TYR:HE1  | 1:12:A:LEU:HD23 | 3        | 0.33          |
| (3,31)  | 1:8:A:TYR:HE2  | 1:12:A:LEU:HD21 | 3        | 0.33          |
| (3,31)  | 1:8:A:TYR:HE2  | 1:12:A:LEU:HD22 | 3        | 0.33          |
| (3,31)  | 1:8:A:TYR:HE2  | 1:12:A:LEU:HD23 | 3        | 0.33          |
| (3,31)  | 1:8:A:TYR:HE1  | 1:12:A:LEU:HD21 | 9        | 0.33          |
| (3,31)  | 1:8:A:TYR:HE1  | 1:12:A:LEU:HD22 | 9        | 0.33          |
| (3,31)  | 1:8:A:TYR:HE1  | 1:12:A:LEU:HD23 | 9        | 0.33          |
| (3,31)  | 1:8:A:TYR:HE2  | 1:12:A:LEU:HD21 | 9        | 0.33          |
| (3,31)  | 1:8:A:TYR:HE2  | 1:12:A:LEU:HD22 | 9        | 0.33          |
| (3,31)  | 1:8:A:TYR:HE2  | 1:12:A:LEU:HD23 | 9        | 0.33          |
| (3,25)  | 1:8:A:TYR:HE1  | 1:12:A:LEU:HG   | 2        | 0.33          |
| (3,25)  | 1:8:A:TYR:HE2  | 1:12:A:LEU:HG   | 2        | 0.33          |
| (2,277) | 1:8:A:TYR:HE1  | 1:24:A:PRO:HD3  | 9        | 0.33          |
| (2,277) | 1:8:A:TYR:HE2  | 1:24:A:PRO:HD3  | 9        | 0.33          |
| (2,197) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD2  | 1        | 0.33          |
| (2,164) | 1:17:A:PRO:HB3 | 1:17:A:PRO:HD2  | 6        | 0.33          |
| (1,543) | 1:5:A:VAL:HG21 | 1:6:A:ARG:HG3   | 9        | 0.33          |
| (1,543) | 1:5:A:VAL:HG22 | 1:6:A:ARG:HG3   | 9        | 0.33          |
| (1,543) | 1:5:A:VAL:HG23 | 1:6:A:ARG:HG3   | 9        | 0.33          |
| (1,444) | 1:11:A:TRP:H   | 1:12:A:LEU:HD11 | 3        | 0.33          |
| (1,444) | 1:11:A:TRP:H   | 1:12:A:LEU:HD12 | 3        | 0.33          |
| (1,444) | 1:11:A:TRP:H   | 1:12:A:LEU:HD13 | 3        | 0.33          |
| (1,321) | 1:8:A:TYR:HE1  | 1:12:A:LEU:HD21 | 3        | 0.33          |
| (1,321) | 1:8:A:TYR:HE1  | 1:12:A:LEU:HD22 | 3        | 0.33          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,321) | 1:8:A:TYR:HE1  | 1:12:A:LEU:HD23 | 3        | 0.33          |
| (1,321) | 1:8:A:TYR:HE2  | 1:12:A:LEU:HD21 | 3        | 0.33          |
| (1,321) | 1:8:A:TYR:HE2  | 1:12:A:LEU:HD22 | 3        | 0.33          |
| (1,321) | 1:8:A:TYR:HE2  | 1:12:A:LEU:HD23 | 3        | 0.33          |
| (1,321) | 1:8:A:TYR:HE1  | 1:12:A:LEU:HD21 | 9        | 0.33          |
| (1,321) | 1:8:A:TYR:HE1  | 1:12:A:LEU:HD22 | 9        | 0.33          |
| (1,321) | 1:8:A:TYR:HE1  | 1:12:A:LEU:HD23 | 9        | 0.33          |
| (1,321) | 1:8:A:TYR:HE2  | 1:12:A:LEU:HD21 | 9        | 0.33          |
| (1,321) | 1:8:A:TYR:HE2  | 1:12:A:LEU:HD22 | 9        | 0.33          |
| (1,321) | 1:8:A:TYR:HE2  | 1:12:A:LEU:HD23 | 9        | 0.33          |
| (1,310) | 1:8:A:TYR:HE1  | 1:12:A:LEU:HG   | 2        | 0.33          |
| (1,310) | 1:8:A:TYR:HE2  | 1:12:A:LEU:HG   | 2        | 0.33          |
| (1,300) | 1:8:A:TYR:HE1  | 1:24:A:PRO:HD3  | 9        | 0.33          |
| (1,300) | 1:8:A:TYR:HE2  | 1:24:A:PRO:HD3  | 9        | 0.33          |
| (1,214) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD2  | 1        | 0.33          |
| (1,179) | 1:17:A:PRO:HB3 | 1:17:A:PRO:HD2  | 6        | 0.33          |
| (3,91)  | 1:7:A:LEU:HD21 | 1:8:A:TYR:HB2   | 9        | 0.32          |
| (3,91)  | 1:7:A:LEU:HD22 | 1:8:A:TYR:HB2   | 9        | 0.32          |
| (3,91)  | 1:7:A:LEU:HD23 | 1:8:A:TYR:HB2   | 9        | 0.32          |
| (3,91)  | 1:7:A:LEU:HD21 | 1:8:A:TYR:HB2   | 10       | 0.32          |
| (3,91)  | 1:7:A:LEU:HD22 | 1:8:A:TYR:HB2   | 10       | 0.32          |
| (3,91)  | 1:7:A:LEU:HD23 | 1:8:A:TYR:HB2   | 10       | 0.32          |
| (3,60)  | 1:11:A:TRP:H   | 1:12:A:LEU:HD11 | 10       | 0.32          |
| (3,60)  | 1:11:A:TRP:H   | 1:12:A:LEU:HD12 | 10       | 0.32          |
| (3,60)  | 1:11:A:TRP:H   | 1:12:A:LEU:HD13 | 10       | 0.32          |
| (3,43)  | 1:8:A:TYR:HE1  | 1:11:A:TRP:HE3  | 9        | 0.32          |
| (3,43)  | 1:8:A:TYR:HE2  | 1:11:A:TRP:HE3  | 9        | 0.32          |
| (3,31)  | 1:8:A:TYR:HE1  | 1:12:A:LEU:HD21 | 5        | 0.32          |
| (3,31)  | 1:8:A:TYR:HE1  | 1:12:A:LEU:HD22 | 5        | 0.32          |
| (3,31)  | 1:8:A:TYR:HE1  | 1:12:A:LEU:HD23 | 5        | 0.32          |
| (3,31)  | 1:8:A:TYR:HE2  | 1:12:A:LEU:HD21 | 5        | 0.32          |
| (3,31)  | 1:8:A:TYR:HE2  | 1:12:A:LEU:HD22 | 5        | 0.32          |
| (3,31)  | 1:8:A:TYR:HE2  | 1:12:A:LEU:HD23 | 5        | 0.32          |
| (3,30)  | 1:7:A:LEU:HD11 | 1:8:A:TYR:HD1   | 10       | 0.32          |
| (3,30)  | 1:7:A:LEU:HD11 | 1:8:A:TYR:HD2   | 10       | 0.32          |
| (3,30)  | 1:7:A:LEU:HD12 | 1:8:A:TYR:HD1   | 10       | 0.32          |
| (3,30)  | 1:7:A:LEU:HD12 | 1:8:A:TYR:HD2   | 10       | 0.32          |
| (3,30)  | 1:7:A:LEU:HD13 | 1:8:A:TYR:HD1   | 10       | 0.32          |
| (3,30)  | 1:7:A:LEU:HD13 | 1:8:A:TYR:HD2   | 10       | 0.32          |
| (3,24)  | 1:11:A:TRP:HD1 | 1:21:A:ARG:HG2  | 7        | 0.32          |
| (3,24)  | 1:11:A:TRP:HD1 | 1:21:A:ARG:HG3  | 7        | 0.32          |
| (3,20)  | 1:8:A:TYR:HA   | 1:8:A:TYR:HE1   | 4        | 0.32          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (3,20)  | 1:8:A:TYR:HA   | 1:8:A:TYR:HE2   | 4        | 0.32          |
| (1,595) | 1:7:A:LEU:HD21 | 1:8:A:TYR:HB2   | 9        | 0.32          |
| (1,595) | 1:7:A:LEU:HD22 | 1:8:A:TYR:HB2   | 9        | 0.32          |
| (1,595) | 1:7:A:LEU:HD23 | 1:8:A:TYR:HB2   | 9        | 0.32          |
| (1,595) | 1:7:A:LEU:HD21 | 1:8:A:TYR:HB2   | 10       | 0.32          |
| (1,595) | 1:7:A:LEU:HD22 | 1:8:A:TYR:HB2   | 10       | 0.32          |
| (1,595) | 1:7:A:LEU:HD23 | 1:8:A:TYR:HB2   | 10       | 0.32          |
| (1,444) | 1:11:A:TRP:H   | 1:12:A:LEU:HD11 | 10       | 0.32          |
| (1,444) | 1:11:A:TRP:H   | 1:12:A:LEU:HD12 | 10       | 0.32          |
| (1,444) | 1:11:A:TRP:H   | 1:12:A:LEU:HD13 | 10       | 0.32          |
| (1,377) | 1:8:A:TYR:HE1  | 1:11:A:TRP:HE3  | 9        | 0.32          |
| (1,377) | 1:8:A:TYR:HE2  | 1:11:A:TRP:HE3  | 9        | 0.32          |
| (1,321) | 1:8:A:TYR:HE1  | 1:12:A:LEU:HD21 | 5        | 0.32          |
| (1,321) | 1:8:A:TYR:HE1  | 1:12:A:LEU:HD22 | 5        | 0.32          |
| (1,321) | 1:8:A:TYR:HE1  | 1:12:A:LEU:HD23 | 5        | 0.32          |
| (1,321) | 1:8:A:TYR:HE2  | 1:12:A:LEU:HD21 | 5        | 0.32          |
| (1,321) | 1:8:A:TYR:HE2  | 1:12:A:LEU:HD22 | 5        | 0.32          |
| (1,321) | 1:8:A:TYR:HE2  | 1:12:A:LEU:HD23 | 5        | 0.32          |
| (1,318) | 1:7:A:LEU:HD11 | 1:8:A:TYR:HD1   | 10       | 0.32          |
| (1,318) | 1:7:A:LEU:HD11 | 1:8:A:TYR:HD2   | 10       | 0.32          |
| (1,318) | 1:7:A:LEU:HD12 | 1:8:A:TYR:HD1   | 10       | 0.32          |
| (1,318) | 1:7:A:LEU:HD12 | 1:8:A:TYR:HD2   | 10       | 0.32          |
| (1,318) | 1:7:A:LEU:HD13 | 1:8:A:TYR:HD1   | 10       | 0.32          |
| (1,318) | 1:7:A:LEU:HD13 | 1:8:A:TYR:HD2   | 10       | 0.32          |
| (1,308) | 1:11:A:TRP:HD1 | 1:21:A:ARG:HG2  | 7        | 0.32          |
| (1,308) | 1:11:A:TRP:HD1 | 1:21:A:ARG:HG3  | 7        | 0.32          |
| (1,287) | 1:8:A:TYR:HA   | 1:8:A:TYR:HE1   | 4        | 0.32          |
| (1,287) | 1:8:A:TYR:HA   | 1:8:A:TYR:HE2   | 4        | 0.32          |
| (3,82)  | 1:6:A:ARG:HG3  | 1:7:A:LEU:HD21  | 10       | 0.31          |
| (3,82)  | 1:6:A:ARG:HG3  | 1:7:A:LEU:HD22  | 10       | 0.31          |
| (3,82)  | 1:6:A:ARG:HG3  | 1:7:A:LEU:HD23  | 10       | 0.31          |
| (3,79)  | 1:7:A:LEU:HD21 | 1:10:A:GLN:HB3  | 9        | 0.31          |
| (3,79)  | 1:7:A:LEU:HD22 | 1:10:A:GLN:HB3  | 9        | 0.31          |
| (3,79)  | 1:7:A:LEU:HD23 | 1:10:A:GLN:HB3  | 9        | 0.31          |
| (3,79)  | 1:7:A:LEU:HD21 | 1:10:A:GLN:HB3  | 10       | 0.31          |
| (3,79)  | 1:7:A:LEU:HD22 | 1:10:A:GLN:HB3  | 10       | 0.31          |
| (3,79)  | 1:7:A:LEU:HD23 | 1:10:A:GLN:HB3  | 10       | 0.31          |
| (3,75)  | 1:5:A:VAL:HG21 | 1:6:A:ARG:HG3   | 1        | 0.31          |
| (3,75)  | 1:5:A:VAL:HG22 | 1:6:A:ARG:HG3   | 1        | 0.31          |
| (3,75)  | 1:5:A:VAL:HG23 | 1:6:A:ARG:HG3   | 1        | 0.31          |
| (3,75)  | 1:5:A:VAL:HG21 | 1:6:A:ARG:HG3   | 2        | 0.31          |
| (3,75)  | 1:5:A:VAL:HG22 | 1:6:A:ARG:HG3   | 2        | 0.31          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (3,75)  | 1:5:A:VAL:HG23 | 1:6:A:ARG:HG3   | 2        | 0.31          |
| (3,67)  | 1:22:A:PRO:HG2 | 1:23:A:PRO:HD2  | 9        | 0.31          |
| (3,67)  | 1:22:A:PRO:HG2 | 1:23:A:PRO:HD3  | 9        | 0.31          |
| (3,67)  | 1:22:A:PRO:HG3 | 1:23:A:PRO:HD2  | 9        | 0.31          |
| (3,67)  | 1:22:A:PRO:HG3 | 1:23:A:PRO:HD3  | 9        | 0.31          |
| (3,31)  | 1:8:A:TYR:HE1  | 1:12:A:LEU:HD21 | 6        | 0.31          |
| (3,31)  | 1:8:A:TYR:HE1  | 1:12:A:LEU:HD22 | 6        | 0.31          |
| (3,31)  | 1:8:A:TYR:HE1  | 1:12:A:LEU:HD23 | 6        | 0.31          |
| (3,31)  | 1:8:A:TYR:HE2  | 1:12:A:LEU:HD21 | 6        | 0.31          |
| (3,31)  | 1:8:A:TYR:HE2  | 1:12:A:LEU:HD22 | 6        | 0.31          |
| (3,31)  | 1:8:A:TYR:HE2  | 1:12:A:LEU:HD23 | 6        | 0.31          |
| (3,20)  | 1:8:A:TYR:HA   | 1:8:A:TYR:HE1   | 2        | 0.31          |
| (3,20)  | 1:8:A:TYR:HA   | 1:8:A:TYR:HE2   | 2        | 0.31          |
| (2,127) | 1:13:A:LYS:HB2 | 1:13:A:LYS:HE2  | 7        | 0.31          |
| (2,127) | 1:13:A:LYS:HB3 | 1:13:A:LYS:HE2  | 7        | 0.31          |
| (2,127) | 1:13:A:LYS:HB3 | 1:13:A:LYS:HE3  | 7        | 0.31          |
| (1,560) | 1:6:A:ARG:HG3  | 1:7:A:LEU:HD21  | 10       | 0.31          |
| (1,560) | 1:6:A:ARG:HG3  | 1:7:A:LEU:HD22  | 10       | 0.31          |
| (1,560) | 1:6:A:ARG:HG3  | 1:7:A:LEU:HD23  | 10       | 0.31          |
| (1,555) | 1:7:A:LEU:HD21 | 1:10:A:GLN:HB3  | 9        | 0.31          |
| (1,555) | 1:7:A:LEU:HD22 | 1:10:A:GLN:HB3  | 9        | 0.31          |
| (1,555) | 1:7:A:LEU:HD23 | 1:10:A:GLN:HB3  | 9        | 0.31          |
| (1,555) | 1:7:A:LEU:HD21 | 1:10:A:GLN:HB3  | 10       | 0.31          |
| (1,555) | 1:7:A:LEU:HD22 | 1:10:A:GLN:HB3  | 10       | 0.31          |
| (1,555) | 1:7:A:LEU:HD23 | 1:10:A:GLN:HB3  | 10       | 0.31          |
| (1,543) | 1:5:A:VAL:HG21 | 1:6:A:ARG:HG3   | 1        | 0.31          |
| (1,543) | 1:5:A:VAL:HG22 | 1:6:A:ARG:HG3   | 1        | 0.31          |
| (1,543) | 1:5:A:VAL:HG23 | 1:6:A:ARG:HG3   | 1        | 0.31          |
| (1,543) | 1:5:A:VAL:HG21 | 1:6:A:ARG:HG3   | 2        | 0.31          |
| (1,543) | 1:5:A:VAL:HG22 | 1:6:A:ARG:HG3   | 2        | 0.31          |
| (1,543) | 1:5:A:VAL:HG23 | 1:6:A:ARG:HG3   | 2        | 0.31          |
| (1,491) | 1:22:A:PRO:HG2 | 1:23:A:PRO:HD2  | 9        | 0.31          |
| (1,491) | 1:22:A:PRO:HG2 | 1:23:A:PRO:HD3  | 9        | 0.31          |
| (1,491) | 1:22:A:PRO:HG3 | 1:23:A:PRO:HD2  | 9        | 0.31          |
| (1,491) | 1:22:A:PRO:HG3 | 1:23:A:PRO:HD3  | 9        | 0.31          |
| (1,321) | 1:8:A:TYR:HE1  | 1:12:A:LEU:HD21 | 6        | 0.31          |
| (1,321) | 1:8:A:TYR:HE1  | 1:12:A:LEU:HD22 | 6        | 0.31          |
| (1,321) | 1:8:A:TYR:HE1  | 1:12:A:LEU:HD23 | 6        | 0.31          |
| (1,321) | 1:8:A:TYR:HE2  | 1:12:A:LEU:HD21 | 6        | 0.31          |
| (1,321) | 1:8:A:TYR:HE2  | 1:12:A:LEU:HD22 | 6        | 0.31          |
| (1,321) | 1:8:A:TYR:HE2  | 1:12:A:LEU:HD23 | 6        | 0.31          |
| (1,287) | 1:8:A:TYR:HA   | 1:8:A:TYR:HE1   | 2        | 0.31          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,287) | 1:8:A:TYR:HA   | 1:8:A:TYR:HE2  | 2        | 0.31          |
| (1,141) | 1:13:A:LYS:HB2 | 1:13:A:LYS:HE2 | 7        | 0.31          |
| (1,141) | 1:13:A:LYS:HB3 | 1:13:A:LYS:HE2 | 7        | 0.31          |
| (1,141) | 1:13:A:LYS:HB3 | 1:13:A:LYS:HE3 | 7        | 0.31          |
| (3,67)  | 1:22:A:PRO:HG2 | 1:23:A:PRO:HD2 | 3        | 0.3           |
| (3,67)  | 1:22:A:PRO:HG2 | 1:23:A:PRO:HD3 | 3        | 0.3           |
| (3,67)  | 1:22:A:PRO:HG3 | 1:23:A:PRO:HD2 | 3        | 0.3           |
| (3,67)  | 1:22:A:PRO:HG3 | 1:23:A:PRO:HD3 | 3        | 0.3           |
| (3,53)  | 1:14:A:ASP:H   | 1:15:A:GLY:HA2 | 6        | 0.3           |
| (3,25)  | 1:8:A:TYR:HE1  | 1:12:A:LEU:HG  | 10       | 0.3           |
| (3,25)  | 1:8:A:TYR:HE2  | 1:12:A:LEU:HG  | 10       | 0.3           |
| (3,24)  | 1:11:A:TRP:HD1 | 1:21:A:ARG:HG2 | 2        | 0.3           |
| (3,24)  | 1:11:A:TRP:HD1 | 1:21:A:ARG:HG3 | 2        | 0.3           |
| (3,24)  | 1:11:A:TRP:HD1 | 1:21:A:ARG:HG2 | 5        | 0.3           |
| (3,24)  | 1:11:A:TRP:HD1 | 1:21:A:ARG:HG3 | 5        | 0.3           |
| (3,22)  | 1:8:A:TYR:HB2  | 1:8:A:TYR:HE1  | 10       | 0.3           |
| (3,22)  | 1:8:A:TYR:HB2  | 1:8:A:TYR:HE2  | 10       | 0.3           |
| (3,20)  | 1:8:A:TYR:HA   | 1:8:A:TYR:HE1  | 6        | 0.3           |
| (3,20)  | 1:8:A:TYR:HA   | 1:8:A:TYR:HE2  | 6        | 0.3           |
| (2,386) | 1:23:A:PRO:HB3 | 1:25:A:SER:H   | 7        | 0.3           |
| (2,351) | 1:3:A:GLU:HB2  | 1:4:A:ALA:H    | 4        | 0.3           |
| (2,292) | 1:8:A:TYR:HD1  | 1:23:A:PRO:HB2 | 2        | 0.3           |
| (2,292) | 1:8:A:TYR:HD2  | 1:23:A:PRO:HB2 | 2        | 0.3           |
| (2,292) | 1:8:A:TYR:HD1  | 1:23:A:PRO:HB2 | 7        | 0.3           |
| (2,292) | 1:8:A:TYR:HD2  | 1:23:A:PRO:HB2 | 7        | 0.3           |
| (2,277) | 1:8:A:TYR:HE1  | 1:24:A:PRO:HD3 | 10       | 0.3           |
| (2,277) | 1:8:A:TYR:HE2  | 1:24:A:PRO:HD3 | 10       | 0.3           |
| (2,127) | 1:13:A:LYS:HB2 | 1:13:A:LYS:HE2 | 9        | 0.3           |
| (2,127) | 1:13:A:LYS:HB3 | 1:13:A:LYS:HE2 | 9        | 0.3           |
| (2,127) | 1:13:A:LYS:HB3 | 1:13:A:LYS:HE3 | 9        | 0.3           |
| (2,127) | 1:13:A:LYS:HB2 | 1:13:A:LYS:HE2 | 10       | 0.3           |
| (2,127) | 1:13:A:LYS:HB3 | 1:13:A:LYS:HE2 | 10       | 0.3           |
| (2,127) | 1:13:A:LYS:HB3 | 1:13:A:LYS:HE3 | 10       | 0.3           |
| (1,491) | 1:22:A:PRO:HG2 | 1:23:A:PRO:HD2 | 3        | 0.3           |
| (1,491) | 1:22:A:PRO:HG2 | 1:23:A:PRO:HD3 | 3        | 0.3           |
| (1,491) | 1:22:A:PRO:HG3 | 1:23:A:PRO:HD2 | 3        | 0.3           |
| (1,491) | 1:22:A:PRO:HG3 | 1:23:A:PRO:HD3 | 3        | 0.3           |
| (1,448) | 1:23:A:PRO:HB3 | 1:25:A:SER:H   | 7        | 0.3           |
| (1,421) | 1:14:A:ASP:H   | 1:15:A:GLY:HA2 | 6        | 0.3           |
| (1,398) | 1:3:A:GLU:HB2  | 1:4:A:ALA:H    | 4        | 0.3           |
| (1,323) | 1:8:A:TYR:HD1  | 1:23:A:PRO:HB2 | 2        | 0.3           |
| (1,323) | 1:8:A:TYR:HD2  | 1:23:A:PRO:HB2 | 2        | 0.3           |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,323) | 1:8:A:TYR:HD1  | 1:23:A:PRO:HB2  | 7        | 0.3           |
| (1,323) | 1:8:A:TYR:HD2  | 1:23:A:PRO:HB2  | 7        | 0.3           |
| (1,310) | 1:8:A:TYR:HE1  | 1:12:A:LEU:HG   | 10       | 0.3           |
| (1,310) | 1:8:A:TYR:HE2  | 1:12:A:LEU:HG   | 10       | 0.3           |
| (1,308) | 1:11:A:TRP:HD1 | 1:21:A:ARG:HG2  | 2        | 0.3           |
| (1,308) | 1:11:A:TRP:HD1 | 1:21:A:ARG:HG3  | 2        | 0.3           |
| (1,308) | 1:11:A:TRP:HD1 | 1:21:A:ARG:HG2  | 5        | 0.3           |
| (1,308) | 1:11:A:TRP:HD1 | 1:21:A:ARG:HG3  | 5        | 0.3           |
| (1,300) | 1:8:A:TYR:HE1  | 1:24:A:PRO:HD3  | 10       | 0.3           |
| (1,300) | 1:8:A:TYR:HE2  | 1:24:A:PRO:HD3  | 10       | 0.3           |
| (1,296) | 1:8:A:TYR:HB2  | 1:8:A:TYR:HE1   | 10       | 0.3           |
| (1,296) | 1:8:A:TYR:HB2  | 1:8:A:TYR:HE2   | 10       | 0.3           |
| (1,287) | 1:8:A:TYR:HA   | 1:8:A:TYR:HE1   | 6        | 0.3           |
| (1,287) | 1:8:A:TYR:HA   | 1:8:A:TYR:HE2   | 6        | 0.3           |
| (1,141) | 1:13:A:LYS:HB2 | 1:13:A:LYS:HE2  | 9        | 0.3           |
| (1,141) | 1:13:A:LYS:HB3 | 1:13:A:LYS:HE2  | 9        | 0.3           |
| (1,141) | 1:13:A:LYS:HB3 | 1:13:A:LYS:HE3  | 9        | 0.3           |
| (1,141) | 1:13:A:LYS:HB2 | 1:13:A:LYS:HE2  | 10       | 0.3           |
| (1,141) | 1:13:A:LYS:HB3 | 1:13:A:LYS:HE2  | 10       | 0.3           |
| (1,141) | 1:13:A:LYS:HB3 | 1:13:A:LYS:HE3  | 10       | 0.3           |
| (3,88)  | 1:1:A:GLU:HB2  | 1:3:A:GLU:HA    | 1        | 0.29          |
| (3,80)  | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD11  | 8        | 0.29          |
| (3,80)  | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD12  | 8        | 0.29          |
| (3,80)  | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD13  | 8        | 0.29          |
| (3,80)  | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD11  | 8        | 0.29          |
| (3,80)  | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD12  | 8        | 0.29          |
| (3,80)  | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD13  | 8        | 0.29          |
| (3,80)  | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD11  | 8        | 0.29          |
| (3,80)  | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD12  | 8        | 0.29          |
| (3,80)  | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD13  | 8        | 0.29          |
| (3,77)  | 1:3:A:GLU:HG2  | 1:7:A:LEU:HD11  | 10       | 0.29          |
| (3,77)  | 1:3:A:GLU:HG2  | 1:7:A:LEU:HD12  | 10       | 0.29          |
| (3,77)  | 1:3:A:GLU:HG2  | 1:7:A:LEU:HD13  | 10       | 0.29          |
| (3,77)  | 1:3:A:GLU:HG3  | 1:7:A:LEU:HD11  | 10       | 0.29          |
| (3,77)  | 1:3:A:GLU:HG3  | 1:7:A:LEU:HD12  | 10       | 0.29          |
| (3,77)  | 1:3:A:GLU:HG3  | 1:7:A:LEU:HD13  | 10       | 0.29          |
| (3,62)  | 1:6:A:ARG:H    | 1:7:A:LEU:HD11  | 4        | 0.29          |
| (3,62)  | 1:6:A:ARG:H    | 1:7:A:LEU:HD12  | 4        | 0.29          |
| (3,62)  | 1:6:A:ARG:H    | 1:7:A:LEU:HD13  | 4        | 0.29          |
| (3,60)  | 1:11:A:TRP:H   | 1:12:A:LEU:HD11 | 6        | 0.29          |
| (3,60)  | 1:11:A:TRP:H   | 1:12:A:LEU:HD12 | 6        | 0.29          |
| (3,60)  | 1:11:A:TRP:H   | 1:12:A:LEU:HD13 | 6        | 0.29          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (3,60)  | 1:11:A:TRP:H   | 1:12:A:LEU:HD11 | 9        | 0.29          |
| (3,60)  | 1:11:A:TRP:H   | 1:12:A:LEU:HD12 | 9        | 0.29          |
| (3,60)  | 1:11:A:TRP:H   | 1:12:A:LEU:HD13 | 9        | 0.29          |
| (3,24)  | 1:11:A:TRP:HD1 | 1:21:A:ARG:HG2  | 4        | 0.29          |
| (3,24)  | 1:11:A:TRP:HD1 | 1:21:A:ARG:HG3  | 4        | 0.29          |
| (3,22)  | 1:8:A:TYR:HB2  | 1:8:A:TYR:HE1   | 9        | 0.29          |
| (3,22)  | 1:8:A:TYR:HB2  | 1:8:A:TYR:HE2   | 9        | 0.29          |
| (3,20)  | 1:8:A:TYR:HA   | 1:8:A:TYR:HE1   | 3        | 0.29          |
| (3,20)  | 1:8:A:TYR:HA   | 1:8:A:TYR:HE2   | 3        | 0.29          |
| (3,20)  | 1:8:A:TYR:HA   | 1:8:A:TYR:HE1   | 5        | 0.29          |
| (3,20)  | 1:8:A:TYR:HA   | 1:8:A:TYR:HE2   | 5        | 0.29          |
| (2,127) | 1:13:A:LYS:HB2 | 1:13:A:LYS:HE2  | 3        | 0.29          |
| (2,127) | 1:13:A:LYS:HB3 | 1:13:A:LYS:HE2  | 3        | 0.29          |
| (2,127) | 1:13:A:LYS:HB3 | 1:13:A:LYS:HE3  | 3        | 0.29          |
| (2,127) | 1:13:A:LYS:HB2 | 1:13:A:LYS:HE2  | 5        | 0.29          |
| (2,127) | 1:13:A:LYS:HB3 | 1:13:A:LYS:HE2  | 5        | 0.29          |
| (2,127) | 1:13:A:LYS:HB3 | 1:13:A:LYS:HE3  | 5        | 0.29          |
| (2,94)  | 1:10:A:GLN:H   | 1:10:A:GLN:HG2  | 2        | 0.29          |
| (2,94)  | 1:10:A:GLN:H   | 1:10:A:GLN:HG3  | 2        | 0.29          |
| (2,94)  | 1:10:A:GLN:H   | 1:10:A:GLN:HG2  | 3        | 0.29          |
| (2,94)  | 1:10:A:GLN:H   | 1:10:A:GLN:HG3  | 3        | 0.29          |
| (1,578) | 1:1:A:GLU:HB2  | 1:3:A:GLU:HA    | 1        | 0.29          |
| (1,558) | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD11  | 8        | 0.29          |
| (1,558) | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD12  | 8        | 0.29          |
| (1,558) | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD13  | 8        | 0.29          |
| (1,558) | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD11  | 8        | 0.29          |
| (1,558) | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD12  | 8        | 0.29          |
| (1,558) | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD13  | 8        | 0.29          |
| (1,558) | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD11  | 8        | 0.29          |
| (1,558) | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD12  | 8        | 0.29          |
| (1,558) | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD13  | 8        | 0.29          |
| (1,552) | 1:3:A:GLU:HG2  | 1:7:A:LEU:HD11  | 10       | 0.29          |
| (1,552) | 1:3:A:GLU:HG2  | 1:7:A:LEU:HD12  | 10       | 0.29          |
| (1,552) | 1:3:A:GLU:HG2  | 1:7:A:LEU:HD13  | 10       | 0.29          |
| (1,552) | 1:3:A:GLU:HG3  | 1:7:A:LEU:HD11  | 10       | 0.29          |
| (1,552) | 1:3:A:GLU:HG3  | 1:7:A:LEU:HD12  | 10       | 0.29          |
| (1,552) | 1:3:A:GLU:HG3  | 1:7:A:LEU:HD13  | 10       | 0.29          |
| (1,447) | 1:6:A:ARG:H    | 1:7:A:LEU:HD11  | 4        | 0.29          |
| (1,447) | 1:6:A:ARG:H    | 1:7:A:LEU:HD12  | 4        | 0.29          |
| (1,447) | 1:6:A:ARG:H    | 1:7:A:LEU:HD13  | 4        | 0.29          |
| (1,444) | 1:11:A:TRP:H   | 1:12:A:LEU:HD11 | 6        | 0.29          |
| (1,444) | 1:11:A:TRP:H   | 1:12:A:LEU:HD12 | 6        | 0.29          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,444) | 1:11:A:TRP:H   | 1:12:A:LEU:HD13 | 6        | 0.29          |
| (1,444) | 1:11:A:TRP:H   | 1:12:A:LEU:HD11 | 9        | 0.29          |
| (1,444) | 1:11:A:TRP:H   | 1:12:A:LEU:HD12 | 9        | 0.29          |
| (1,444) | 1:11:A:TRP:H   | 1:12:A:LEU:HD13 | 9        | 0.29          |
| (1,308) | 1:11:A:TRP:HD1 | 1:21:A:ARG:HG2  | 4        | 0.29          |
| (1,308) | 1:11:A:TRP:HD1 | 1:21:A:ARG:HG3  | 4        | 0.29          |
| (1,296) | 1:8:A:TYR:HB2  | 1:8:A:TYR:HE1   | 9        | 0.29          |
| (1,296) | 1:8:A:TYR:HB2  | 1:8:A:TYR:HE2   | 9        | 0.29          |
| (1,287) | 1:8:A:TYR:HA   | 1:8:A:TYR:HE1   | 3        | 0.29          |
| (1,287) | 1:8:A:TYR:HA   | 1:8:A:TYR:HE2   | 3        | 0.29          |
| (1,287) | 1:8:A:TYR:HA   | 1:8:A:TYR:HE1   | 5        | 0.29          |
| (1,287) | 1:8:A:TYR:HA   | 1:8:A:TYR:HE2   | 5        | 0.29          |
| (1,141) | 1:13:A:LYS:HB2 | 1:13:A:LYS:HE2  | 3        | 0.29          |
| (1,141) | 1:13:A:LYS:HB3 | 1:13:A:LYS:HE2  | 3        | 0.29          |
| (1,141) | 1:13:A:LYS:HB3 | 1:13:A:LYS:HE3  | 3        | 0.29          |
| (1,141) | 1:13:A:LYS:HB2 | 1:13:A:LYS:HE2  | 5        | 0.29          |
| (1,141) | 1:13:A:LYS:HB3 | 1:13:A:LYS:HE2  | 5        | 0.29          |
| (1,141) | 1:13:A:LYS:HB3 | 1:13:A:LYS:HE3  | 5        | 0.29          |
| (1,104) | 1:10:A:GLN:H   | 1:10:A:GLN:HG2  | 2        | 0.29          |
| (1,104) | 1:10:A:GLN:H   | 1:10:A:GLN:HG3  | 2        | 0.29          |
| (1,104) | 1:10:A:GLN:H   | 1:10:A:GLN:HG2  | 3        | 0.29          |
| (1,104) | 1:10:A:GLN:H   | 1:10:A:GLN:HG3  | 3        | 0.29          |
| (3,88)  | 1:1:A:GLU:HB2  | 1:3:A:GLU:HA    | 4        | 0.28          |
| (3,85)  | 1:7:A:LEU:HA   | 1:8:A:TYR:H     | 5        | 0.28          |
| (3,80)  | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD11  | 9        | 0.28          |
| (3,80)  | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD12  | 9        | 0.28          |
| (3,80)  | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD13  | 9        | 0.28          |
| (3,80)  | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD11  | 9        | 0.28          |
| (3,80)  | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD12  | 9        | 0.28          |
| (3,80)  | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD13  | 9        | 0.28          |
| (3,80)  | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD11  | 9        | 0.28          |
| (3,80)  | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD12  | 9        | 0.28          |
| (3,80)  | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD13  | 9        | 0.28          |
| (3,80)  | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD11  | 10       | 0.28          |
| (3,80)  | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD12  | 10       | 0.28          |
| (3,80)  | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD13  | 10       | 0.28          |
| (3,80)  | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD11  | 10       | 0.28          |
| (3,80)  | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD12  | 10       | 0.28          |
| (3,80)  | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD13  | 10       | 0.28          |
| (3,80)  | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD11  | 10       | 0.28          |
| (3,80)  | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD12  | 10       | 0.28          |
| (3,80)  | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD13  | 10       | 0.28          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (3,64)  | 1:6:A:ARG:HA   | 1:10:A:GLN:HB2  | 9        | 0.28          |
| (3,53)  | 1:14:A:ASP:H   | 1:15:A:GLY:HA2  | 10       | 0.28          |
| (3,31)  | 1:8:A:TYR:HE1  | 1:12:A:LEU:HD21 | 2        | 0.28          |
| (3,31)  | 1:8:A:TYR:HE1  | 1:12:A:LEU:HD22 | 2        | 0.28          |
| (3,31)  | 1:8:A:TYR:HE1  | 1:12:A:LEU:HD23 | 2        | 0.28          |
| (3,31)  | 1:8:A:TYR:HE2  | 1:12:A:LEU:HD21 | 2        | 0.28          |
| (3,31)  | 1:8:A:TYR:HE2  | 1:12:A:LEU:HD22 | 2        | 0.28          |
| (3,31)  | 1:8:A:TYR:HE2  | 1:12:A:LEU:HD23 | 2        | 0.28          |
| (3,14)  | 1:13:A:LYS:HA  | 1:13:A:LYS:HD2  | 8        | 0.28          |
| (3,14)  | 1:13:A:LYS:HA  | 1:13:A:LYS:HD3  | 8        | 0.28          |
| (2,387) | 1:24:A:PRO:HB3 | 1:25:A:SER:H    | 1        | 0.28          |
| (2,127) | 1:13:A:LYS:HB2 | 1:13:A:LYS:HE2  | 1        | 0.28          |
| (2,127) | 1:13:A:LYS:HB3 | 1:13:A:LYS:HE2  | 1        | 0.28          |
| (2,127) | 1:13:A:LYS:HB3 | 1:13:A:LYS:HE3  | 1        | 0.28          |
| (2,127) | 1:13:A:LYS:HB2 | 1:13:A:LYS:HE2  | 2        | 0.28          |
| (2,127) | 1:13:A:LYS:HB3 | 1:13:A:LYS:HE2  | 2        | 0.28          |
| (2,127) | 1:13:A:LYS:HB3 | 1:13:A:LYS:HE3  | 2        | 0.28          |
| (2,127) | 1:13:A:LYS:HB2 | 1:13:A:LYS:HE2  | 6        | 0.28          |
| (2,127) | 1:13:A:LYS:HB3 | 1:13:A:LYS:HE2  | 6        | 0.28          |
| (2,127) | 1:13:A:LYS:HB3 | 1:13:A:LYS:HE3  | 6        | 0.28          |
| (2,127) | 1:13:A:LYS:HB2 | 1:13:A:LYS:HE2  | 8        | 0.28          |
| (2,127) | 1:13:A:LYS:HB3 | 1:13:A:LYS:HE2  | 8        | 0.28          |
| (2,127) | 1:13:A:LYS:HB3 | 1:13:A:LYS:HE3  | 8        | 0.28          |
| (2,94)  | 1:10:A:GLN:H   | 1:10:A:GLN:HG2  | 1        | 0.28          |
| (2,94)  | 1:10:A:GLN:H   | 1:10:A:GLN:HG3  | 1        | 0.28          |
| (1,578) | 1:1:A:GLU:HB2  | 1:3:A:GLU:HA    | 4        | 0.28          |
| (1,570) | 1:7:A:LEU:HA   | 1:8:A:TYR:H     | 5        | 0.28          |
| (1,558) | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD11  | 9        | 0.28          |
| (1,558) | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD12  | 9        | 0.28          |
| (1,558) | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD13  | 9        | 0.28          |
| (1,558) | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD11  | 9        | 0.28          |
| (1,558) | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD12  | 9        | 0.28          |
| (1,558) | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD13  | 9        | 0.28          |
| (1,558) | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD11  | 9        | 0.28          |
| (1,558) | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD12  | 9        | 0.28          |
| (1,558) | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD13  | 9        | 0.28          |
| (1,558) | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD11  | 10       | 0.28          |
| (1,558) | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD12  | 10       | 0.28          |
| (1,558) | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD13  | 10       | 0.28          |
| (1,558) | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD11  | 10       | 0.28          |
| (1,558) | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD12  | 10       | 0.28          |
| (1,558) | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD13  | 10       | 0.28          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,558) | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD11  | 10       | 0.28          |
| (1,558) | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD12  | 10       | 0.28          |
| (1,558) | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD13  | 10       | 0.28          |
| (1,480) | 1:6:A:ARG:HA   | 1:10:A:GLN:HB2  | 9        | 0.28          |
| (1,449) | 1:24:A:PRO:HB3 | 1:25:A:SER:H    | 1        | 0.28          |
| (1,421) | 1:14:A:ASP:H   | 1:15:A:GLY:HA2  | 10       | 0.28          |
| (1,321) | 1:8:A:TYR:HE1  | 1:12:A:LEU:HD21 | 2        | 0.28          |
| (1,321) | 1:8:A:TYR:HE1  | 1:12:A:LEU:HD22 | 2        | 0.28          |
| (1,321) | 1:8:A:TYR:HE1  | 1:12:A:LEU:HD23 | 2        | 0.28          |
| (1,321) | 1:8:A:TYR:HE2  | 1:12:A:LEU:HD21 | 2        | 0.28          |
| (1,321) | 1:8:A:TYR:HE2  | 1:12:A:LEU:HD22 | 2        | 0.28          |
| (1,321) | 1:8:A:TYR:HE2  | 1:12:A:LEU:HD23 | 2        | 0.28          |
| (1,141) | 1:13:A:LYS:HB2 | 1:13:A:LYS:HE2  | 1        | 0.28          |
| (1,141) | 1:13:A:LYS:HB3 | 1:13:A:LYS:HE2  | 1        | 0.28          |
| (1,141) | 1:13:A:LYS:HB3 | 1:13:A:LYS:HE3  | 1        | 0.28          |
| (1,141) | 1:13:A:LYS:HB2 | 1:13:A:LYS:HE2  | 2        | 0.28          |
| (1,141) | 1:13:A:LYS:HB3 | 1:13:A:LYS:HE2  | 2        | 0.28          |
| (1,141) | 1:13:A:LYS:HB3 | 1:13:A:LYS:HE3  | 2        | 0.28          |
| (1,141) | 1:13:A:LYS:HB2 | 1:13:A:LYS:HE2  | 6        | 0.28          |
| (1,141) | 1:13:A:LYS:HB3 | 1:13:A:LYS:HE2  | 6        | 0.28          |
| (1,141) | 1:13:A:LYS:HB3 | 1:13:A:LYS:HE3  | 6        | 0.28          |
| (1,141) | 1:13:A:LYS:HB2 | 1:13:A:LYS:HE2  | 8        | 0.28          |
| (1,141) | 1:13:A:LYS:HB3 | 1:13:A:LYS:HE2  | 8        | 0.28          |
| (1,141) | 1:13:A:LYS:HB3 | 1:13:A:LYS:HE3  | 8        | 0.28          |
| (1,138) | 1:13:A:LYS:HA  | 1:13:A:LYS:HD2  | 8        | 0.28          |
| (1,138) | 1:13:A:LYS:HA  | 1:13:A:LYS:HD3  | 8        | 0.28          |
| (1,104) | 1:10:A:GLN:H   | 1:10:A:GLN:HG2  | 1        | 0.28          |
| (1,104) | 1:10:A:GLN:H   | 1:10:A:GLN:HG3  | 1        | 0.28          |
| (3,93)  | 1:10:A:GLN:HA  | 1:13:A:LYS:H    | 9        | 0.27          |
| (3,85)  | 1:7:A:LEU:HA   | 1:8:A:TYR:H     | 1        | 0.27          |
| (3,85)  | 1:7:A:LEU:HA   | 1:8:A:TYR:H     | 3        | 0.27          |
| (3,85)  | 1:7:A:LEU:HA   | 1:8:A:TYR:H     | 4        | 0.27          |
| (3,85)  | 1:7:A:LEU:HA   | 1:8:A:TYR:H     | 7        | 0.27          |
| (3,85)  | 1:7:A:LEU:HA   | 1:8:A:TYR:H     | 8        | 0.27          |
| (3,85)  | 1:7:A:LEU:HA   | 1:8:A:TYR:H     | 9        | 0.27          |
| (3,85)  | 1:7:A:LEU:HA   | 1:8:A:TYR:H     | 10       | 0.27          |
| (3,80)  | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD11  | 5        | 0.27          |
| (3,80)  | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD12  | 5        | 0.27          |
| (3,80)  | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD13  | 5        | 0.27          |
| (3,80)  | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD11  | 5        | 0.27          |
| (3,80)  | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD12  | 5        | 0.27          |
| (3,80)  | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD13  | 5        | 0.27          |

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| Key    | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|--------|----------------|----------------|----------|---------------|
| (3,80) | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD11 | 5        | 0.27          |
| (3,80) | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD12 | 5        | 0.27          |
| (3,80) | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD13 | 5        | 0.27          |
| (3,80) | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD11 | 7        | 0.27          |
| (3,80) | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD12 | 7        | 0.27          |
| (3,80) | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD13 | 7        | 0.27          |
| (3,80) | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD11 | 7        | 0.27          |
| (3,80) | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD12 | 7        | 0.27          |
| (3,80) | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD13 | 7        | 0.27          |
| (3,80) | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD11 | 7        | 0.27          |
| (3,80) | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD12 | 7        | 0.27          |
| (3,80) | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD13 | 7        | 0.27          |
| (3,79) | 1:7:A:LEU:HD21 | 1:10:A:GLN:HB3 | 5        | 0.27          |
| (3,79) | 1:7:A:LEU:HD22 | 1:10:A:GLN:HB3 | 5        | 0.27          |
| (3,79) | 1:7:A:LEU:HD23 | 1:10:A:GLN:HB3 | 5        | 0.27          |
| (3,79) | 1:7:A:LEU:HD21 | 1:10:A:GLN:HB3 | 7        | 0.27          |
| (3,79) | 1:7:A:LEU:HD22 | 1:10:A:GLN:HB3 | 7        | 0.27          |
| (3,79) | 1:7:A:LEU:HD23 | 1:10:A:GLN:HB3 | 7        | 0.27          |
| (3,79) | 1:7:A:LEU:HD21 | 1:10:A:GLN:HB3 | 8        | 0.27          |
| (3,79) | 1:7:A:LEU:HD22 | 1:10:A:GLN:HB3 | 8        | 0.27          |
| (3,79) | 1:7:A:LEU:HD23 | 1:10:A:GLN:HB3 | 8        | 0.27          |
| (3,75) | 1:5:A:VAL:HG21 | 1:6:A:ARG:HG3  | 7        | 0.27          |
| (3,75) | 1:5:A:VAL:HG22 | 1:6:A:ARG:HG3  | 7        | 0.27          |
| (3,75) | 1:5:A:VAL:HG23 | 1:6:A:ARG:HG3  | 7        | 0.27          |
| (3,75) | 1:5:A:VAL:HG21 | 1:6:A:ARG:HG3  | 8        | 0.27          |
| (3,75) | 1:5:A:VAL:HG22 | 1:6:A:ARG:HG3  | 8        | 0.27          |
| (3,75) | 1:5:A:VAL:HG23 | 1:6:A:ARG:HG3  | 8        | 0.27          |
| (3,73) | 1:2:A:GLU:HG2  | 1:5:A:VAL:HG21 | 10       | 0.27          |
| (3,73) | 1:2:A:GLU:HG2  | 1:5:A:VAL:HG22 | 10       | 0.27          |
| (3,73) | 1:2:A:GLU:HG2  | 1:5:A:VAL:HG23 | 10       | 0.27          |
| (3,73) | 1:2:A:GLU:HG3  | 1:5:A:VAL:HG21 | 10       | 0.27          |
| (3,73) | 1:2:A:GLU:HG3  | 1:5:A:VAL:HG22 | 10       | 0.27          |
| (3,73) | 1:2:A:GLU:HG3  | 1:5:A:VAL:HG23 | 10       | 0.27          |
| (3,67) | 1:22:A:PRO:HG2 | 1:23:A:PRO:HD2 | 2        | 0.27          |
| (3,67) | 1:22:A:PRO:HG2 | 1:23:A:PRO:HD3 | 2        | 0.27          |
| (3,67) | 1:22:A:PRO:HG3 | 1:23:A:PRO:HD2 | 2        | 0.27          |
| (3,67) | 1:22:A:PRO:HG3 | 1:23:A:PRO:HD3 | 2        | 0.27          |
| (3,67) | 1:22:A:PRO:HG2 | 1:23:A:PRO:HD2 | 5        | 0.27          |
| (3,67) | 1:22:A:PRO:HG2 | 1:23:A:PRO:HD3 | 5        | 0.27          |
| (3,67) | 1:22:A:PRO:HG3 | 1:23:A:PRO:HD2 | 5        | 0.27          |
| (3,67) | 1:22:A:PRO:HG3 | 1:23:A:PRO:HD3 | 5        | 0.27          |
| (3,67) | 1:22:A:PRO:HG2 | 1:23:A:PRO:HD2 | 6        | 0.27          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (3,67)  | 1:22:A:PRO:HG2 | 1:23:A:PRO:HD3 | 6        | 0.27          |
| (3,67)  | 1:22:A:PRO:HG3 | 1:23:A:PRO:HD2 | 6        | 0.27          |
| (3,67)  | 1:22:A:PRO:HG3 | 1:23:A:PRO:HD3 | 6        | 0.27          |
| (3,67)  | 1:22:A:PRO:HG2 | 1:23:A:PRO:HD2 | 10       | 0.27          |
| (3,67)  | 1:22:A:PRO:HG2 | 1:23:A:PRO:HD3 | 10       | 0.27          |
| (3,67)  | 1:22:A:PRO:HG3 | 1:23:A:PRO:HD2 | 10       | 0.27          |
| (3,67)  | 1:22:A:PRO:HG3 | 1:23:A:PRO:HD3 | 10       | 0.27          |
| (3,53)  | 1:14:A:ASP:H   | 1:15:A:GLY:HA2 | 1        | 0.27          |
| (3,53)  | 1:14:A:ASP:H   | 1:15:A:GLY:HA2 | 3        | 0.27          |
| (3,53)  | 1:14:A:ASP:H   | 1:15:A:GLY:HA2 | 5        | 0.27          |
| (3,49)  | 1:9:A:ILE:H    | 1:9:A:ILE:HG12 | 2        | 0.27          |
| (3,49)  | 1:9:A:ILE:H    | 1:9:A:ILE:HG12 | 3        | 0.27          |
| (3,49)  | 1:9:A:ILE:H    | 1:9:A:ILE:HG12 | 4        | 0.27          |
| (3,49)  | 1:9:A:ILE:H    | 1:9:A:ILE:HG12 | 7        | 0.27          |
| (3,49)  | 1:9:A:ILE:H    | 1:9:A:ILE:HG12 | 9        | 0.27          |
| (3,49)  | 1:9:A:ILE:H    | 1:9:A:ILE:HG12 | 10       | 0.27          |
| (3,25)  | 1:8:A:TYR:HE1  | 1:12:A:LEU:HG  | 4        | 0.27          |
| (3,25)  | 1:8:A:TYR:HE2  | 1:12:A:LEU:HG  | 4        | 0.27          |
| (3,22)  | 1:8:A:TYR:HB2  | 1:8:A:TYR:HE1  | 8        | 0.27          |
| (3,22)  | 1:8:A:TYR:HB2  | 1:8:A:TYR:HE2  | 8        | 0.27          |
| (2,292) | 1:8:A:TYR:HD1  | 1:23:A:PRO:HB2 | 8        | 0.27          |
| (2,292) | 1:8:A:TYR:HD2  | 1:23:A:PRO:HB2 | 8        | 0.27          |
| (2,127) | 1:13:A:LYS:HB2 | 1:13:A:LYS:HE2 | 4        | 0.27          |
| (2,127) | 1:13:A:LYS:HB3 | 1:13:A:LYS:HE2 | 4        | 0.27          |
| (2,127) | 1:13:A:LYS:HB3 | 1:13:A:LYS:HE3 | 4        | 0.27          |
| (2,123) | 1:13:A:LYS:HA  | 1:13:A:LYS:HE2 | 9        | 0.27          |
| (2,123) | 1:13:A:LYS:HA  | 1:13:A:LYS:HE3 | 9        | 0.27          |
| (2,94)  | 1:10:A:GLN:H   | 1:10:A:GLN:HG2 | 6        | 0.27          |
| (2,94)  | 1:10:A:GLN:H   | 1:10:A:GLN:HG3 | 6        | 0.27          |
| (2,94)  | 1:10:A:GLN:H   | 1:10:A:GLN:HG2 | 8        | 0.27          |
| (2,94)  | 1:10:A:GLN:H   | 1:10:A:GLN:HG3 | 8        | 0.27          |
| (1,601) | 1:10:A:GLN:HA  | 1:13:A:LYS:H   | 9        | 0.27          |
| (1,570) | 1:7:A:LEU:HA   | 1:8:A:TYR:H    | 1        | 0.27          |
| (1,570) | 1:7:A:LEU:HA   | 1:8:A:TYR:H    | 3        | 0.27          |
| (1,570) | 1:7:A:LEU:HA   | 1:8:A:TYR:H    | 4        | 0.27          |
| (1,570) | 1:7:A:LEU:HA   | 1:8:A:TYR:H    | 7        | 0.27          |
| (1,570) | 1:7:A:LEU:HA   | 1:8:A:TYR:H    | 8        | 0.27          |
| (1,570) | 1:7:A:LEU:HA   | 1:8:A:TYR:H    | 9        | 0.27          |
| (1,570) | 1:7:A:LEU:HA   | 1:8:A:TYR:H    | 10       | 0.27          |
| (1,558) | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD11 | 5        | 0.27          |
| (1,558) | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD12 | 5        | 0.27          |
| (1,558) | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD13 | 5        | 0.27          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,558) | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD11 | 5        | 0.27          |
| (1,558) | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD12 | 5        | 0.27          |
| (1,558) | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD13 | 5        | 0.27          |
| (1,558) | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD11 | 5        | 0.27          |
| (1,558) | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD12 | 5        | 0.27          |
| (1,558) | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD13 | 5        | 0.27          |
| (1,558) | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD11 | 7        | 0.27          |
| (1,558) | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD12 | 7        | 0.27          |
| (1,558) | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD13 | 7        | 0.27          |
| (1,558) | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD11 | 7        | 0.27          |
| (1,558) | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD12 | 7        | 0.27          |
| (1,558) | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD13 | 7        | 0.27          |
| (1,558) | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD11 | 7        | 0.27          |
| (1,558) | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD12 | 7        | 0.27          |
| (1,558) | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD13 | 7        | 0.27          |
| (1,555) | 1:7:A:LEU:HD21 | 1:10:A:GLN:HB3 | 5        | 0.27          |
| (1,555) | 1:7:A:LEU:HD22 | 1:10:A:GLN:HB3 | 5        | 0.27          |
| (1,555) | 1:7:A:LEU:HD23 | 1:10:A:GLN:HB3 | 5        | 0.27          |
| (1,555) | 1:7:A:LEU:HD21 | 1:10:A:GLN:HB3 | 7        | 0.27          |
| (1,555) | 1:7:A:LEU:HD22 | 1:10:A:GLN:HB3 | 7        | 0.27          |
| (1,555) | 1:7:A:LEU:HD23 | 1:10:A:GLN:HB3 | 7        | 0.27          |
| (1,555) | 1:7:A:LEU:HD21 | 1:10:A:GLN:HB3 | 8        | 0.27          |
| (1,555) | 1:7:A:LEU:HD22 | 1:10:A:GLN:HB3 | 8        | 0.27          |
| (1,555) | 1:7:A:LEU:HD23 | 1:10:A:GLN:HB3 | 8        | 0.27          |
| (1,543) | 1:5:A:VAL:HG21 | 1:6:A:ARG:HG3  | 7        | 0.27          |
| (1,543) | 1:5:A:VAL:HG22 | 1:6:A:ARG:HG3  | 7        | 0.27          |
| (1,543) | 1:5:A:VAL:HG23 | 1:6:A:ARG:HG3  | 7        | 0.27          |
| (1,543) | 1:5:A:VAL:HG21 | 1:6:A:ARG:HG3  | 8        | 0.27          |
| (1,543) | 1:5:A:VAL:HG22 | 1:6:A:ARG:HG3  | 8        | 0.27          |
| (1,543) | 1:5:A:VAL:HG23 | 1:6:A:ARG:HG3  | 8        | 0.27          |
| (1,539) | 1:2:A:GLU:HG2  | 1:5:A:VAL:HG21 | 10       | 0.27          |
| (1,539) | 1:2:A:GLU:HG2  | 1:5:A:VAL:HG22 | 10       | 0.27          |
| (1,539) | 1:2:A:GLU:HG2  | 1:5:A:VAL:HG23 | 10       | 0.27          |
| (1,539) | 1:2:A:GLU:HG3  | 1:5:A:VAL:HG21 | 10       | 0.27          |
| (1,539) | 1:2:A:GLU:HG3  | 1:5:A:VAL:HG22 | 10       | 0.27          |
| (1,539) | 1:2:A:GLU:HG3  | 1:5:A:VAL:HG23 | 10       | 0.27          |
| (1,491) | 1:22:A:PRO:HG2 | 1:23:A:PRO:HD2 | 2        | 0.27          |
| (1,491) | 1:22:A:PRO:HG2 | 1:23:A:PRO:HD3 | 2        | 0.27          |
| (1,491) | 1:22:A:PRO:HG3 | 1:23:A:PRO:HD2 | 2        | 0.27          |
| (1,491) | 1:22:A:PRO:HG3 | 1:23:A:PRO:HD3 | 2        | 0.27          |
| (1,491) | 1:22:A:PRO:HG2 | 1:23:A:PRO:HD2 | 5        | 0.27          |
| (1,491) | 1:22:A:PRO:HG2 | 1:23:A:PRO:HD3 | 5        | 0.27          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,491) | 1:22:A:PRO:HG3 | 1:23:A:PRO:HD2 | 5        | 0.27          |
| (1,491) | 1:22:A:PRO:HG3 | 1:23:A:PRO:HD3 | 5        | 0.27          |
| (1,491) | 1:22:A:PRO:HG2 | 1:23:A:PRO:HD2 | 6        | 0.27          |
| (1,491) | 1:22:A:PRO:HG2 | 1:23:A:PRO:HD3 | 6        | 0.27          |
| (1,491) | 1:22:A:PRO:HG3 | 1:23:A:PRO:HD2 | 6        | 0.27          |
| (1,491) | 1:22:A:PRO:HG3 | 1:23:A:PRO:HD3 | 6        | 0.27          |
| (1,491) | 1:22:A:PRO:HG2 | 1:23:A:PRO:HD2 | 10       | 0.27          |
| (1,491) | 1:22:A:PRO:HG2 | 1:23:A:PRO:HD3 | 10       | 0.27          |
| (1,491) | 1:22:A:PRO:HG3 | 1:23:A:PRO:HD2 | 10       | 0.27          |
| (1,491) | 1:22:A:PRO:HG3 | 1:23:A:PRO:HD3 | 10       | 0.27          |
| (1,421) | 1:14:A:ASP:H   | 1:15:A:GLY:HA2 | 1        | 0.27          |
| (1,421) | 1:14:A:ASP:H   | 1:15:A:GLY:HA2 | 3        | 0.27          |
| (1,421) | 1:14:A:ASP:H   | 1:15:A:GLY:HA2 | 5        | 0.27          |
| (1,401) | 1:9:A:ILE:H    | 1:9:A:ILE:HG12 | 2        | 0.27          |
| (1,401) | 1:9:A:ILE:H    | 1:9:A:ILE:HG12 | 3        | 0.27          |
| (1,401) | 1:9:A:ILE:H    | 1:9:A:ILE:HG12 | 4        | 0.27          |
| (1,401) | 1:9:A:ILE:H    | 1:9:A:ILE:HG12 | 7        | 0.27          |
| (1,401) | 1:9:A:ILE:H    | 1:9:A:ILE:HG12 | 9        | 0.27          |
| (1,401) | 1:9:A:ILE:H    | 1:9:A:ILE:HG12 | 10       | 0.27          |
| (1,323) | 1:8:A:TYR:HD1  | 1:23:A:PRO:HB2 | 8        | 0.27          |
| (1,323) | 1:8:A:TYR:HD2  | 1:23:A:PRO:HB2 | 8        | 0.27          |
| (1,310) | 1:8:A:TYR:HE1  | 1:12:A:LEU:HG  | 4        | 0.27          |
| (1,310) | 1:8:A:TYR:HE2  | 1:12:A:LEU:HG  | 4        | 0.27          |
| (1,296) | 1:8:A:TYR:HB2  | 1:8:A:TYR:HE1  | 8        | 0.27          |
| (1,296) | 1:8:A:TYR:HB2  | 1:8:A:TYR:HE2  | 8        | 0.27          |
| (1,141) | 1:13:A:LYS:HB2 | 1:13:A:LYS:HE2 | 4        | 0.27          |
| (1,141) | 1:13:A:LYS:HB3 | 1:13:A:LYS:HE2 | 4        | 0.27          |
| (1,141) | 1:13:A:LYS:HB3 | 1:13:A:LYS:HE3 | 4        | 0.27          |
| (1,136) | 1:13:A:LYS:HA  | 1:13:A:LYS:HE2 | 9        | 0.27          |
| (1,136) | 1:13:A:LYS:HA  | 1:13:A:LYS:HE3 | 9        | 0.27          |
| (1,104) | 1:10:A:GLN:H   | 1:10:A:GLN:HG2 | 6        | 0.27          |
| (1,104) | 1:10:A:GLN:H   | 1:10:A:GLN:HG3 | 6        | 0.27          |
| (1,104) | 1:10:A:GLN:H   | 1:10:A:GLN:HG2 | 8        | 0.27          |
| (1,104) | 1:10:A:GLN:H   | 1:10:A:GLN:HG3 | 8        | 0.27          |
| (3,85)  | 1:7:A:LEU:HA   | 1:8:A:TYR:H    | 2        | 0.26          |
| (3,85)  | 1:7:A:LEU:HA   | 1:8:A:TYR:H    | 6        | 0.26          |
| (3,82)  | 1:6:A:ARG:HG3  | 1:7:A:LEU:HD21 | 9        | 0.26          |
| (3,82)  | 1:6:A:ARG:HG3  | 1:7:A:LEU:HD22 | 9        | 0.26          |
| (3,82)  | 1:6:A:ARG:HG3  | 1:7:A:LEU:HD23 | 9        | 0.26          |
| (3,80)  | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD11 | 6        | 0.26          |
| (3,80)  | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD12 | 6        | 0.26          |
| (3,80)  | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD13 | 6        | 0.26          |

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| Key    | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|--------|----------------|----------------|----------|---------------|
| (3,80) | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD11 | 6        | 0.26          |
| (3,80) | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD12 | 6        | 0.26          |
| (3,80) | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD13 | 6        | 0.26          |
| (3,80) | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD11 | 6        | 0.26          |
| (3,80) | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD12 | 6        | 0.26          |
| (3,80) | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD13 | 6        | 0.26          |
| (3,79) | 1:7:A:LEU:HD21 | 1:10:A:GLN:HB3 | 1        | 0.26          |
| (3,79) | 1:7:A:LEU:HD22 | 1:10:A:GLN:HB3 | 1        | 0.26          |
| (3,79) | 1:7:A:LEU:HD23 | 1:10:A:GLN:HB3 | 1        | 0.26          |
| (3,79) | 1:7:A:LEU:HD21 | 1:10:A:GLN:HB3 | 3        | 0.26          |
| (3,79) | 1:7:A:LEU:HD22 | 1:10:A:GLN:HB3 | 3        | 0.26          |
| (3,79) | 1:7:A:LEU:HD23 | 1:10:A:GLN:HB3 | 3        | 0.26          |
| (3,79) | 1:7:A:LEU:HD21 | 1:10:A:GLN:HB3 | 6        | 0.26          |
| (3,79) | 1:7:A:LEU:HD22 | 1:10:A:GLN:HB3 | 6        | 0.26          |
| (3,79) | 1:7:A:LEU:HD23 | 1:10:A:GLN:HB3 | 6        | 0.26          |
| (3,73) | 1:2:A:GLU:HG2  | 1:5:A:VAL:HG21 | 9        | 0.26          |
| (3,73) | 1:2:A:GLU:HG2  | 1:5:A:VAL:HG22 | 9        | 0.26          |
| (3,73) | 1:2:A:GLU:HG2  | 1:5:A:VAL:HG23 | 9        | 0.26          |
| (3,73) | 1:2:A:GLU:HG3  | 1:5:A:VAL:HG21 | 9        | 0.26          |
| (3,73) | 1:2:A:GLU:HG3  | 1:5:A:VAL:HG22 | 9        | 0.26          |
| (3,73) | 1:2:A:GLU:HG3  | 1:5:A:VAL:HG23 | 9        | 0.26          |
| (3,58) | 1:13:A:LYS:HD2 | 1:14:A:ASP:H   | 6        | 0.26          |
| (3,58) | 1:13:A:LYS:HD3 | 1:14:A:ASP:H   | 6        | 0.26          |
| (3,58) | 1:13:A:LYS:HD2 | 1:14:A:ASP:H   | 9        | 0.26          |
| (3,58) | 1:13:A:LYS:HD3 | 1:14:A:ASP:H   | 9        | 0.26          |
| (3,53) | 1:14:A:ASP:H   | 1:15:A:GLY:HA2 | 2        | 0.26          |
| (3,53) | 1:14:A:ASP:H   | 1:15:A:GLY:HA2 | 4        | 0.26          |
| (3,53) | 1:14:A:ASP:H   | 1:15:A:GLY:HA2 | 8        | 0.26          |
| (3,53) | 1:14:A:ASP:H   | 1:15:A:GLY:HA2 | 9        | 0.26          |
| (3,49) | 1:9:A:ILE:H    | 1:9:A:ILE:HG12 | 1        | 0.26          |
| (3,49) | 1:9:A:ILE:H    | 1:9:A:ILE:HG12 | 5        | 0.26          |
| (3,49) | 1:9:A:ILE:H    | 1:9:A:ILE:HG12 | 6        | 0.26          |
| (3,49) | 1:9:A:ILE:H    | 1:9:A:ILE:HG12 | 8        | 0.26          |
| (3,39) | 1:11:A:TRP:HH2 | 1:17:A:PRO:HD2 | 3        | 0.26          |
| (3,26) | 1:8:A:TYR:HE1  | 1:24:A:PRO:HG2 | 8        | 0.26          |
| (3,26) | 1:8:A:TYR:HE2  | 1:24:A:PRO:HG2 | 8        | 0.26          |
| (3,22) | 1:8:A:TYR:HB2  | 1:8:A:TYR:HE1  | 1        | 0.26          |
| (3,22) | 1:8:A:TYR:HB2  | 1:8:A:TYR:HE2  | 1        | 0.26          |
| (3,22) | 1:8:A:TYR:HB2  | 1:8:A:TYR:HE1  | 7        | 0.26          |
| (3,22) | 1:8:A:TYR:HB2  | 1:8:A:TYR:HE2  | 7        | 0.26          |
| (3,14) | 1:13:A:LYS:HA  | 1:13:A:LYS:HD2 | 6        | 0.26          |
| (3,14) | 1:13:A:LYS:HA  | 1:13:A:LYS:HD3 | 6        | 0.26          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (2,445) | 1:1:A:GLU:HB2  | 1:2:A:GLU:HG2  | 3        | 0.26          |
| (2,164) | 1:17:A:PRO:HB3 | 1:17:A:PRO:HD2 | 9        | 0.26          |
| (2,94)  | 1:10:A:GLN:H   | 1:10:A:GLN:HG2 | 4        | 0.26          |
| (2,94)  | 1:10:A:GLN:H   | 1:10:A:GLN:HG3 | 4        | 0.26          |
| (2,94)  | 1:10:A:GLN:H   | 1:10:A:GLN:HG2 | 5        | 0.26          |
| (2,94)  | 1:10:A:GLN:H   | 1:10:A:GLN:HG3 | 5        | 0.26          |
| (2,94)  | 1:10:A:GLN:H   | 1:10:A:GLN:HG2 | 7        | 0.26          |
| (2,94)  | 1:10:A:GLN:H   | 1:10:A:GLN:HG3 | 7        | 0.26          |
| (1,570) | 1:7:A:LEU:HA   | 1:8:A:TYR:H    | 2        | 0.26          |
| (1,570) | 1:7:A:LEU:HA   | 1:8:A:TYR:H    | 6        | 0.26          |
| (1,560) | 1:6:A:ARG:HG3  | 1:7:A:LEU:HD21 | 9        | 0.26          |
| (1,560) | 1:6:A:ARG:HG3  | 1:7:A:LEU:HD22 | 9        | 0.26          |
| (1,560) | 1:6:A:ARG:HG3  | 1:7:A:LEU:HD23 | 9        | 0.26          |
| (1,558) | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD11 | 6        | 0.26          |
| (1,558) | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD12 | 6        | 0.26          |
| (1,558) | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD13 | 6        | 0.26          |
| (1,558) | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD11 | 6        | 0.26          |
| (1,558) | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD12 | 6        | 0.26          |
| (1,558) | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD13 | 6        | 0.26          |
| (1,558) | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD11 | 6        | 0.26          |
| (1,558) | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD12 | 6        | 0.26          |
| (1,558) | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD13 | 6        | 0.26          |
| (1,555) | 1:7:A:LEU:HD21 | 1:10:A:GLN:HB3 | 1        | 0.26          |
| (1,555) | 1:7:A:LEU:HD22 | 1:10:A:GLN:HB3 | 1        | 0.26          |
| (1,555) | 1:7:A:LEU:HD23 | 1:10:A:GLN:HB3 | 1        | 0.26          |
| (1,555) | 1:7:A:LEU:HD21 | 1:10:A:GLN:HB3 | 3        | 0.26          |
| (1,555) | 1:7:A:LEU:HD22 | 1:10:A:GLN:HB3 | 3        | 0.26          |
| (1,555) | 1:7:A:LEU:HD23 | 1:10:A:GLN:HB3 | 3        | 0.26          |
| (1,555) | 1:7:A:LEU:HD21 | 1:10:A:GLN:HB3 | 6        | 0.26          |
| (1,555) | 1:7:A:LEU:HD22 | 1:10:A:GLN:HB3 | 6        | 0.26          |
| (1,555) | 1:7:A:LEU:HD23 | 1:10:A:GLN:HB3 | 6        | 0.26          |
| (1,539) | 1:2:A:GLU:HG2  | 1:5:A:VAL:HG21 | 9        | 0.26          |
| (1,539) | 1:2:A:GLU:HG2  | 1:5:A:VAL:HG22 | 9        | 0.26          |
| (1,539) | 1:2:A:GLU:HG2  | 1:5:A:VAL:HG23 | 9        | 0.26          |
| (1,539) | 1:2:A:GLU:HG3  | 1:5:A:VAL:HG21 | 9        | 0.26          |
| (1,539) | 1:2:A:GLU:HG3  | 1:5:A:VAL:HG22 | 9        | 0.26          |
| (1,539) | 1:2:A:GLU:HG3  | 1:5:A:VAL:HG23 | 9        | 0.26          |
| (1,512) | 1:1:A:GLU:HB2  | 1:2:A:GLU:HG2  | 3        | 0.26          |
| (1,437) | 1:13:A:LYS:HD2 | 1:14:A:ASP:H   | 6        | 0.26          |
| (1,437) | 1:13:A:LYS:HD3 | 1:14:A:ASP:H   | 6        | 0.26          |
| (1,437) | 1:13:A:LYS:HD2 | 1:14:A:ASP:H   | 9        | 0.26          |
| (1,437) | 1:13:A:LYS:HD3 | 1:14:A:ASP:H   | 9        | 0.26          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,421) | 1:14:A:ASP:H   | 1:15:A:GLY:HA2  | 2        | 0.26          |
| (1,421) | 1:14:A:ASP:H   | 1:15:A:GLY:HA2  | 4        | 0.26          |
| (1,421) | 1:14:A:ASP:H   | 1:15:A:GLY:HA2  | 8        | 0.26          |
| (1,421) | 1:14:A:ASP:H   | 1:15:A:GLY:HA2  | 9        | 0.26          |
| (1,401) | 1:9:A:ILE:H    | 1:9:A:ILE:HG12  | 1        | 0.26          |
| (1,401) | 1:9:A:ILE:H    | 1:9:A:ILE:HG12  | 5        | 0.26          |
| (1,401) | 1:9:A:ILE:H    | 1:9:A:ILE:HG12  | 6        | 0.26          |
| (1,401) | 1:9:A:ILE:H    | 1:9:A:ILE:HG12  | 8        | 0.26          |
| (1,354) | 1:11:A:TRP:HH2 | 1:17:A:PRO:HD2  | 3        | 0.26          |
| (1,311) | 1:8:A:TYR:HE1  | 1:24:A:PRO:HG2  | 8        | 0.26          |
| (1,311) | 1:8:A:TYR:HE2  | 1:24:A:PRO:HG2  | 8        | 0.26          |
| (1,296) | 1:8:A:TYR:HB2  | 1:8:A:TYR:HE1   | 1        | 0.26          |
| (1,296) | 1:8:A:TYR:HB2  | 1:8:A:TYR:HE2   | 1        | 0.26          |
| (1,296) | 1:8:A:TYR:HB2  | 1:8:A:TYR:HE1   | 7        | 0.26          |
| (1,296) | 1:8:A:TYR:HB2  | 1:8:A:TYR:HE2   | 7        | 0.26          |
| (1,179) | 1:17:A:PRO:HB3 | 1:17:A:PRO:HD2  | 9        | 0.26          |
| (1,138) | 1:13:A:LYS:HA  | 1:13:A:LYS:HD2  | 6        | 0.26          |
| (1,138) | 1:13:A:LYS:HA  | 1:13:A:LYS:HD3  | 6        | 0.26          |
| (1,104) | 1:10:A:GLN:H   | 1:10:A:GLN:HG2  | 4        | 0.26          |
| (1,104) | 1:10:A:GLN:H   | 1:10:A:GLN:HG3  | 4        | 0.26          |
| (1,104) | 1:10:A:GLN:H   | 1:10:A:GLN:HG2  | 5        | 0.26          |
| (1,104) | 1:10:A:GLN:H   | 1:10:A:GLN:HG3  | 5        | 0.26          |
| (1,104) | 1:10:A:GLN:H   | 1:10:A:GLN:HG2  | 7        | 0.26          |
| (1,104) | 1:10:A:GLN:H   | 1:10:A:GLN:HG3  | 7        | 0.26          |
| (3,93)  | 1:10:A:GLN:HA  | 1:13:A:LYS:H    | 10       | 0.25          |
| (3,84)  | 1:3:A:GLU:HA   | 1:7:A:LEU:H     | 1        | 0.25          |
| (3,70)  | 1:6:A:ARG:HA   | 1:9:A:ILE:HG21  | 9        | 0.25          |
| (3,70)  | 1:6:A:ARG:HA   | 1:9:A:ILE:HG22  | 9        | 0.25          |
| (3,70)  | 1:6:A:ARG:HA   | 1:9:A:ILE:HG23  | 9        | 0.25          |
| (3,70)  | 1:6:A:ARG:HA   | 1:9:A:ILE:HG21  | 10       | 0.25          |
| (3,70)  | 1:6:A:ARG:HA   | 1:9:A:ILE:HG22  | 10       | 0.25          |
| (3,70)  | 1:6:A:ARG:HA   | 1:9:A:ILE:HG23  | 10       | 0.25          |
| (3,58)  | 1:13:A:LYS:HD2 | 1:14:A:ASP:H    | 7        | 0.25          |
| (3,58)  | 1:13:A:LYS:HD3 | 1:14:A:ASP:H    | 7        | 0.25          |
| (3,53)  | 1:14:A:ASP:H   | 1:15:A:GLY:HA2  | 7        | 0.25          |
| (3,39)  | 1:11:A:TRP:HH2 | 1:17:A:PRO:HD2  | 1        | 0.25          |
| (3,39)  | 1:11:A:TRP:HH2 | 1:17:A:PRO:HD2  | 4        | 0.25          |
| (3,39)  | 1:11:A:TRP:HH2 | 1:17:A:PRO:HD2  | 7        | 0.25          |
| (3,39)  | 1:11:A:TRP:HH2 | 1:17:A:PRO:HD2  | 8        | 0.25          |
| (3,33)  | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD21 | 6        | 0.25          |
| (3,33)  | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD22 | 6        | 0.25          |
| (3,33)  | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD23 | 6        | 0.25          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (3,24)  | 1:11:A:TRP:HD1 | 1:21:A:ARG:HG2  | 8        | 0.25          |
| (3,24)  | 1:11:A:TRP:HD1 | 1:21:A:ARG:HG3  | 8        | 0.25          |
| (3,24)  | 1:11:A:TRP:HD1 | 1:21:A:ARG:HG2  | 9        | 0.25          |
| (3,24)  | 1:11:A:TRP:HD1 | 1:21:A:ARG:HG3  | 9        | 0.25          |
| (3,20)  | 1:8:A:TYR:HA   | 1:8:A:TYR:HE1   | 7        | 0.25          |
| (3,20)  | 1:8:A:TYR:HA   | 1:8:A:TYR:HE2   | 7        | 0.25          |
| (3,20)  | 1:8:A:TYR:HA   | 1:8:A:TYR:HE1   | 8        | 0.25          |
| (3,20)  | 1:8:A:TYR:HA   | 1:8:A:TYR:HE2   | 8        | 0.25          |
| (2,360) | 1:5:A:VAL:HG21 | 1:7:A:LEU:H     | 10       | 0.25          |
| (2,360) | 1:5:A:VAL:HG22 | 1:7:A:LEU:H     | 10       | 0.25          |
| (2,360) | 1:5:A:VAL:HG23 | 1:7:A:LEU:H     | 10       | 0.25          |
| (2,272) | 1:11:A:TRP:HD1 | 1:19:A:SER:HB3  | 4        | 0.25          |
| (2,164) | 1:17:A:PRO:HB3 | 1:17:A:PRO:HD2  | 1        | 0.25          |
| (2,164) | 1:17:A:PRO:HB3 | 1:17:A:PRO:HD2  | 2        | 0.25          |
| (2,123) | 1:13:A:LYS:HA  | 1:13:A:LYS:HE2  | 7        | 0.25          |
| (2,123) | 1:13:A:LYS:HA  | 1:13:A:LYS:HE3  | 7        | 0.25          |
| (1,601) | 1:10:A:GLN:HA  | 1:13:A:LYS:H    | 10       | 0.25          |
| (1,569) | 1:3:A:GLU:HA   | 1:7:A:LEU:H     | 1        | 0.25          |
| (1,521) | 1:6:A:ARG:HA   | 1:9:A:ILE:HG21  | 9        | 0.25          |
| (1,521) | 1:6:A:ARG:HA   | 1:9:A:ILE:HG22  | 9        | 0.25          |
| (1,521) | 1:6:A:ARG:HA   | 1:9:A:ILE:HG23  | 9        | 0.25          |
| (1,521) | 1:6:A:ARG:HA   | 1:9:A:ILE:HG21  | 10       | 0.25          |
| (1,521) | 1:6:A:ARG:HA   | 1:9:A:ILE:HG22  | 10       | 0.25          |
| (1,521) | 1:6:A:ARG:HA   | 1:9:A:ILE:HG23  | 10       | 0.25          |
| (1,437) | 1:13:A:LYS:HD2 | 1:14:A:ASP:H    | 7        | 0.25          |
| (1,437) | 1:13:A:LYS:HD3 | 1:14:A:ASP:H    | 7        | 0.25          |
| (1,421) | 1:14:A:ASP:H   | 1:15:A:GLY:HA2  | 7        | 0.25          |
| (1,411) | 1:5:A:VAL:HG21 | 1:7:A:LEU:H     | 10       | 0.25          |
| (1,411) | 1:5:A:VAL:HG22 | 1:7:A:LEU:H     | 10       | 0.25          |
| (1,411) | 1:5:A:VAL:HG23 | 1:7:A:LEU:H     | 10       | 0.25          |
| (1,354) | 1:11:A:TRP:HH2 | 1:17:A:PRO:HD2  | 1        | 0.25          |
| (1,354) | 1:11:A:TRP:HH2 | 1:17:A:PRO:HD2  | 4        | 0.25          |
| (1,354) | 1:11:A:TRP:HH2 | 1:17:A:PRO:HD2  | 7        | 0.25          |
| (1,354) | 1:11:A:TRP:HH2 | 1:17:A:PRO:HD2  | 8        | 0.25          |
| (1,329) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD21 | 6        | 0.25          |
| (1,329) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD22 | 6        | 0.25          |
| (1,329) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD23 | 6        | 0.25          |
| (1,308) | 1:11:A:TRP:HD1 | 1:21:A:ARG:HG2  | 8        | 0.25          |
| (1,308) | 1:11:A:TRP:HD1 | 1:21:A:ARG:HG3  | 8        | 0.25          |
| (1,308) | 1:11:A:TRP:HD1 | 1:21:A:ARG:HG2  | 9        | 0.25          |
| (1,308) | 1:11:A:TRP:HD1 | 1:21:A:ARG:HG3  | 9        | 0.25          |
| (1,293) | 1:11:A:TRP:HD1 | 1:19:A:SER:HB3  | 4        | 0.25          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,287) | 1:8:A:TYR:HA   | 1:8:A:TYR:HE1  | 7        | 0.25          |
| (1,287) | 1:8:A:TYR:HA   | 1:8:A:TYR:HE2  | 7        | 0.25          |
| (1,287) | 1:8:A:TYR:HA   | 1:8:A:TYR:HE1  | 8        | 0.25          |
| (1,287) | 1:8:A:TYR:HA   | 1:8:A:TYR:HE2  | 8        | 0.25          |
| (1,179) | 1:17:A:PRO:HB3 | 1:17:A:PRO:HD2 | 1        | 0.25          |
| (1,179) | 1:17:A:PRO:HB3 | 1:17:A:PRO:HD2 | 2        | 0.25          |
| (1,136) | 1:13:A:LYS:HA  | 1:13:A:LYS:HE2 | 7        | 0.25          |
| (1,136) | 1:13:A:LYS:HA  | 1:13:A:LYS:HE3 | 7        | 0.25          |
| (3,79)  | 1:7:A:LEU:HD21 | 1:10:A:GLN:HB3 | 4        | 0.24          |
| (3,79)  | 1:7:A:LEU:HD22 | 1:10:A:GLN:HB3 | 4        | 0.24          |
| (3,79)  | 1:7:A:LEU:HD23 | 1:10:A:GLN:HB3 | 4        | 0.24          |
| (3,77)  | 1:3:A:GLU:HG2  | 1:7:A:LEU:HD11 | 1        | 0.24          |
| (3,77)  | 1:3:A:GLU:HG2  | 1:7:A:LEU:HD12 | 1        | 0.24          |
| (3,77)  | 1:3:A:GLU:HG2  | 1:7:A:LEU:HD13 | 1        | 0.24          |
| (3,77)  | 1:3:A:GLU:HG3  | 1:7:A:LEU:HD11 | 1        | 0.24          |
| (3,77)  | 1:3:A:GLU:HG3  | 1:7:A:LEU:HD12 | 1        | 0.24          |
| (3,77)  | 1:3:A:GLU:HG3  | 1:7:A:LEU:HD13 | 1        | 0.24          |
| (3,75)  | 1:5:A:VAL:HG21 | 1:6:A:ARG:HG3  | 4        | 0.24          |
| (3,75)  | 1:5:A:VAL:HG22 | 1:6:A:ARG:HG3  | 4        | 0.24          |
| (3,75)  | 1:5:A:VAL:HG23 | 1:6:A:ARG:HG3  | 4        | 0.24          |
| (3,73)  | 1:2:A:GLU:HG2  | 1:5:A:VAL:HG21 | 5        | 0.24          |
| (3,73)  | 1:2:A:GLU:HG2  | 1:5:A:VAL:HG22 | 5        | 0.24          |
| (3,73)  | 1:2:A:GLU:HG2  | 1:5:A:VAL:HG23 | 5        | 0.24          |
| (3,73)  | 1:2:A:GLU:HG3  | 1:5:A:VAL:HG21 | 5        | 0.24          |
| (3,73)  | 1:2:A:GLU:HG3  | 1:5:A:VAL:HG22 | 5        | 0.24          |
| (3,73)  | 1:2:A:GLU:HG3  | 1:5:A:VAL:HG23 | 5        | 0.24          |
| (3,67)  | 1:22:A:PRO:HG2 | 1:23:A:PRO:HD2 | 1        | 0.24          |
| (3,67)  | 1:22:A:PRO:HG2 | 1:23:A:PRO:HD3 | 1        | 0.24          |
| (3,67)  | 1:22:A:PRO:HG3 | 1:23:A:PRO:HD2 | 1        | 0.24          |
| (3,67)  | 1:22:A:PRO:HG3 | 1:23:A:PRO:HD3 | 1        | 0.24          |
| (3,62)  | 1:6:A:ARG:H    | 1:7:A:LEU:HD11 | 10       | 0.24          |
| (3,62)  | 1:6:A:ARG:H    | 1:7:A:LEU:HD12 | 10       | 0.24          |
| (3,62)  | 1:6:A:ARG:H    | 1:7:A:LEU:HD13 | 10       | 0.24          |
| (3,39)  | 1:11:A:TRP:HH2 | 1:17:A:PRO:HD2 | 2        | 0.24          |
| (3,39)  | 1:11:A:TRP:HH2 | 1:17:A:PRO:HD2 | 5        | 0.24          |
| (3,39)  | 1:11:A:TRP:HH2 | 1:17:A:PRO:HD2 | 9        | 0.24          |
| (3,39)  | 1:11:A:TRP:HH2 | 1:17:A:PRO:HD2 | 10       | 0.24          |
| (3,28)  | 1:4:A:ALA:HB1  | 1:8:A:TYR:HE1  | 1        | 0.24          |
| (3,28)  | 1:4:A:ALA:HB1  | 1:8:A:TYR:HE2  | 1        | 0.24          |
| (3,28)  | 1:4:A:ALA:HB2  | 1:8:A:TYR:HE1  | 1        | 0.24          |
| (3,28)  | 1:4:A:ALA:HB2  | 1:8:A:TYR:HE2  | 1        | 0.24          |
| (3,28)  | 1:4:A:ALA:HB3  | 1:8:A:TYR:HE1  | 1        | 0.24          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (3,28)  | 1:4:A:ALA:HB3  | 1:8:A:TYR:HE2  | 1        | 0.24          |
| (3,28)  | 1:4:A:ALA:HB1  | 1:8:A:TYR:HE1  | 7        | 0.24          |
| (3,28)  | 1:4:A:ALA:HB1  | 1:8:A:TYR:HE2  | 7        | 0.24          |
| (3,28)  | 1:4:A:ALA:HB2  | 1:8:A:TYR:HE1  | 7        | 0.24          |
| (3,28)  | 1:4:A:ALA:HB2  | 1:8:A:TYR:HE2  | 7        | 0.24          |
| (3,28)  | 1:4:A:ALA:HB3  | 1:8:A:TYR:HE1  | 7        | 0.24          |
| (3,28)  | 1:4:A:ALA:HB3  | 1:8:A:TYR:HE2  | 7        | 0.24          |
| (3,22)  | 1:8:A:TYR:HB2  | 1:8:A:TYR:HE1  | 4        | 0.24          |
| (3,22)  | 1:8:A:TYR:HB2  | 1:8:A:TYR:HE2  | 4        | 0.24          |
| (3,22)  | 1:8:A:TYR:HB2  | 1:8:A:TYR:HE1  | 5        | 0.24          |
| (3,22)  | 1:8:A:TYR:HB2  | 1:8:A:TYR:HE2  | 5        | 0.24          |
| (3,22)  | 1:8:A:TYR:HB2  | 1:8:A:TYR:HE1  | 6        | 0.24          |
| (3,22)  | 1:8:A:TYR:HB2  | 1:8:A:TYR:HE2  | 6        | 0.24          |
| (3,14)  | 1:13:A:LYS:HA  | 1:13:A:LYS:HD2 | 1        | 0.24          |
| (3,14)  | 1:13:A:LYS:HA  | 1:13:A:LYS:HD3 | 1        | 0.24          |
| (3,14)  | 1:13:A:LYS:HA  | 1:13:A:LYS:HD2 | 4        | 0.24          |
| (3,14)  | 1:13:A:LYS:HA  | 1:13:A:LYS:HD3 | 4        | 0.24          |
| (2,414) | 1:14:A:ASP:HB2 | 1:19:A:SER:HB2 | 5        | 0.24          |
| (2,387) | 1:24:A:PRO:HB3 | 1:25:A:SER:H   | 4        | 0.24          |
| (2,387) | 1:24:A:PRO:HB3 | 1:25:A:SER:H   | 5        | 0.24          |
| (2,387) | 1:24:A:PRO:HB3 | 1:25:A:SER:H   | 9        | 0.24          |
| (2,283) | 1:11:A:TRP:HD1 | 1:21:A:ARG:HB3 | 7        | 0.24          |
| (2,164) | 1:17:A:PRO:HB3 | 1:17:A:PRO:HD2 | 4        | 0.24          |
| (2,164) | 1:17:A:PRO:HB3 | 1:17:A:PRO:HD2 | 8        | 0.24          |
| (1,555) | 1:7:A:LEU:HD21 | 1:10:A:GLN:HB3 | 4        | 0.24          |
| (1,555) | 1:7:A:LEU:HD22 | 1:10:A:GLN:HB3 | 4        | 0.24          |
| (1,555) | 1:7:A:LEU:HD23 | 1:10:A:GLN:HB3 | 4        | 0.24          |
| (1,552) | 1:3:A:GLU:HG2  | 1:7:A:LEU:HD11 | 1        | 0.24          |
| (1,552) | 1:3:A:GLU:HG2  | 1:7:A:LEU:HD12 | 1        | 0.24          |
| (1,552) | 1:3:A:GLU:HG2  | 1:7:A:LEU:HD13 | 1        | 0.24          |
| (1,552) | 1:3:A:GLU:HG3  | 1:7:A:LEU:HD11 | 1        | 0.24          |
| (1,552) | 1:3:A:GLU:HG3  | 1:7:A:LEU:HD12 | 1        | 0.24          |
| (1,552) | 1:3:A:GLU:HG3  | 1:7:A:LEU:HD13 | 1        | 0.24          |
| (1,543) | 1:5:A:VAL:HG21 | 1:6:A:ARG:HG3  | 4        | 0.24          |
| (1,543) | 1:5:A:VAL:HG22 | 1:6:A:ARG:HG3  | 4        | 0.24          |
| (1,543) | 1:5:A:VAL:HG23 | 1:6:A:ARG:HG3  | 4        | 0.24          |
| (1,539) | 1:2:A:GLU:HG2  | 1:5:A:VAL:HG21 | 5        | 0.24          |
| (1,539) | 1:2:A:GLU:HG2  | 1:5:A:VAL:HG22 | 5        | 0.24          |
| (1,539) | 1:2:A:GLU:HG2  | 1:5:A:VAL:HG23 | 5        | 0.24          |
| (1,539) | 1:2:A:GLU:HG3  | 1:5:A:VAL:HG21 | 5        | 0.24          |
| (1,539) | 1:2:A:GLU:HG3  | 1:5:A:VAL:HG22 | 5        | 0.24          |
| (1,539) | 1:2:A:GLU:HG3  | 1:5:A:VAL:HG23 | 5        | 0.24          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,491) | 1:22:A:PRO:HG2 | 1:23:A:PRO:HD2 | 1        | 0.24          |
| (1,491) | 1:22:A:PRO:HG2 | 1:23:A:PRO:HD3 | 1        | 0.24          |
| (1,491) | 1:22:A:PRO:HG3 | 1:23:A:PRO:HD2 | 1        | 0.24          |
| (1,491) | 1:22:A:PRO:HG3 | 1:23:A:PRO:HD3 | 1        | 0.24          |
| (1,477) | 1:14:A:ASP:HB2 | 1:19:A:SER:HB2 | 5        | 0.24          |
| (1,449) | 1:24:A:PRO:HB3 | 1:25:A:SER:H   | 4        | 0.24          |
| (1,449) | 1:24:A:PRO:HB3 | 1:25:A:SER:H   | 5        | 0.24          |
| (1,449) | 1:24:A:PRO:HB3 | 1:25:A:SER:H   | 9        | 0.24          |
| (1,447) | 1:6:A:ARG:H    | 1:7:A:LEU:HD11 | 10       | 0.24          |
| (1,447) | 1:6:A:ARG:H    | 1:7:A:LEU:HD12 | 10       | 0.24          |
| (1,447) | 1:6:A:ARG:H    | 1:7:A:LEU:HD13 | 10       | 0.24          |
| (1,354) | 1:11:A:TRP:HH2 | 1:17:A:PRO:HD2 | 2        | 0.24          |
| (1,354) | 1:11:A:TRP:HH2 | 1:17:A:PRO:HD2 | 5        | 0.24          |
| (1,354) | 1:11:A:TRP:HH2 | 1:17:A:PRO:HD2 | 9        | 0.24          |
| (1,354) | 1:11:A:TRP:HH2 | 1:17:A:PRO:HD2 | 10       | 0.24          |
| (1,315) | 1:4:A:ALA:HB1  | 1:8:A:TYR:HE1  | 1        | 0.24          |
| (1,315) | 1:4:A:ALA:HB1  | 1:8:A:TYR:HE2  | 1        | 0.24          |
| (1,315) | 1:4:A:ALA:HB2  | 1:8:A:TYR:HE1  | 1        | 0.24          |
| (1,315) | 1:4:A:ALA:HB2  | 1:8:A:TYR:HE2  | 1        | 0.24          |
| (1,315) | 1:4:A:ALA:HB3  | 1:8:A:TYR:HE1  | 1        | 0.24          |
| (1,315) | 1:4:A:ALA:HB3  | 1:8:A:TYR:HE2  | 1        | 0.24          |
| (1,315) | 1:4:A:ALA:HB1  | 1:8:A:TYR:HE1  | 7        | 0.24          |
| (1,315) | 1:4:A:ALA:HB1  | 1:8:A:TYR:HE2  | 7        | 0.24          |
| (1,315) | 1:4:A:ALA:HB2  | 1:8:A:TYR:HE1  | 7        | 0.24          |
| (1,315) | 1:4:A:ALA:HB2  | 1:8:A:TYR:HE2  | 7        | 0.24          |
| (1,315) | 1:4:A:ALA:HB3  | 1:8:A:TYR:HE1  | 7        | 0.24          |
| (1,315) | 1:4:A:ALA:HB3  | 1:8:A:TYR:HE2  | 7        | 0.24          |
| (1,306) | 1:11:A:TRP:HD1 | 1:21:A:ARG:HB3 | 7        | 0.24          |
| (1,296) | 1:8:A:TYR:HB2  | 1:8:A:TYR:HE1  | 4        | 0.24          |
| (1,296) | 1:8:A:TYR:HB2  | 1:8:A:TYR:HE2  | 4        | 0.24          |
| (1,296) | 1:8:A:TYR:HB2  | 1:8:A:TYR:HE1  | 5        | 0.24          |
| (1,296) | 1:8:A:TYR:HB2  | 1:8:A:TYR:HE2  | 5        | 0.24          |
| (1,296) | 1:8:A:TYR:HB2  | 1:8:A:TYR:HE1  | 6        | 0.24          |
| (1,296) | 1:8:A:TYR:HB2  | 1:8:A:TYR:HE2  | 6        | 0.24          |
| (1,179) | 1:17:A:PRO:HB3 | 1:17:A:PRO:HD2 | 4        | 0.24          |
| (1,179) | 1:17:A:PRO:HB3 | 1:17:A:PRO:HD2 | 8        | 0.24          |
| (1,138) | 1:13:A:LYS:HA  | 1:13:A:LYS:HD2 | 1        | 0.24          |
| (1,138) | 1:13:A:LYS:HA  | 1:13:A:LYS:HD3 | 1        | 0.24          |
| (1,138) | 1:13:A:LYS:HA  | 1:13:A:LYS:HD2 | 4        | 0.24          |
| (1,138) | 1:13:A:LYS:HA  | 1:13:A:LYS:HD3 | 4        | 0.24          |
| (3,88)  | 1:1:A:GLU:HB2  | 1:3:A:GLU:HA   | 3        | 0.23          |
| (3,79)  | 1:7:A:LEU:HD21 | 1:10:A:GLN:HB3 | 2        | 0.23          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (3,79)  | 1:7:A:LEU:HD22 | 1:10:A:GLN:HB3  | 2        | 0.23          |
| (3,79)  | 1:7:A:LEU:HD23 | 1:10:A:GLN:HB3  | 2        | 0.23          |
| (3,66)  | 1:22:A:PRO:HB3 | 1:23:A:PRO:HD2  | 8        | 0.23          |
| (3,66)  | 1:22:A:PRO:HB3 | 1:23:A:PRO:HD3  | 8        | 0.23          |
| (3,64)  | 1:6:A:ARG:HA   | 1:10:A:GLN:HB2  | 4        | 0.23          |
| (3,62)  | 1:6:A:ARG:H    | 1:7:A:LEU:HD11  | 9        | 0.23          |
| (3,62)  | 1:6:A:ARG:H    | 1:7:A:LEU:HD12  | 9        | 0.23          |
| (3,62)  | 1:6:A:ARG:H    | 1:7:A:LEU:HD13  | 9        | 0.23          |
| (3,58)  | 1:13:A:LYS:HD2 | 1:14:A:ASP:H    | 4        | 0.23          |
| (3,58)  | 1:13:A:LYS:HD3 | 1:14:A:ASP:H    | 4        | 0.23          |
| (3,31)  | 1:8:A:TYR:HE1  | 1:12:A:LEU:HD21 | 4        | 0.23          |
| (3,31)  | 1:8:A:TYR:HE1  | 1:12:A:LEU:HD22 | 4        | 0.23          |
| (3,31)  | 1:8:A:TYR:HE1  | 1:12:A:LEU:HD23 | 4        | 0.23          |
| (3,31)  | 1:8:A:TYR:HE2  | 1:12:A:LEU:HD21 | 4        | 0.23          |
| (3,31)  | 1:8:A:TYR:HE2  | 1:12:A:LEU:HD22 | 4        | 0.23          |
| (3,31)  | 1:8:A:TYR:HE2  | 1:12:A:LEU:HD23 | 4        | 0.23          |
| (3,25)  | 1:8:A:TYR:HE1  | 1:12:A:LEU:HG   | 7        | 0.23          |
| (3,25)  | 1:8:A:TYR:HE2  | 1:12:A:LEU:HG   | 7        | 0.23          |
| (3,25)  | 1:8:A:TYR:HE1  | 1:12:A:LEU:HG   | 9        | 0.23          |
| (3,25)  | 1:8:A:TYR:HE2  | 1:12:A:LEU:HG   | 9        | 0.23          |
| (3,22)  | 1:8:A:TYR:HB2  | 1:8:A:TYR:HE1   | 2        | 0.23          |
| (3,22)  | 1:8:A:TYR:HB2  | 1:8:A:TYR:HE2   | 2        | 0.23          |
| (3,22)  | 1:8:A:TYR:HB2  | 1:8:A:TYR:HE1   | 3        | 0.23          |
| (3,22)  | 1:8:A:TYR:HB2  | 1:8:A:TYR:HE2   | 3        | 0.23          |
| (3,14)  | 1:13:A:LYS:HA  | 1:13:A:LYS:HD2  | 5        | 0.23          |
| (3,14)  | 1:13:A:LYS:HA  | 1:13:A:LYS:HD3  | 5        | 0.23          |
| (2,485) | 1:16:A:GLY:H   | 1:19:A:SER:HB3  | 10       | 0.23          |
| (2,360) | 1:5:A:VAL:HG21 | 1:7:A:LEU:H     | 4        | 0.23          |
| (2,360) | 1:5:A:VAL:HG22 | 1:7:A:LEU:H     | 4        | 0.23          |
| (2,360) | 1:5:A:VAL:HG23 | 1:7:A:LEU:H     | 4        | 0.23          |
| (2,360) | 1:5:A:VAL:HG21 | 1:7:A:LEU:H     | 9        | 0.23          |
| (2,360) | 1:5:A:VAL:HG22 | 1:7:A:LEU:H     | 9        | 0.23          |
| (2,360) | 1:5:A:VAL:HG23 | 1:7:A:LEU:H     | 9        | 0.23          |
| (2,283) | 1:11:A:TRP:HD1 | 1:21:A:ARG:HB3  | 10       | 0.23          |
| (1,578) | 1:1:A:GLU:HB2  | 1:3:A:GLU:HA    | 3        | 0.23          |
| (1,568) | 1:16:A:GLY:H   | 1:19:A:SER:HB3  | 10       | 0.23          |
| (1,555) | 1:7:A:LEU:HD21 | 1:10:A:GLN:HB3  | 2        | 0.23          |
| (1,555) | 1:7:A:LEU:HD22 | 1:10:A:GLN:HB3  | 2        | 0.23          |
| (1,555) | 1:7:A:LEU:HD23 | 1:10:A:GLN:HB3  | 2        | 0.23          |
| (1,490) | 1:22:A:PRO:HB3 | 1:23:A:PRO:HD2  | 8        | 0.23          |
| (1,490) | 1:22:A:PRO:HB3 | 1:23:A:PRO:HD3  | 8        | 0.23          |
| (1,480) | 1:6:A:ARG:HA   | 1:10:A:GLN:HB2  | 4        | 0.23          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,447) | 1:6:A:ARG:H    | 1:7:A:LEU:HD11  | 9        | 0.23          |
| (1,447) | 1:6:A:ARG:H    | 1:7:A:LEU:HD12  | 9        | 0.23          |
| (1,447) | 1:6:A:ARG:H    | 1:7:A:LEU:HD13  | 9        | 0.23          |
| (1,437) | 1:13:A:LYS:HD2 | 1:14:A:ASP:H    | 4        | 0.23          |
| (1,437) | 1:13:A:LYS:HD3 | 1:14:A:ASP:H    | 4        | 0.23          |
| (1,411) | 1:5:A:VAL:HG21 | 1:7:A:LEU:H     | 4        | 0.23          |
| (1,411) | 1:5:A:VAL:HG22 | 1:7:A:LEU:H     | 4        | 0.23          |
| (1,411) | 1:5:A:VAL:HG23 | 1:7:A:LEU:H     | 4        | 0.23          |
| (1,411) | 1:5:A:VAL:HG21 | 1:7:A:LEU:H     | 9        | 0.23          |
| (1,411) | 1:5:A:VAL:HG22 | 1:7:A:LEU:H     | 9        | 0.23          |
| (1,411) | 1:5:A:VAL:HG23 | 1:7:A:LEU:H     | 9        | 0.23          |
| (1,321) | 1:8:A:TYR:HE1  | 1:12:A:LEU:HD21 | 4        | 0.23          |
| (1,321) | 1:8:A:TYR:HE1  | 1:12:A:LEU:HD22 | 4        | 0.23          |
| (1,321) | 1:8:A:TYR:HE1  | 1:12:A:LEU:HD23 | 4        | 0.23          |
| (1,321) | 1:8:A:TYR:HE2  | 1:12:A:LEU:HD21 | 4        | 0.23          |
| (1,321) | 1:8:A:TYR:HE2  | 1:12:A:LEU:HD22 | 4        | 0.23          |
| (1,321) | 1:8:A:TYR:HE2  | 1:12:A:LEU:HD23 | 4        | 0.23          |
| (1,310) | 1:8:A:TYR:HE1  | 1:12:A:LEU:HG   | 7        | 0.23          |
| (1,310) | 1:8:A:TYR:HE2  | 1:12:A:LEU:HG   | 7        | 0.23          |
| (1,310) | 1:8:A:TYR:HE1  | 1:12:A:LEU:HG   | 9        | 0.23          |
| (1,310) | 1:8:A:TYR:HE2  | 1:12:A:LEU:HG   | 9        | 0.23          |
| (1,306) | 1:11:A:TRP:HD1 | 1:21:A:ARG:HB3  | 10       | 0.23          |
| (1,296) | 1:8:A:TYR:HB2  | 1:8:A:TYR:HE1   | 2        | 0.23          |
| (1,296) | 1:8:A:TYR:HB2  | 1:8:A:TYR:HE2   | 2        | 0.23          |
| (1,296) | 1:8:A:TYR:HB2  | 1:8:A:TYR:HE1   | 3        | 0.23          |
| (1,296) | 1:8:A:TYR:HB2  | 1:8:A:TYR:HE2   | 3        | 0.23          |
| (1,138) | 1:13:A:LYS:HA  | 1:13:A:LYS:HD2  | 5        | 0.23          |
| (1,138) | 1:13:A:LYS:HA  | 1:13:A:LYS:HD3  | 5        | 0.23          |
| (3,80)  | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD11  | 2        | 0.22          |
| (3,80)  | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD12  | 2        | 0.22          |
| (3,80)  | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD13  | 2        | 0.22          |
| (3,80)  | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD11  | 2        | 0.22          |
| (3,80)  | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD12  | 2        | 0.22          |
| (3,80)  | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD13  | 2        | 0.22          |
| (3,80)  | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD11  | 2        | 0.22          |
| (3,80)  | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD12  | 2        | 0.22          |
| (3,80)  | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD13  | 2        | 0.22          |
| (3,75)  | 1:5:A:VAL:HG21 | 1:6:A:ARG:HG3   | 5        | 0.22          |
| (3,75)  | 1:5:A:VAL:HG22 | 1:6:A:ARG:HG3   | 5        | 0.22          |
| (3,75)  | 1:5:A:VAL:HG23 | 1:6:A:ARG:HG3   | 5        | 0.22          |
| (3,75)  | 1:5:A:VAL:HG21 | 1:6:A:ARG:HG3   | 6        | 0.22          |
| (3,75)  | 1:5:A:VAL:HG22 | 1:6:A:ARG:HG3   | 6        | 0.22          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (3,75)  | 1:5:A:VAL:HG23 | 1:6:A:ARG:HG3   | 6        | 0.22          |
| (3,66)  | 1:22:A:PRO:HB3 | 1:23:A:PRO:HD2  | 4        | 0.22          |
| (3,66)  | 1:22:A:PRO:HB3 | 1:23:A:PRO:HD3  | 4        | 0.22          |
| (3,66)  | 1:22:A:PRO:HB3 | 1:23:A:PRO:HD2  | 7        | 0.22          |
| (3,66)  | 1:22:A:PRO:HB3 | 1:23:A:PRO:HD3  | 7        | 0.22          |
| (3,62)  | 1:6:A:ARG:H    | 1:7:A:LEU:HD11  | 8        | 0.22          |
| (3,62)  | 1:6:A:ARG:H    | 1:7:A:LEU:HD12  | 8        | 0.22          |
| (3,62)  | 1:6:A:ARG:H    | 1:7:A:LEU:HD13  | 8        | 0.22          |
| (3,58)  | 1:13:A:LYS:HD2 | 1:14:A:ASP:H    | 5        | 0.22          |
| (3,58)  | 1:13:A:LYS:HD3 | 1:14:A:ASP:H    | 5        | 0.22          |
| (3,58)  | 1:13:A:LYS:HD2 | 1:14:A:ASP:H    | 8        | 0.22          |
| (3,58)  | 1:13:A:LYS:HD3 | 1:14:A:ASP:H    | 8        | 0.22          |
| (3,33)  | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD21 | 2        | 0.22          |
| (3,33)  | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD22 | 2        | 0.22          |
| (3,33)  | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD23 | 2        | 0.22          |
| (3,33)  | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD21 | 5        | 0.22          |
| (3,33)  | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD22 | 5        | 0.22          |
| (3,33)  | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD23 | 5        | 0.22          |
| (3,33)  | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD21 | 7        | 0.22          |
| (3,33)  | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD22 | 7        | 0.22          |
| (3,33)  | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD23 | 7        | 0.22          |
| (3,31)  | 1:8:A:TYR:HE1  | 1:12:A:LEU:HD21 | 8        | 0.22          |
| (3,31)  | 1:8:A:TYR:HE1  | 1:12:A:LEU:HD22 | 8        | 0.22          |
| (3,31)  | 1:8:A:TYR:HE1  | 1:12:A:LEU:HD23 | 8        | 0.22          |
| (3,31)  | 1:8:A:TYR:HE2  | 1:12:A:LEU:HD21 | 8        | 0.22          |
| (3,31)  | 1:8:A:TYR:HE2  | 1:12:A:LEU:HD22 | 8        | 0.22          |
| (3,31)  | 1:8:A:TYR:HE2  | 1:12:A:LEU:HD23 | 8        | 0.22          |
| (3,28)  | 1:4:A:ALA:HB1  | 1:8:A:TYR:HE1   | 8        | 0.22          |
| (3,28)  | 1:4:A:ALA:HB1  | 1:8:A:TYR:HE2   | 8        | 0.22          |
| (3,28)  | 1:4:A:ALA:HB2  | 1:8:A:TYR:HE1   | 8        | 0.22          |
| (3,28)  | 1:4:A:ALA:HB2  | 1:8:A:TYR:HE2   | 8        | 0.22          |
| (3,28)  | 1:4:A:ALA:HB3  | 1:8:A:TYR:HE1   | 8        | 0.22          |
| (3,28)  | 1:4:A:ALA:HB3  | 1:8:A:TYR:HE2   | 8        | 0.22          |
| (3,25)  | 1:8:A:TYR:HE1  | 1:12:A:LEU:HG   | 8        | 0.22          |
| (3,25)  | 1:8:A:TYR:HE2  | 1:12:A:LEU:HG   | 8        | 0.22          |
| (3,24)  | 1:11:A:TRP:HD1 | 1:21:A:ARG:HG2  | 3        | 0.22          |
| (3,24)  | 1:11:A:TRP:HD1 | 1:21:A:ARG:HG3  | 3        | 0.22          |
| (3,14)  | 1:13:A:LYS:HA  | 1:13:A:LYS:HD2  | 3        | 0.22          |
| (3,14)  | 1:13:A:LYS:HA  | 1:13:A:LYS:HD3  | 3        | 0.22          |
| (2,461) | 1:5:A:VAL:HG11 | 1:8:A:TYR:HB2   | 2        | 0.22          |
| (2,461) | 1:5:A:VAL:HG12 | 1:8:A:TYR:HB2   | 2        | 0.22          |
| (2,461) | 1:5:A:VAL:HG13 | 1:8:A:TYR:HB2   | 2        | 0.22          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (2,461) | 1:5:A:VAL:HG11 | 1:8:A:TYR:HB2  | 4        | 0.22          |
| (2,461) | 1:5:A:VAL:HG12 | 1:8:A:TYR:HB2  | 4        | 0.22          |
| (2,461) | 1:5:A:VAL:HG13 | 1:8:A:TYR:HB2  | 4        | 0.22          |
| (2,387) | 1:24:A:PRO:HB3 | 1:25:A:SER:H   | 3        | 0.22          |
| (2,362) | 1:7:A:LEU:HD21 | 1:8:A:TYR:H    | 3        | 0.22          |
| (2,362) | 1:7:A:LEU:HD22 | 1:8:A:TYR:H    | 3        | 0.22          |
| (2,362) | 1:7:A:LEU:HD23 | 1:8:A:TYR:H    | 3        | 0.22          |
| (2,362) | 1:7:A:LEU:HD21 | 1:8:A:TYR:H    | 4        | 0.22          |
| (2,362) | 1:7:A:LEU:HD22 | 1:8:A:TYR:H    | 4        | 0.22          |
| (2,362) | 1:7:A:LEU:HD23 | 1:8:A:TYR:H    | 4        | 0.22          |
| (2,198) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD3 | 6        | 0.22          |
| (1,558) | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD11 | 2        | 0.22          |
| (1,558) | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD12 | 2        | 0.22          |
| (1,558) | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD13 | 2        | 0.22          |
| (1,558) | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD11 | 2        | 0.22          |
| (1,558) | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD12 | 2        | 0.22          |
| (1,558) | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD13 | 2        | 0.22          |
| (1,558) | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD11 | 2        | 0.22          |
| (1,558) | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD12 | 2        | 0.22          |
| (1,558) | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD13 | 2        | 0.22          |
| (1,543) | 1:5:A:VAL:HG21 | 1:6:A:ARG:HG3  | 5        | 0.22          |
| (1,543) | 1:5:A:VAL:HG22 | 1:6:A:ARG:HG3  | 5        | 0.22          |
| (1,543) | 1:5:A:VAL:HG23 | 1:6:A:ARG:HG3  | 5        | 0.22          |
| (1,543) | 1:5:A:VAL:HG21 | 1:6:A:ARG:HG3  | 6        | 0.22          |
| (1,543) | 1:5:A:VAL:HG22 | 1:6:A:ARG:HG3  | 6        | 0.22          |
| (1,543) | 1:5:A:VAL:HG23 | 1:6:A:ARG:HG3  | 6        | 0.22          |
| (1,532) | 1:5:A:VAL:HG11 | 1:8:A:TYR:HB2  | 2        | 0.22          |
| (1,532) | 1:5:A:VAL:HG12 | 1:8:A:TYR:HB2  | 2        | 0.22          |
| (1,532) | 1:5:A:VAL:HG13 | 1:8:A:TYR:HB2  | 2        | 0.22          |
| (1,532) | 1:5:A:VAL:HG11 | 1:8:A:TYR:HB2  | 4        | 0.22          |
| (1,532) | 1:5:A:VAL:HG12 | 1:8:A:TYR:HB2  | 4        | 0.22          |
| (1,532) | 1:5:A:VAL:HG13 | 1:8:A:TYR:HB2  | 4        | 0.22          |
| (1,490) | 1:22:A:PRO:HB3 | 1:23:A:PRO:HD2 | 4        | 0.22          |
| (1,490) | 1:22:A:PRO:HB3 | 1:23:A:PRO:HD3 | 4        | 0.22          |
| (1,490) | 1:22:A:PRO:HB3 | 1:23:A:PRO:HD2 | 7        | 0.22          |
| (1,490) | 1:22:A:PRO:HB3 | 1:23:A:PRO:HD3 | 7        | 0.22          |
| (1,449) | 1:24:A:PRO:HB3 | 1:25:A:SER:H   | 3        | 0.22          |
| (1,447) | 1:6:A:ARG:H    | 1:7:A:LEU:HD11 | 8        | 0.22          |
| (1,447) | 1:6:A:ARG:H    | 1:7:A:LEU:HD12 | 8        | 0.22          |
| (1,447) | 1:6:A:ARG:H    | 1:7:A:LEU:HD13 | 8        | 0.22          |
| (1,437) | 1:13:A:LYS:HD2 | 1:14:A:ASP:H   | 5        | 0.22          |
| (1,437) | 1:13:A:LYS:HD3 | 1:14:A:ASP:H   | 5        | 0.22          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,437) | 1:13:A:LYS:HD2 | 1:14:A:ASP:H    | 8        | 0.22          |
| (1,437) | 1:13:A:LYS:HD3 | 1:14:A:ASP:H    | 8        | 0.22          |
| (1,413) | 1:7:A:LEU:HD21 | 1:8:A:TYR:H     | 3        | 0.22          |
| (1,413) | 1:7:A:LEU:HD22 | 1:8:A:TYR:H     | 3        | 0.22          |
| (1,413) | 1:7:A:LEU:HD23 | 1:8:A:TYR:H     | 3        | 0.22          |
| (1,413) | 1:7:A:LEU:HD21 | 1:8:A:TYR:H     | 4        | 0.22          |
| (1,413) | 1:7:A:LEU:HD22 | 1:8:A:TYR:H     | 4        | 0.22          |
| (1,413) | 1:7:A:LEU:HD23 | 1:8:A:TYR:H     | 4        | 0.22          |
| (1,329) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD21 | 2        | 0.22          |
| (1,329) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD22 | 2        | 0.22          |
| (1,329) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD23 | 2        | 0.22          |
| (1,329) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD21 | 5        | 0.22          |
| (1,329) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD22 | 5        | 0.22          |
| (1,329) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD23 | 5        | 0.22          |
| (1,329) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD21 | 7        | 0.22          |
| (1,329) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD22 | 7        | 0.22          |
| (1,329) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD23 | 7        | 0.22          |
| (1,321) | 1:8:A:TYR:HE1  | 1:12:A:LEU:HD21 | 8        | 0.22          |
| (1,321) | 1:8:A:TYR:HE1  | 1:12:A:LEU:HD22 | 8        | 0.22          |
| (1,321) | 1:8:A:TYR:HE1  | 1:12:A:LEU:HD23 | 8        | 0.22          |
| (1,321) | 1:8:A:TYR:HE2  | 1:12:A:LEU:HD21 | 8        | 0.22          |
| (1,321) | 1:8:A:TYR:HE2  | 1:12:A:LEU:HD22 | 8        | 0.22          |
| (1,321) | 1:8:A:TYR:HE2  | 1:12:A:LEU:HD23 | 8        | 0.22          |
| (1,315) | 1:4:A:ALA:HB1  | 1:8:A:TYR:HE1   | 8        | 0.22          |
| (1,315) | 1:4:A:ALA:HB1  | 1:8:A:TYR:HE2   | 8        | 0.22          |
| (1,315) | 1:4:A:ALA:HB2  | 1:8:A:TYR:HE1   | 8        | 0.22          |
| (1,315) | 1:4:A:ALA:HB2  | 1:8:A:TYR:HE2   | 8        | 0.22          |
| (1,315) | 1:4:A:ALA:HB3  | 1:8:A:TYR:HE1   | 8        | 0.22          |
| (1,315) | 1:4:A:ALA:HB3  | 1:8:A:TYR:HE2   | 8        | 0.22          |
| (1,310) | 1:8:A:TYR:HE1  | 1:12:A:LEU:HG   | 8        | 0.22          |
| (1,310) | 1:8:A:TYR:HE2  | 1:12:A:LEU:HG   | 8        | 0.22          |
| (1,308) | 1:11:A:TRP:HD1 | 1:21:A:ARG:HG2  | 3        | 0.22          |
| (1,308) | 1:11:A:TRP:HD1 | 1:21:A:ARG:HG3  | 3        | 0.22          |
| (1,215) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD3  | 6        | 0.22          |
| (1,138) | 1:13:A:LYS:HA  | 1:13:A:LYS:HD2  | 3        | 0.22          |
| (1,138) | 1:13:A:LYS:HA  | 1:13:A:LYS:HD3  | 3        | 0.22          |
| (3,80)  | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD11  | 3        | 0.21          |
| (3,80)  | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD12  | 3        | 0.21          |
| (3,80)  | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD13  | 3        | 0.21          |
| (3,80)  | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD11  | 3        | 0.21          |
| (3,80)  | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD12  | 3        | 0.21          |
| (3,80)  | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD13  | 3        | 0.21          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (3,80)  | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD11  | 3        | 0.21          |
| (3,80)  | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD12  | 3        | 0.21          |
| (3,80)  | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD13  | 3        | 0.21          |
| (3,73)  | 1:2:A:GLU:HG2  | 1:5:A:VAL:HG21  | 4        | 0.21          |
| (3,73)  | 1:2:A:GLU:HG2  | 1:5:A:VAL:HG22  | 4        | 0.21          |
| (3,73)  | 1:2:A:GLU:HG2  | 1:5:A:VAL:HG23  | 4        | 0.21          |
| (3,73)  | 1:2:A:GLU:HG3  | 1:5:A:VAL:HG21  | 4        | 0.21          |
| (3,73)  | 1:2:A:GLU:HG3  | 1:5:A:VAL:HG22  | 4        | 0.21          |
| (3,73)  | 1:2:A:GLU:HG3  | 1:5:A:VAL:HG23  | 4        | 0.21          |
| (3,62)  | 1:6:A:ARG:H    | 1:7:A:LEU:HD11  | 5        | 0.21          |
| (3,62)  | 1:6:A:ARG:H    | 1:7:A:LEU:HD12  | 5        | 0.21          |
| (3,62)  | 1:6:A:ARG:H    | 1:7:A:LEU:HD13  | 5        | 0.21          |
| (3,62)  | 1:6:A:ARG:H    | 1:7:A:LEU:HD11  | 6        | 0.21          |
| (3,62)  | 1:6:A:ARG:H    | 1:7:A:LEU:HD12  | 6        | 0.21          |
| (3,62)  | 1:6:A:ARG:H    | 1:7:A:LEU:HD13  | 6        | 0.21          |
| (3,62)  | 1:6:A:ARG:H    | 1:7:A:LEU:HD11  | 7        | 0.21          |
| (3,62)  | 1:6:A:ARG:H    | 1:7:A:LEU:HD12  | 7        | 0.21          |
| (3,62)  | 1:6:A:ARG:H    | 1:7:A:LEU:HD13  | 7        | 0.21          |
| (3,33)  | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD21 | 3        | 0.21          |
| (3,33)  | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD22 | 3        | 0.21          |
| (3,33)  | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD23 | 3        | 0.21          |
| (3,33)  | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD21 | 9        | 0.21          |
| (3,33)  | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD22 | 9        | 0.21          |
| (3,33)  | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD23 | 9        | 0.21          |
| (3,31)  | 1:8:A:TYR:HE1  | 1:12:A:LEU:HD21 | 7        | 0.21          |
| (3,31)  | 1:8:A:TYR:HE1  | 1:12:A:LEU:HD22 | 7        | 0.21          |
| (3,31)  | 1:8:A:TYR:HE1  | 1:12:A:LEU:HD23 | 7        | 0.21          |
| (3,31)  | 1:8:A:TYR:HE2  | 1:12:A:LEU:HD21 | 7        | 0.21          |
| (3,31)  | 1:8:A:TYR:HE2  | 1:12:A:LEU:HD22 | 7        | 0.21          |
| (3,31)  | 1:8:A:TYR:HE2  | 1:12:A:LEU:HD23 | 7        | 0.21          |
| (3,20)  | 1:8:A:TYR:HA   | 1:8:A:TYR:HE1   | 1        | 0.21          |
| (3,20)  | 1:8:A:TYR:HA   | 1:8:A:TYR:HE2   | 1        | 0.21          |
| (3,14)  | 1:13:A:LYS:HA  | 1:13:A:LYS:HD2  | 2        | 0.21          |
| (3,14)  | 1:13:A:LYS:HA  | 1:13:A:LYS:HD3  | 2        | 0.21          |
| (2,461) | 1:5:A:VAL:HG11 | 1:8:A:TYR:HB2   | 6        | 0.21          |
| (2,461) | 1:5:A:VAL:HG12 | 1:8:A:TYR:HB2   | 6        | 0.21          |
| (2,461) | 1:5:A:VAL:HG13 | 1:8:A:TYR:HB2   | 6        | 0.21          |
| (2,461) | 1:5:A:VAL:HG11 | 1:8:A:TYR:HB2   | 7        | 0.21          |
| (2,461) | 1:5:A:VAL:HG12 | 1:8:A:TYR:HB2   | 7        | 0.21          |
| (2,461) | 1:5:A:VAL:HG13 | 1:8:A:TYR:HB2   | 7        | 0.21          |
| (2,414) | 1:14:A:ASP:HB2 | 1:19:A:SER:HB2  | 6        | 0.21          |
| (2,404) | 1:11:A:TRP:HA  | 1:14:A:ASP:HB3  | 6        | 0.21          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (2,362) | 1:7:A:LEU:HD21 | 1:8:A:TYR:H    | 1        | 0.21          |
| (2,362) | 1:7:A:LEU:HD22 | 1:8:A:TYR:H    | 1        | 0.21          |
| (2,362) | 1:7:A:LEU:HD23 | 1:8:A:TYR:H    | 1        | 0.21          |
| (2,362) | 1:7:A:LEU:HD21 | 1:8:A:TYR:H    | 2        | 0.21          |
| (2,362) | 1:7:A:LEU:HD22 | 1:8:A:TYR:H    | 2        | 0.21          |
| (2,362) | 1:7:A:LEU:HD23 | 1:8:A:TYR:H    | 2        | 0.21          |
| (2,272) | 1:11:A:TRP:HD1 | 1:19:A:SER:HB3 | 5        | 0.21          |
| (2,263) | 1:11:A:TRP:HE1 | 1:19:A:SER:HB2 | 3        | 0.21          |
| (2,263) | 1:11:A:TRP:HE1 | 1:19:A:SER:HB2 | 4        | 0.21          |
| (2,164) | 1:17:A:PRO:HB3 | 1:17:A:PRO:HD2 | 3        | 0.21          |
| (2,164) | 1:17:A:PRO:HB3 | 1:17:A:PRO:HD2 | 10       | 0.21          |
| (1,558) | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD11 | 3        | 0.21          |
| (1,558) | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD12 | 3        | 0.21          |
| (1,558) | 1:4:A:ALA:HB1  | 1:7:A:LEU:HD13 | 3        | 0.21          |
| (1,558) | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD11 | 3        | 0.21          |
| (1,558) | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD12 | 3        | 0.21          |
| (1,558) | 1:4:A:ALA:HB2  | 1:7:A:LEU:HD13 | 3        | 0.21          |
| (1,558) | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD11 | 3        | 0.21          |
| (1,558) | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD12 | 3        | 0.21          |
| (1,558) | 1:4:A:ALA:HB3  | 1:7:A:LEU:HD13 | 3        | 0.21          |
| (1,539) | 1:2:A:GLU:HG2  | 1:5:A:VAL:HG21 | 4        | 0.21          |
| (1,539) | 1:2:A:GLU:HG2  | 1:5:A:VAL:HG22 | 4        | 0.21          |
| (1,539) | 1:2:A:GLU:HG2  | 1:5:A:VAL:HG23 | 4        | 0.21          |
| (1,539) | 1:2:A:GLU:HG3  | 1:5:A:VAL:HG21 | 4        | 0.21          |
| (1,539) | 1:2:A:GLU:HG3  | 1:5:A:VAL:HG22 | 4        | 0.21          |
| (1,539) | 1:2:A:GLU:HG3  | 1:5:A:VAL:HG23 | 4        | 0.21          |
| (1,532) | 1:5:A:VAL:HG11 | 1:8:A:TYR:HB2  | 6        | 0.21          |
| (1,532) | 1:5:A:VAL:HG12 | 1:8:A:TYR:HB2  | 6        | 0.21          |
| (1,532) | 1:5:A:VAL:HG13 | 1:8:A:TYR:HB2  | 6        | 0.21          |
| (1,532) | 1:5:A:VAL:HG11 | 1:8:A:TYR:HB2  | 7        | 0.21          |
| (1,532) | 1:5:A:VAL:HG12 | 1:8:A:TYR:HB2  | 7        | 0.21          |
| (1,532) | 1:5:A:VAL:HG13 | 1:8:A:TYR:HB2  | 7        | 0.21          |
| (1,477) | 1:14:A:ASP:HB2 | 1:19:A:SER:HB2 | 6        | 0.21          |
| (1,466) | 1:11:A:TRP:HA  | 1:14:A:ASP:HB3 | 6        | 0.21          |
| (1,447) | 1:6:A:ARG:H    | 1:7:A:LEU:HD11 | 5        | 0.21          |
| (1,447) | 1:6:A:ARG:H    | 1:7:A:LEU:HD12 | 5        | 0.21          |
| (1,447) | 1:6:A:ARG:H    | 1:7:A:LEU:HD13 | 5        | 0.21          |
| (1,447) | 1:6:A:ARG:H    | 1:7:A:LEU:HD11 | 6        | 0.21          |
| (1,447) | 1:6:A:ARG:H    | 1:7:A:LEU:HD12 | 6        | 0.21          |
| (1,447) | 1:6:A:ARG:H    | 1:7:A:LEU:HD13 | 6        | 0.21          |
| (1,447) | 1:6:A:ARG:H    | 1:7:A:LEU:HD11 | 7        | 0.21          |
| (1,447) | 1:6:A:ARG:H    | 1:7:A:LEU:HD12 | 7        | 0.21          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,447) | 1:6:A:ARG:H    | 1:7:A:LEU:HD13  | 7        | 0.21          |
| (1,413) | 1:7:A:LEU:HD21 | 1:8:A:TYR:H     | 1        | 0.21          |
| (1,413) | 1:7:A:LEU:HD22 | 1:8:A:TYR:H     | 1        | 0.21          |
| (1,413) | 1:7:A:LEU:HD23 | 1:8:A:TYR:H     | 1        | 0.21          |
| (1,413) | 1:7:A:LEU:HD21 | 1:8:A:TYR:H     | 2        | 0.21          |
| (1,413) | 1:7:A:LEU:HD22 | 1:8:A:TYR:H     | 2        | 0.21          |
| (1,413) | 1:7:A:LEU:HD23 | 1:8:A:TYR:H     | 2        | 0.21          |
| (1,329) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD21 | 3        | 0.21          |
| (1,329) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD22 | 3        | 0.21          |
| (1,329) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD23 | 3        | 0.21          |
| (1,329) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD21 | 9        | 0.21          |
| (1,329) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD22 | 9        | 0.21          |
| (1,329) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD23 | 9        | 0.21          |
| (1,321) | 1:8:A:TYR:HE1  | 1:12:A:LEU:HD21 | 7        | 0.21          |
| (1,321) | 1:8:A:TYR:HE1  | 1:12:A:LEU:HD22 | 7        | 0.21          |
| (1,321) | 1:8:A:TYR:HE1  | 1:12:A:LEU:HD23 | 7        | 0.21          |
| (1,321) | 1:8:A:TYR:HE2  | 1:12:A:LEU:HD21 | 7        | 0.21          |
| (1,321) | 1:8:A:TYR:HE2  | 1:12:A:LEU:HD22 | 7        | 0.21          |
| (1,321) | 1:8:A:TYR:HE2  | 1:12:A:LEU:HD23 | 7        | 0.21          |
| (1,293) | 1:11:A:TRP:HD1 | 1:19:A:SER:HB3  | 5        | 0.21          |
| (1,287) | 1:8:A:TYR:HA   | 1:8:A:TYR:HE1   | 1        | 0.21          |
| (1,287) | 1:8:A:TYR:HA   | 1:8:A:TYR:HE2   | 1        | 0.21          |
| (1,282) | 1:11:A:TRP:HE1 | 1:19:A:SER:HB2  | 3        | 0.21          |
| (1,282) | 1:11:A:TRP:HE1 | 1:19:A:SER:HB2  | 4        | 0.21          |
| (1,179) | 1:17:A:PRO:HB3 | 1:17:A:PRO:HD2  | 3        | 0.21          |
| (1,179) | 1:17:A:PRO:HB3 | 1:17:A:PRO:HD2  | 10       | 0.21          |
| (1,138) | 1:13:A:LYS:HA  | 1:13:A:LYS:HD2  | 2        | 0.21          |
| (1,138) | 1:13:A:LYS:HA  | 1:13:A:LYS:HD3  | 2        | 0.21          |
| (3,93)  | 1:10:A:GLN:HA  | 1:13:A:LYS:H    | 1        | 0.2           |
| (3,84)  | 1:3:A:GLU:HA   | 1:7:A:LEU:H     | 2        | 0.2           |
| (3,84)  | 1:3:A:GLU:HA   | 1:7:A:LEU:H     | 3        | 0.2           |
| (3,77)  | 1:3:A:GLU:HG2  | 1:7:A:LEU:HD11  | 2        | 0.2           |
| (3,77)  | 1:3:A:GLU:HG2  | 1:7:A:LEU:HD12  | 2        | 0.2           |
| (3,77)  | 1:3:A:GLU:HG2  | 1:7:A:LEU:HD13  | 2        | 0.2           |
| (3,77)  | 1:3:A:GLU:HG3  | 1:7:A:LEU:HD11  | 2        | 0.2           |
| (3,77)  | 1:3:A:GLU:HG3  | 1:7:A:LEU:HD12  | 2        | 0.2           |
| (3,77)  | 1:3:A:GLU:HG3  | 1:7:A:LEU:HD13  | 2        | 0.2           |
| (3,77)  | 1:3:A:GLU:HG2  | 1:7:A:LEU:HD11  | 3        | 0.2           |
| (3,77)  | 1:3:A:GLU:HG2  | 1:7:A:LEU:HD12  | 3        | 0.2           |
| (3,77)  | 1:3:A:GLU:HG2  | 1:7:A:LEU:HD13  | 3        | 0.2           |
| (3,77)  | 1:3:A:GLU:HG3  | 1:7:A:LEU:HD11  | 3        | 0.2           |
| (3,77)  | 1:3:A:GLU:HG3  | 1:7:A:LEU:HD12  | 3        | 0.2           |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (3,77)  | 1:3:A:GLU:HG3  | 1:7:A:LEU:HD13  | 3        | 0.2           |
| (3,73)  | 1:2:A:GLU:HG2  | 1:5:A:VAL:HG21  | 7        | 0.2           |
| (3,73)  | 1:2:A:GLU:HG2  | 1:5:A:VAL:HG22  | 7        | 0.2           |
| (3,73)  | 1:2:A:GLU:HG2  | 1:5:A:VAL:HG23  | 7        | 0.2           |
| (3,73)  | 1:2:A:GLU:HG3  | 1:5:A:VAL:HG21  | 7        | 0.2           |
| (3,73)  | 1:2:A:GLU:HG3  | 1:5:A:VAL:HG22  | 7        | 0.2           |
| (3,73)  | 1:2:A:GLU:HG3  | 1:5:A:VAL:HG23  | 7        | 0.2           |
| (3,64)  | 1:6:A:ARG:HA   | 1:10:A:GLN:HB2  | 1        | 0.2           |
| (3,62)  | 1:6:A:ARG:H    | 1:7:A:LEU:HD11  | 1        | 0.2           |
| (3,62)  | 1:6:A:ARG:H    | 1:7:A:LEU:HD12  | 1        | 0.2           |
| (3,62)  | 1:6:A:ARG:H    | 1:7:A:LEU:HD13  | 1        | 0.2           |
| (3,62)  | 1:6:A:ARG:H    | 1:7:A:LEU:HD11  | 2        | 0.2           |
| (3,62)  | 1:6:A:ARG:H    | 1:7:A:LEU:HD12  | 2        | 0.2           |
| (3,62)  | 1:6:A:ARG:H    | 1:7:A:LEU:HD13  | 2        | 0.2           |
| (3,58)  | 1:13:A:LYS:HD2 | 1:14:A:ASP:H    | 1        | 0.2           |
| (3,58)  | 1:13:A:LYS:HD3 | 1:14:A:ASP:H    | 1        | 0.2           |
| (3,40)  | 1:11:A:TRP:HA  | 1:11:A:TRP:HE3  | 8        | 0.2           |
| (3,33)  | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD21 | 8        | 0.2           |
| (3,33)  | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD22 | 8        | 0.2           |
| (3,33)  | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD23 | 8        | 0.2           |
| (3,28)  | 1:4:A:ALA:HB1  | 1:8:A:TYR:HE1   | 4        | 0.2           |
| (3,28)  | 1:4:A:ALA:HB1  | 1:8:A:TYR:HE2   | 4        | 0.2           |
| (3,28)  | 1:4:A:ALA:HB2  | 1:8:A:TYR:HE1   | 4        | 0.2           |
| (3,28)  | 1:4:A:ALA:HB2  | 1:8:A:TYR:HE2   | 4        | 0.2           |
| (3,28)  | 1:4:A:ALA:HB3  | 1:8:A:TYR:HE1   | 4        | 0.2           |
| (3,28)  | 1:4:A:ALA:HB3  | 1:8:A:TYR:HE2   | 4        | 0.2           |
| (3,14)  | 1:13:A:LYS:HA  | 1:13:A:LYS:HD2  | 10       | 0.2           |
| (3,14)  | 1:13:A:LYS:HA  | 1:13:A:LYS:HD3  | 10       | 0.2           |
| (2,461) | 1:5:A:VAL:HG11 | 1:8:A:TYR:HB2   | 1        | 0.2           |
| (2,461) | 1:5:A:VAL:HG12 | 1:8:A:TYR:HB2   | 1        | 0.2           |
| (2,461) | 1:5:A:VAL:HG13 | 1:8:A:TYR:HB2   | 1        | 0.2           |
| (2,461) | 1:5:A:VAL:HG11 | 1:8:A:TYR:HB2   | 3        | 0.2           |
| (2,461) | 1:5:A:VAL:HG12 | 1:8:A:TYR:HB2   | 3        | 0.2           |
| (2,461) | 1:5:A:VAL:HG13 | 1:8:A:TYR:HB2   | 3        | 0.2           |
| (2,461) | 1:5:A:VAL:HG11 | 1:8:A:TYR:HB2   | 5        | 0.2           |
| (2,461) | 1:5:A:VAL:HG12 | 1:8:A:TYR:HB2   | 5        | 0.2           |
| (2,461) | 1:5:A:VAL:HG13 | 1:8:A:TYR:HB2   | 5        | 0.2           |
| (2,461) | 1:5:A:VAL:HG11 | 1:8:A:TYR:HB2   | 8        | 0.2           |
| (2,461) | 1:5:A:VAL:HG12 | 1:8:A:TYR:HB2   | 8        | 0.2           |
| (2,461) | 1:5:A:VAL:HG13 | 1:8:A:TYR:HB2   | 8        | 0.2           |
| (2,387) | 1:24:A:PRO:HB3 | 1:25:A:SER:H    | 2        | 0.2           |
| (2,362) | 1:7:A:LEU:HD21 | 1:8:A:TYR:H     | 6        | 0.2           |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (2,362) | 1:7:A:LEU:HD22 | 1:8:A:TYR:H    | 6        | 0.2           |
| (2,362) | 1:7:A:LEU:HD23 | 1:8:A:TYR:H    | 6        | 0.2           |
| (2,362) | 1:7:A:LEU:HD21 | 1:8:A:TYR:H    | 7        | 0.2           |
| (2,362) | 1:7:A:LEU:HD22 | 1:8:A:TYR:H    | 7        | 0.2           |
| (2,362) | 1:7:A:LEU:HD23 | 1:8:A:TYR:H    | 7        | 0.2           |
| (2,362) | 1:7:A:LEU:HD21 | 1:8:A:TYR:H    | 8        | 0.2           |
| (2,362) | 1:7:A:LEU:HD22 | 1:8:A:TYR:H    | 8        | 0.2           |
| (2,362) | 1:7:A:LEU:HD23 | 1:8:A:TYR:H    | 8        | 0.2           |
| (2,360) | 1:5:A:VAL:HG21 | 1:7:A:LEU:H    | 1        | 0.2           |
| (2,360) | 1:5:A:VAL:HG22 | 1:7:A:LEU:H    | 1        | 0.2           |
| (2,360) | 1:5:A:VAL:HG23 | 1:7:A:LEU:H    | 1        | 0.2           |
| (2,272) | 1:11:A:TRP:HD1 | 1:19:A:SER:HB3 | 6        | 0.2           |
| (1,601) | 1:10:A:GLN:HA  | 1:13:A:LYS:H   | 1        | 0.2           |
| (1,569) | 1:3:A:GLU:HA   | 1:7:A:LEU:H    | 2        | 0.2           |
| (1,569) | 1:3:A:GLU:HA   | 1:7:A:LEU:H    | 3        | 0.2           |
| (1,552) | 1:3:A:GLU:HG2  | 1:7:A:LEU:HD11 | 2        | 0.2           |
| (1,552) | 1:3:A:GLU:HG2  | 1:7:A:LEU:HD12 | 2        | 0.2           |
| (1,552) | 1:3:A:GLU:HG2  | 1:7:A:LEU:HD13 | 2        | 0.2           |
| (1,552) | 1:3:A:GLU:HG3  | 1:7:A:LEU:HD11 | 2        | 0.2           |
| (1,552) | 1:3:A:GLU:HG3  | 1:7:A:LEU:HD12 | 2        | 0.2           |
| (1,552) | 1:3:A:GLU:HG3  | 1:7:A:LEU:HD13 | 2        | 0.2           |
| (1,552) | 1:3:A:GLU:HG2  | 1:7:A:LEU:HD11 | 3        | 0.2           |
| (1,552) | 1:3:A:GLU:HG2  | 1:7:A:LEU:HD12 | 3        | 0.2           |
| (1,552) | 1:3:A:GLU:HG2  | 1:7:A:LEU:HD13 | 3        | 0.2           |
| (1,552) | 1:3:A:GLU:HG3  | 1:7:A:LEU:HD11 | 3        | 0.2           |
| (1,552) | 1:3:A:GLU:HG3  | 1:7:A:LEU:HD12 | 3        | 0.2           |
| (1,552) | 1:3:A:GLU:HG3  | 1:7:A:LEU:HD13 | 3        | 0.2           |
| (1,539) | 1:2:A:GLU:HG2  | 1:5:A:VAL:HG21 | 7        | 0.2           |
| (1,539) | 1:2:A:GLU:HG2  | 1:5:A:VAL:HG22 | 7        | 0.2           |
| (1,539) | 1:2:A:GLU:HG2  | 1:5:A:VAL:HG23 | 7        | 0.2           |
| (1,539) | 1:2:A:GLU:HG3  | 1:5:A:VAL:HG21 | 7        | 0.2           |
| (1,539) | 1:2:A:GLU:HG3  | 1:5:A:VAL:HG22 | 7        | 0.2           |
| (1,539) | 1:2:A:GLU:HG3  | 1:5:A:VAL:HG23 | 7        | 0.2           |
| (1,532) | 1:5:A:VAL:HG11 | 1:8:A:TYR:HB2  | 1        | 0.2           |
| (1,532) | 1:5:A:VAL:HG12 | 1:8:A:TYR:HB2  | 1        | 0.2           |
| (1,532) | 1:5:A:VAL:HG13 | 1:8:A:TYR:HB2  | 1        | 0.2           |
| (1,532) | 1:5:A:VAL:HG11 | 1:8:A:TYR:HB2  | 3        | 0.2           |
| (1,532) | 1:5:A:VAL:HG12 | 1:8:A:TYR:HB2  | 3        | 0.2           |
| (1,532) | 1:5:A:VAL:HG13 | 1:8:A:TYR:HB2  | 3        | 0.2           |
| (1,532) | 1:5:A:VAL:HG11 | 1:8:A:TYR:HB2  | 5        | 0.2           |
| (1,532) | 1:5:A:VAL:HG12 | 1:8:A:TYR:HB2  | 5        | 0.2           |
| (1,532) | 1:5:A:VAL:HG13 | 1:8:A:TYR:HB2  | 5        | 0.2           |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,532) | 1:5:A:VAL:HG11 | 1:8:A:TYR:HB2   | 8        | 0.2           |
| (1,532) | 1:5:A:VAL:HG12 | 1:8:A:TYR:HB2   | 8        | 0.2           |
| (1,532) | 1:5:A:VAL:HG13 | 1:8:A:TYR:HB2   | 8        | 0.2           |
| (1,480) | 1:6:A:ARG:HA   | 1:10:A:GLN:HB2  | 1        | 0.2           |
| (1,449) | 1:24:A:PRO:HB3 | 1:25:A:SER:H    | 2        | 0.2           |
| (1,447) | 1:6:A:ARG:H    | 1:7:A:LEU:HD11  | 1        | 0.2           |
| (1,447) | 1:6:A:ARG:H    | 1:7:A:LEU:HD12  | 1        | 0.2           |
| (1,447) | 1:6:A:ARG:H    | 1:7:A:LEU:HD13  | 1        | 0.2           |
| (1,447) | 1:6:A:ARG:H    | 1:7:A:LEU:HD11  | 2        | 0.2           |
| (1,447) | 1:6:A:ARG:H    | 1:7:A:LEU:HD12  | 2        | 0.2           |
| (1,447) | 1:6:A:ARG:H    | 1:7:A:LEU:HD13  | 2        | 0.2           |
| (1,437) | 1:13:A:LYS:HD2 | 1:14:A:ASP:H    | 1        | 0.2           |
| (1,437) | 1:13:A:LYS:HD3 | 1:14:A:ASP:H    | 1        | 0.2           |
| (1,413) | 1:7:A:LEU:HD21 | 1:8:A:TYR:H     | 6        | 0.2           |
| (1,413) | 1:7:A:LEU:HD22 | 1:8:A:TYR:H     | 6        | 0.2           |
| (1,413) | 1:7:A:LEU:HD23 | 1:8:A:TYR:H     | 6        | 0.2           |
| (1,413) | 1:7:A:LEU:HD21 | 1:8:A:TYR:H     | 7        | 0.2           |
| (1,413) | 1:7:A:LEU:HD22 | 1:8:A:TYR:H     | 7        | 0.2           |
| (1,413) | 1:7:A:LEU:HD23 | 1:8:A:TYR:H     | 7        | 0.2           |
| (1,413) | 1:7:A:LEU:HD21 | 1:8:A:TYR:H     | 8        | 0.2           |
| (1,413) | 1:7:A:LEU:HD22 | 1:8:A:TYR:H     | 8        | 0.2           |
| (1,413) | 1:7:A:LEU:HD23 | 1:8:A:TYR:H     | 8        | 0.2           |
| (1,411) | 1:5:A:VAL:HG21 | 1:7:A:LEU:H     | 1        | 0.2           |
| (1,411) | 1:5:A:VAL:HG22 | 1:7:A:LEU:H     | 1        | 0.2           |
| (1,411) | 1:5:A:VAL:HG23 | 1:7:A:LEU:H     | 1        | 0.2           |
| (1,357) | 1:11:A:TRP:HA  | 1:11:A:TRP:HE3  | 8        | 0.2           |
| (1,329) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD21 | 8        | 0.2           |
| (1,329) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD22 | 8        | 0.2           |
| (1,329) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD23 | 8        | 0.2           |
| (1,315) | 1:4:A:ALA:HB1  | 1:8:A:TYR:HE1   | 4        | 0.2           |
| (1,315) | 1:4:A:ALA:HB1  | 1:8:A:TYR:HE2   | 4        | 0.2           |
| (1,315) | 1:4:A:ALA:HB2  | 1:8:A:TYR:HE1   | 4        | 0.2           |
| (1,315) | 1:4:A:ALA:HB2  | 1:8:A:TYR:HE2   | 4        | 0.2           |
| (1,315) | 1:4:A:ALA:HB3  | 1:8:A:TYR:HE1   | 4        | 0.2           |
| (1,315) | 1:4:A:ALA:HB3  | 1:8:A:TYR:HE2   | 4        | 0.2           |
| (1,293) | 1:11:A:TRP:HD1 | 1:19:A:SER:HB3  | 6        | 0.2           |
| (1,138) | 1:13:A:LYS:HA  | 1:13:A:LYS:HD2  | 10       | 0.2           |
| (1,138) | 1:13:A:LYS:HA  | 1:13:A:LYS:HD3  | 10       | 0.2           |
| (3,77)  | 1:3:A:GLU:HG2  | 1:7:A:LEU:HD11  | 6        | 0.19          |
| (3,77)  | 1:3:A:GLU:HG2  | 1:7:A:LEU:HD12  | 6        | 0.19          |
| (3,77)  | 1:3:A:GLU:HG2  | 1:7:A:LEU:HD13  | 6        | 0.19          |
| (3,77)  | 1:3:A:GLU:HG3  | 1:7:A:LEU:HD11  | 6        | 0.19          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (3,77)  | 1:3:A:GLU:HG3  | 1:7:A:LEU:HD12  | 6        | 0.19          |
| (3,77)  | 1:3:A:GLU:HG3  | 1:7:A:LEU:HD13  | 6        | 0.19          |
| (3,66)  | 1:22:A:PRO:HB3 | 1:23:A:PRO:HD2  | 3        | 0.19          |
| (3,66)  | 1:22:A:PRO:HB3 | 1:23:A:PRO:HD3  | 3        | 0.19          |
| (3,66)  | 1:22:A:PRO:HB3 | 1:23:A:PRO:HD2  | 10       | 0.19          |
| (3,66)  | 1:22:A:PRO:HB3 | 1:23:A:PRO:HD3  | 10       | 0.19          |
| (3,64)  | 1:6:A:ARG:HA   | 1:10:A:GLN:HB2  | 7        | 0.19          |
| (3,40)  | 1:11:A:TRP:HA  | 1:11:A:TRP:HE3  | 4        | 0.19          |
| (3,40)  | 1:11:A:TRP:HA  | 1:11:A:TRP:HE3  | 9        | 0.19          |
| (3,33)  | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD21 | 4        | 0.19          |
| (3,33)  | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD22 | 4        | 0.19          |
| (3,33)  | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD23 | 4        | 0.19          |
| (3,33)  | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD21 | 10       | 0.19          |
| (3,33)  | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD22 | 10       | 0.19          |
| (3,33)  | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD23 | 10       | 0.19          |
| (3,28)  | 1:4:A:ALA:HB1  | 1:8:A:TYR:HE1   | 9        | 0.19          |
| (3,28)  | 1:4:A:ALA:HB1  | 1:8:A:TYR:HE2   | 9        | 0.19          |
| (3,28)  | 1:4:A:ALA:HB2  | 1:8:A:TYR:HE1   | 9        | 0.19          |
| (3,28)  | 1:4:A:ALA:HB2  | 1:8:A:TYR:HE2   | 9        | 0.19          |
| (3,28)  | 1:4:A:ALA:HB3  | 1:8:A:TYR:HE1   | 9        | 0.19          |
| (3,28)  | 1:4:A:ALA:HB3  | 1:8:A:TYR:HE2   | 9        | 0.19          |
| (2,437) | 1:16:A:GLY:HA2 | 1:17:A:PRO:HG2  | 6        | 0.19          |
| (2,437) | 1:16:A:GLY:HA2 | 1:17:A:PRO:HG3  | 6        | 0.19          |
| (2,362) | 1:7:A:LEU:HD21 | 1:8:A:TYR:H     | 5        | 0.19          |
| (2,362) | 1:7:A:LEU:HD22 | 1:8:A:TYR:H     | 5        | 0.19          |
| (2,362) | 1:7:A:LEU:HD23 | 1:8:A:TYR:H     | 5        | 0.19          |
| (2,360) | 1:5:A:VAL:HG21 | 1:7:A:LEU:H     | 3        | 0.19          |
| (2,360) | 1:5:A:VAL:HG22 | 1:7:A:LEU:H     | 3        | 0.19          |
| (2,360) | 1:5:A:VAL:HG23 | 1:7:A:LEU:H     | 3        | 0.19          |
| (2,272) | 1:11:A:TRP:HD1 | 1:19:A:SER:HB3  | 7        | 0.19          |
| (2,1)   | 1:2:A:GLU:HA   | 1:3:A:GLU:H     | 3        | 0.19          |
| (1,552) | 1:3:A:GLU:HG2  | 1:7:A:LEU:HD11  | 6        | 0.19          |
| (1,552) | 1:3:A:GLU:HG2  | 1:7:A:LEU:HD12  | 6        | 0.19          |
| (1,552) | 1:3:A:GLU:HG2  | 1:7:A:LEU:HD13  | 6        | 0.19          |
| (1,552) | 1:3:A:GLU:HG3  | 1:7:A:LEU:HD11  | 6        | 0.19          |
| (1,552) | 1:3:A:GLU:HG3  | 1:7:A:LEU:HD12  | 6        | 0.19          |
| (1,552) | 1:3:A:GLU:HG3  | 1:7:A:LEU:HD13  | 6        | 0.19          |
| (1,504) | 1:16:A:GLY:HA2 | 1:17:A:PRO:HG2  | 6        | 0.19          |
| (1,504) | 1:16:A:GLY:HA2 | 1:17:A:PRO:HG3  | 6        | 0.19          |
| (1,490) | 1:22:A:PRO:HB3 | 1:23:A:PRO:HD2  | 3        | 0.19          |
| (1,490) | 1:22:A:PRO:HB3 | 1:23:A:PRO:HD3  | 3        | 0.19          |
| (1,490) | 1:22:A:PRO:HB3 | 1:23:A:PRO:HD2  | 10       | 0.19          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,490) | 1:22:A:PRO:HB3  | 1:23:A:PRO:HD3  | 10       | 0.19          |
| (1,480) | 1:6:A:ARG:HA    | 1:10:A:GLN:HB2  | 7        | 0.19          |
| (1,413) | 1:7:A:LEU:HD21  | 1:8:A:TYR:H     | 5        | 0.19          |
| (1,413) | 1:7:A:LEU:HD22  | 1:8:A:TYR:H     | 5        | 0.19          |
| (1,413) | 1:7:A:LEU:HD23  | 1:8:A:TYR:H     | 5        | 0.19          |
| (1,411) | 1:5:A:VAL:HG21  | 1:7:A:LEU:H     | 3        | 0.19          |
| (1,411) | 1:5:A:VAL:HG22  | 1:7:A:LEU:H     | 3        | 0.19          |
| (1,411) | 1:5:A:VAL:HG23  | 1:7:A:LEU:H     | 3        | 0.19          |
| (1,357) | 1:11:A:TRP:HA   | 1:11:A:TRP:HE3  | 4        | 0.19          |
| (1,357) | 1:11:A:TRP:HA   | 1:11:A:TRP:HE3  | 9        | 0.19          |
| (1,329) | 1:11:A:TRP:HE3  | 1:12:A:LEU:HD21 | 4        | 0.19          |
| (1,329) | 1:11:A:TRP:HE3  | 1:12:A:LEU:HD22 | 4        | 0.19          |
| (1,329) | 1:11:A:TRP:HE3  | 1:12:A:LEU:HD23 | 4        | 0.19          |
| (1,329) | 1:11:A:TRP:HE3  | 1:12:A:LEU:HD21 | 10       | 0.19          |
| (1,329) | 1:11:A:TRP:HE3  | 1:12:A:LEU:HD22 | 10       | 0.19          |
| (1,329) | 1:11:A:TRP:HE3  | 1:12:A:LEU:HD23 | 10       | 0.19          |
| (1,315) | 1:4:A:ALA:HB1   | 1:8:A:TYR:HE1   | 9        | 0.19          |
| (1,315) | 1:4:A:ALA:HB1   | 1:8:A:TYR:HE2   | 9        | 0.19          |
| (1,315) | 1:4:A:ALA:HB2   | 1:8:A:TYR:HE1   | 9        | 0.19          |
| (1,315) | 1:4:A:ALA:HB2   | 1:8:A:TYR:HE2   | 9        | 0.19          |
| (1,315) | 1:4:A:ALA:HB3   | 1:8:A:TYR:HE1   | 9        | 0.19          |
| (1,315) | 1:4:A:ALA:HB3   | 1:8:A:TYR:HE2   | 9        | 0.19          |
| (1,293) | 1:11:A:TRP:HD1  | 1:19:A:SER:HB3  | 7        | 0.19          |
| (1,1)   | 1:2:A:GLU:HA    | 1:3:A:GLU:H     | 3        | 0.19          |
| (3,93)  | 1:10:A:GLN:HA   | 1:13:A:LYS:H    | 3        | 0.18          |
| (3,93)  | 1:10:A:GLN:HA   | 1:13:A:LYS:H    | 8        | 0.18          |
| (3,73)  | 1:2:A:GLU:HG2   | 1:5:A:VAL:HG21  | 6        | 0.18          |
| (3,73)  | 1:2:A:GLU:HG2   | 1:5:A:VAL:HG22  | 6        | 0.18          |
| (3,73)  | 1:2:A:GLU:HG2   | 1:5:A:VAL:HG23  | 6        | 0.18          |
| (3,73)  | 1:2:A:GLU:HG3   | 1:5:A:VAL:HG21  | 6        | 0.18          |
| (3,73)  | 1:2:A:GLU:HG3   | 1:5:A:VAL:HG22  | 6        | 0.18          |
| (3,73)  | 1:2:A:GLU:HG3   | 1:5:A:VAL:HG23  | 6        | 0.18          |
| (3,73)  | 1:2:A:GLU:HG2   | 1:5:A:VAL:HG21  | 8        | 0.18          |
| (3,73)  | 1:2:A:GLU:HG2   | 1:5:A:VAL:HG22  | 8        | 0.18          |
| (3,73)  | 1:2:A:GLU:HG2   | 1:5:A:VAL:HG23  | 8        | 0.18          |
| (3,73)  | 1:2:A:GLU:HG3   | 1:5:A:VAL:HG21  | 8        | 0.18          |
| (3,73)  | 1:2:A:GLU:HG3   | 1:5:A:VAL:HG22  | 8        | 0.18          |
| (3,73)  | 1:2:A:GLU:HG3   | 1:5:A:VAL:HG23  | 8        | 0.18          |
| (3,71)  | 1:12:A:LEU:HD11 | 1:17:A:PRO:HD2  | 6        | 0.18          |
| (3,71)  | 1:12:A:LEU:HD12 | 1:17:A:PRO:HD2  | 6        | 0.18          |
| (3,71)  | 1:12:A:LEU:HD13 | 1:17:A:PRO:HD2  | 6        | 0.18          |
| (3,66)  | 1:22:A:PRO:HB3  | 1:23:A:PRO:HD2  | 9        | 0.18          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (3,66)  | 1:22:A:PRO:HB3 | 1:23:A:PRO:HD3  | 9        | 0.18          |
| (3,64)  | 1:6:A:ARG:HA   | 1:10:A:GLN:HB2  | 5        | 0.18          |
| (3,58)  | 1:13:A:LYS:HD2 | 1:14:A:ASP:H    | 10       | 0.18          |
| (3,58)  | 1:13:A:LYS:HD3 | 1:14:A:ASP:H    | 10       | 0.18          |
| (3,41)  | 1:4:A:ALA:H    | 1:5:A:VAL:H     | 10       | 0.18          |
| (3,40)  | 1:11:A:TRP:HA  | 1:11:A:TRP:HE3  | 1        | 0.18          |
| (3,40)  | 1:11:A:TRP:HA  | 1:11:A:TRP:HE3  | 3        | 0.18          |
| (3,33)  | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD21 | 1        | 0.18          |
| (3,33)  | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD22 | 1        | 0.18          |
| (3,33)  | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD23 | 1        | 0.18          |
| (3,28)  | 1:4:A:ALA:HB1  | 1:8:A:TYR:HE1   | 3        | 0.18          |
| (3,28)  | 1:4:A:ALA:HB1  | 1:8:A:TYR:HE2   | 3        | 0.18          |
| (3,28)  | 1:4:A:ALA:HB2  | 1:8:A:TYR:HE1   | 3        | 0.18          |
| (3,28)  | 1:4:A:ALA:HB2  | 1:8:A:TYR:HE2   | 3        | 0.18          |
| (3,28)  | 1:4:A:ALA:HB3  | 1:8:A:TYR:HE1   | 3        | 0.18          |
| (3,28)  | 1:4:A:ALA:HB3  | 1:8:A:TYR:HE2   | 3        | 0.18          |
| (3,20)  | 1:8:A:TYR:HA   | 1:8:A:TYR:HE1   | 9        | 0.18          |
| (3,20)  | 1:8:A:TYR:HA   | 1:8:A:TYR:HE2   | 9        | 0.18          |
| (3,11)  | 1:12:A:LEU:HA  | 1:12:A:LEU:HD11 | 9        | 0.18          |
| (3,11)  | 1:12:A:LEU:HA  | 1:12:A:LEU:HD12 | 9        | 0.18          |
| (3,11)  | 1:12:A:LEU:HA  | 1:12:A:LEU:HD13 | 9        | 0.18          |
| (2,360) | 1:5:A:VAL:HG21 | 1:7:A:LEU:H     | 2        | 0.18          |
| (2,360) | 1:5:A:VAL:HG22 | 1:7:A:LEU:H     | 2        | 0.18          |
| (2,360) | 1:5:A:VAL:HG23 | 1:7:A:LEU:H     | 2        | 0.18          |
| (2,280) | 1:8:A:TYR:HD1  | 1:24:A:PRO:HB3  | 2        | 0.18          |
| (2,280) | 1:8:A:TYR:HD2  | 1:24:A:PRO:HB3  | 2        | 0.18          |
| (2,280) | 1:8:A:TYR:HD1  | 1:24:A:PRO:HB3  | 3        | 0.18          |
| (2,280) | 1:8:A:TYR:HD2  | 1:24:A:PRO:HB3  | 3        | 0.18          |
| (2,280) | 1:8:A:TYR:HD1  | 1:24:A:PRO:HB3  | 5        | 0.18          |
| (2,280) | 1:8:A:TYR:HD2  | 1:24:A:PRO:HB3  | 5        | 0.18          |
| (2,201) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HG2  | 7        | 0.18          |
| (2,201) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HG3  | 7        | 0.18          |
| (2,201) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HG2  | 10       | 0.18          |
| (2,201) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HG3  | 10       | 0.18          |
| (2,164) | 1:17:A:PRO:HB3 | 1:17:A:PRO:HD2  | 5        | 0.18          |
| (1,601) | 1:10:A:GLN:HA  | 1:13:A:LYS:H    | 3        | 0.18          |
| (1,601) | 1:10:A:GLN:HA  | 1:13:A:LYS:H    | 8        | 0.18          |
| (1,539) | 1:2:A:GLU:HG2  | 1:5:A:VAL:HG21  | 6        | 0.18          |
| (1,539) | 1:2:A:GLU:HG2  | 1:5:A:VAL:HG22  | 6        | 0.18          |
| (1,539) | 1:2:A:GLU:HG2  | 1:5:A:VAL:HG23  | 6        | 0.18          |
| (1,539) | 1:2:A:GLU:HG3  | 1:5:A:VAL:HG21  | 6        | 0.18          |
| (1,539) | 1:2:A:GLU:HG3  | 1:5:A:VAL:HG22  | 6        | 0.18          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,539) | 1:2:A:GLU:HG3   | 1:5:A:VAL:HG23  | 6        | 0.18          |
| (1,539) | 1:2:A:GLU:HG2   | 1:5:A:VAL:HG21  | 8        | 0.18          |
| (1,539) | 1:2:A:GLU:HG2   | 1:5:A:VAL:HG22  | 8        | 0.18          |
| (1,539) | 1:2:A:GLU:HG2   | 1:5:A:VAL:HG23  | 8        | 0.18          |
| (1,539) | 1:2:A:GLU:HG3   | 1:5:A:VAL:HG21  | 8        | 0.18          |
| (1,539) | 1:2:A:GLU:HG3   | 1:5:A:VAL:HG22  | 8        | 0.18          |
| (1,539) | 1:2:A:GLU:HG3   | 1:5:A:VAL:HG23  | 8        | 0.18          |
| (1,529) | 1:12:A:LEU:HD11 | 1:17:A:PRO:HD2  | 6        | 0.18          |
| (1,529) | 1:12:A:LEU:HD12 | 1:17:A:PRO:HD2  | 6        | 0.18          |
| (1,529) | 1:12:A:LEU:HD13 | 1:17:A:PRO:HD2  | 6        | 0.18          |
| (1,490) | 1:22:A:PRO:HB3  | 1:23:A:PRO:HD2  | 9        | 0.18          |
| (1,490) | 1:22:A:PRO:HB3  | 1:23:A:PRO:HD3  | 9        | 0.18          |
| (1,480) | 1:6:A:ARG:HA    | 1:10:A:GLN:HB2  | 5        | 0.18          |
| (1,437) | 1:13:A:LYS:HD2  | 1:14:A:ASP:H    | 10       | 0.18          |
| (1,437) | 1:13:A:LYS:HD3  | 1:14:A:ASP:H    | 10       | 0.18          |
| (1,411) | 1:5:A:VAL:HG21  | 1:7:A:LEU:H     | 2        | 0.18          |
| (1,411) | 1:5:A:VAL:HG22  | 1:7:A:LEU:H     | 2        | 0.18          |
| (1,411) | 1:5:A:VAL:HG23  | 1:7:A:LEU:H     | 2        | 0.18          |
| (1,370) | 1:4:A:ALA:H     | 1:5:A:VAL:H     | 10       | 0.18          |
| (1,357) | 1:11:A:TRP:HA   | 1:11:A:TRP:HE3  | 1        | 0.18          |
| (1,357) | 1:11:A:TRP:HA   | 1:11:A:TRP:HE3  | 3        | 0.18          |
| (1,329) | 1:11:A:TRP:HE3  | 1:12:A:LEU:HD21 | 1        | 0.18          |
| (1,329) | 1:11:A:TRP:HE3  | 1:12:A:LEU:HD22 | 1        | 0.18          |
| (1,329) | 1:11:A:TRP:HE3  | 1:12:A:LEU:HD23 | 1        | 0.18          |
| (1,315) | 1:4:A:ALA:HB1   | 1:8:A:TYR:HE1   | 3        | 0.18          |
| (1,315) | 1:4:A:ALA:HB1   | 1:8:A:TYR:HE2   | 3        | 0.18          |
| (1,315) | 1:4:A:ALA:HB2   | 1:8:A:TYR:HE1   | 3        | 0.18          |
| (1,315) | 1:4:A:ALA:HB2   | 1:8:A:TYR:HE2   | 3        | 0.18          |
| (1,315) | 1:4:A:ALA:HB3   | 1:8:A:TYR:HE1   | 3        | 0.18          |
| (1,315) | 1:4:A:ALA:HB3   | 1:8:A:TYR:HE2   | 3        | 0.18          |
| (1,303) | 1:8:A:TYR:HD1   | 1:24:A:PRO:HB3  | 2        | 0.18          |
| (1,303) | 1:8:A:TYR:HD2   | 1:24:A:PRO:HB3  | 2        | 0.18          |
| (1,303) | 1:8:A:TYR:HD1   | 1:24:A:PRO:HB3  | 3        | 0.18          |
| (1,303) | 1:8:A:TYR:HD2   | 1:24:A:PRO:HB3  | 3        | 0.18          |
| (1,303) | 1:8:A:TYR:HD1   | 1:24:A:PRO:HB3  | 5        | 0.18          |
| (1,303) | 1:8:A:TYR:HD2   | 1:24:A:PRO:HB3  | 5        | 0.18          |
| (1,287) | 1:8:A:TYR:HA    | 1:8:A:TYR:HE1   | 9        | 0.18          |
| (1,287) | 1:8:A:TYR:HA    | 1:8:A:TYR:HE2   | 9        | 0.18          |
| (1,218) | 1:21:A:ARG:HB3  | 1:21:A:ARG:HG2  | 7        | 0.18          |
| (1,218) | 1:21:A:ARG:HB3  | 1:21:A:ARG:HG3  | 7        | 0.18          |
| (1,218) | 1:21:A:ARG:HB3  | 1:21:A:ARG:HG2  | 10       | 0.18          |
| (1,218) | 1:21:A:ARG:HB3  | 1:21:A:ARG:HG3  | 10       | 0.18          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,179) | 1:17:A:PRO:HB3  | 1:17:A:PRO:HD2  | 5        | 0.18          |
| (1,119) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD11 | 9        | 0.18          |
| (1,119) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD12 | 9        | 0.18          |
| (1,119) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD13 | 9        | 0.18          |
| (3,93)  | 1:10:A:GLN:HA   | 1:13:A:LYS:H    | 2        | 0.17          |
| (3,80)  | 1:4:A:ALA:HB1   | 1:7:A:LEU:HD11  | 4        | 0.17          |
| (3,80)  | 1:4:A:ALA:HB1   | 1:7:A:LEU:HD12  | 4        | 0.17          |
| (3,80)  | 1:4:A:ALA:HB1   | 1:7:A:LEU:HD13  | 4        | 0.17          |
| (3,80)  | 1:4:A:ALA:HB2   | 1:7:A:LEU:HD11  | 4        | 0.17          |
| (3,80)  | 1:4:A:ALA:HB2   | 1:7:A:LEU:HD12  | 4        | 0.17          |
| (3,80)  | 1:4:A:ALA:HB2   | 1:7:A:LEU:HD13  | 4        | 0.17          |
| (3,80)  | 1:4:A:ALA:HB3   | 1:7:A:LEU:HD11  | 4        | 0.17          |
| (3,80)  | 1:4:A:ALA:HB3   | 1:7:A:LEU:HD12  | 4        | 0.17          |
| (3,80)  | 1:4:A:ALA:HB3   | 1:7:A:LEU:HD13  | 4        | 0.17          |
| (3,73)  | 1:2:A:GLU:HG2   | 1:5:A:VAL:HG21  | 2        | 0.17          |
| (3,73)  | 1:2:A:GLU:HG2   | 1:5:A:VAL:HG22  | 2        | 0.17          |
| (3,73)  | 1:2:A:GLU:HG2   | 1:5:A:VAL:HG23  | 2        | 0.17          |
| (3,73)  | 1:2:A:GLU:HG3   | 1:5:A:VAL:HG21  | 2        | 0.17          |
| (3,73)  | 1:2:A:GLU:HG3   | 1:5:A:VAL:HG22  | 2        | 0.17          |
| (3,73)  | 1:2:A:GLU:HG3   | 1:5:A:VAL:HG23  | 2        | 0.17          |
| (3,71)  | 1:12:A:LEU:HD11 | 1:17:A:PRO:HD2  | 2        | 0.17          |
| (3,71)  | 1:12:A:LEU:HD12 | 1:17:A:PRO:HD2  | 2        | 0.17          |
| (3,71)  | 1:12:A:LEU:HD13 | 1:17:A:PRO:HD2  | 2        | 0.17          |
| (3,71)  | 1:12:A:LEU:HD11 | 1:17:A:PRO:HD2  | 5        | 0.17          |
| (3,71)  | 1:12:A:LEU:HD12 | 1:17:A:PRO:HD2  | 5        | 0.17          |
| (3,71)  | 1:12:A:LEU:HD13 | 1:17:A:PRO:HD2  | 5        | 0.17          |
| (3,64)  | 1:6:A:ARG:HA    | 1:10:A:GLN:HB2  | 3        | 0.17          |
| (3,64)  | 1:6:A:ARG:HA    | 1:10:A:GLN:HB2  | 8        | 0.17          |
| (3,62)  | 1:6:A:ARG:H     | 1:7:A:LEU:HD11  | 3        | 0.17          |
| (3,62)  | 1:6:A:ARG:H     | 1:7:A:LEU:HD12  | 3        | 0.17          |
| (3,62)  | 1:6:A:ARG:H     | 1:7:A:LEU:HD13  | 3        | 0.17          |
| (3,58)  | 1:13:A:LYS:HD2  | 1:14:A:ASP:H    | 3        | 0.17          |
| (3,58)  | 1:13:A:LYS:HD3  | 1:14:A:ASP:H    | 3        | 0.17          |
| (3,41)  | 1:4:A:ALA:H     | 1:5:A:VAL:H     | 9        | 0.17          |
| (3,40)  | 1:11:A:TRP:HA   | 1:11:A:TRP:HE3  | 2        | 0.17          |
| (3,40)  | 1:11:A:TRP:HA   | 1:11:A:TRP:HE3  | 5        | 0.17          |
| (3,40)  | 1:11:A:TRP:HA   | 1:11:A:TRP:HE3  | 10       | 0.17          |
| (3,28)  | 1:4:A:ALA:HB1   | 1:8:A:TYR:HE1   | 10       | 0.17          |
| (3,28)  | 1:4:A:ALA:HB1   | 1:8:A:TYR:HE2   | 10       | 0.17          |
| (3,28)  | 1:4:A:ALA:HB2   | 1:8:A:TYR:HE1   | 10       | 0.17          |
| (3,28)  | 1:4:A:ALA:HB2   | 1:8:A:TYR:HE2   | 10       | 0.17          |
| (3,28)  | 1:4:A:ALA:HB3   | 1:8:A:TYR:HE1   | 10       | 0.17          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (3,28)  | 1:4:A:ALA:HB3   | 1:8:A:TYR:HE2  | 10       | 0.17          |
| (3,25)  | 1:8:A:TYR:HE1   | 1:12:A:LEU:HG  | 1        | 0.17          |
| (3,25)  | 1:8:A:TYR:HE2   | 1:12:A:LEU:HG  | 1        | 0.17          |
| (2,467) | 1:2:A:GLU:HB3   | 1:5:A:VAL:HG11 | 4        | 0.17          |
| (2,467) | 1:2:A:GLU:HB3   | 1:5:A:VAL:HG12 | 4        | 0.17          |
| (2,467) | 1:2:A:GLU:HB3   | 1:5:A:VAL:HG13 | 4        | 0.17          |
| (2,445) | 1:1:A:GLU:HB2   | 1:2:A:GLU:HG2  | 1        | 0.17          |
| (2,360) | 1:5:A:VAL:HG21  | 1:7:A:LEU:H    | 6        | 0.17          |
| (2,360) | 1:5:A:VAL:HG22  | 1:7:A:LEU:H    | 6        | 0.17          |
| (2,360) | 1:5:A:VAL:HG23  | 1:7:A:LEU:H    | 6        | 0.17          |
| (2,280) | 1:8:A:TYR:HD1   | 1:24:A:PRO:HB3 | 1        | 0.17          |
| (2,280) | 1:8:A:TYR:HD2   | 1:24:A:PRO:HB3 | 1        | 0.17          |
| (2,280) | 1:8:A:TYR:HD1   | 1:24:A:PRO:HB3 | 6        | 0.17          |
| (2,280) | 1:8:A:TYR:HD2   | 1:24:A:PRO:HB3 | 6        | 0.17          |
| (2,280) | 1:8:A:TYR:HD1   | 1:24:A:PRO:HB3 | 7        | 0.17          |
| (2,280) | 1:8:A:TYR:HD2   | 1:24:A:PRO:HB3 | 7        | 0.17          |
| (2,280) | 1:8:A:TYR:HD1   | 1:24:A:PRO:HB3 | 8        | 0.17          |
| (2,280) | 1:8:A:TYR:HD2   | 1:24:A:PRO:HB3 | 8        | 0.17          |
| (2,251) | 1:10:A:GLN:HE22 | 1:10:A:GLN:HG2 | 10       | 0.17          |
| (2,251) | 1:10:A:GLN:HE22 | 1:10:A:GLN:HG3 | 10       | 0.17          |
| (2,201) | 1:21:A:ARG:HB3  | 1:21:A:ARG:HG2 | 8        | 0.17          |
| (2,201) | 1:21:A:ARG:HB3  | 1:21:A:ARG:HG3 | 8        | 0.17          |
| (2,164) | 1:17:A:PRO:HB3  | 1:17:A:PRO:HD2 | 7        | 0.17          |
| (2,142) | 1:14:A:ASP:H    | 1:14:A:ASP:HB3 | 5        | 0.17          |
| (2,1)   | 1:2:A:GLU:HA    | 1:3:A:GLU:H    | 1        | 0.17          |
| (1,601) | 1:10:A:GLN:HA   | 1:13:A:LYS:H   | 2        | 0.17          |
| (1,558) | 1:4:A:ALA:HB1   | 1:7:A:LEU:HD11 | 4        | 0.17          |
| (1,558) | 1:4:A:ALA:HB1   | 1:7:A:LEU:HD12 | 4        | 0.17          |
| (1,558) | 1:4:A:ALA:HB1   | 1:7:A:LEU:HD13 | 4        | 0.17          |
| (1,558) | 1:4:A:ALA:HB2   | 1:7:A:LEU:HD11 | 4        | 0.17          |
| (1,558) | 1:4:A:ALA:HB2   | 1:7:A:LEU:HD12 | 4        | 0.17          |
| (1,558) | 1:4:A:ALA:HB2   | 1:7:A:LEU:HD13 | 4        | 0.17          |
| (1,558) | 1:4:A:ALA:HB3   | 1:7:A:LEU:HD11 | 4        | 0.17          |
| (1,558) | 1:4:A:ALA:HB3   | 1:7:A:LEU:HD12 | 4        | 0.17          |
| (1,558) | 1:4:A:ALA:HB3   | 1:7:A:LEU:HD13 | 4        | 0.17          |
| (1,540) | 1:2:A:GLU:HB3   | 1:5:A:VAL:HG11 | 4        | 0.17          |
| (1,540) | 1:2:A:GLU:HB3   | 1:5:A:VAL:HG12 | 4        | 0.17          |
| (1,540) | 1:2:A:GLU:HB3   | 1:5:A:VAL:HG13 | 4        | 0.17          |
| (1,539) | 1:2:A:GLU:HG2   | 1:5:A:VAL:HG21 | 2        | 0.17          |
| (1,539) | 1:2:A:GLU:HG2   | 1:5:A:VAL:HG22 | 2        | 0.17          |
| (1,539) | 1:2:A:GLU:HG2   | 1:5:A:VAL:HG23 | 2        | 0.17          |
| (1,539) | 1:2:A:GLU:HG3   | 1:5:A:VAL:HG21 | 2        | 0.17          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,539) | 1:2:A:GLU:HG3   | 1:5:A:VAL:HG22 | 2        | 0.17          |
| (1,539) | 1:2:A:GLU:HG3   | 1:5:A:VAL:HG23 | 2        | 0.17          |
| (1,529) | 1:12:A:LEU:HD11 | 1:17:A:PRO:HD2 | 2        | 0.17          |
| (1,529) | 1:12:A:LEU:HD12 | 1:17:A:PRO:HD2 | 2        | 0.17          |
| (1,529) | 1:12:A:LEU:HD13 | 1:17:A:PRO:HD2 | 2        | 0.17          |
| (1,529) | 1:12:A:LEU:HD11 | 1:17:A:PRO:HD2 | 5        | 0.17          |
| (1,529) | 1:12:A:LEU:HD12 | 1:17:A:PRO:HD2 | 5        | 0.17          |
| (1,529) | 1:12:A:LEU:HD13 | 1:17:A:PRO:HD2 | 5        | 0.17          |
| (1,512) | 1:1:A:GLU:HB2   | 1:2:A:GLU:HG2  | 1        | 0.17          |
| (1,480) | 1:6:A:ARG:HA    | 1:10:A:GLN:HB2 | 3        | 0.17          |
| (1,480) | 1:6:A:ARG:HA    | 1:10:A:GLN:HB2 | 8        | 0.17          |
| (1,447) | 1:6:A:ARG:H     | 1:7:A:LEU:HD11 | 3        | 0.17          |
| (1,447) | 1:6:A:ARG:H     | 1:7:A:LEU:HD12 | 3        | 0.17          |
| (1,447) | 1:6:A:ARG:H     | 1:7:A:LEU:HD13 | 3        | 0.17          |
| (1,437) | 1:13:A:LYS:HD2  | 1:14:A:ASP:H   | 3        | 0.17          |
| (1,437) | 1:13:A:LYS:HD3  | 1:14:A:ASP:H   | 3        | 0.17          |
| (1,411) | 1:5:A:VAL:HG21  | 1:7:A:LEU:H    | 6        | 0.17          |
| (1,411) | 1:5:A:VAL:HG22  | 1:7:A:LEU:H    | 6        | 0.17          |
| (1,411) | 1:5:A:VAL:HG23  | 1:7:A:LEU:H    | 6        | 0.17          |
| (1,370) | 1:4:A:ALA:H     | 1:5:A:VAL:H    | 9        | 0.17          |
| (1,357) | 1:11:A:TRP:HA   | 1:11:A:TRP:HE3 | 2        | 0.17          |
| (1,357) | 1:11:A:TRP:HA   | 1:11:A:TRP:HE3 | 5        | 0.17          |
| (1,357) | 1:11:A:TRP:HA   | 1:11:A:TRP:HE3 | 10       | 0.17          |
| (1,315) | 1:4:A:ALA:HB1   | 1:8:A:TYR:HE1  | 10       | 0.17          |
| (1,315) | 1:4:A:ALA:HB1   | 1:8:A:TYR:HE2  | 10       | 0.17          |
| (1,315) | 1:4:A:ALA:HB2   | 1:8:A:TYR:HE1  | 10       | 0.17          |
| (1,315) | 1:4:A:ALA:HB2   | 1:8:A:TYR:HE2  | 10       | 0.17          |
| (1,315) | 1:4:A:ALA:HB3   | 1:8:A:TYR:HE1  | 10       | 0.17          |
| (1,315) | 1:4:A:ALA:HB3   | 1:8:A:TYR:HE2  | 10       | 0.17          |
| (1,310) | 1:8:A:TYR:HE1   | 1:12:A:LEU:HG  | 1        | 0.17          |
| (1,310) | 1:8:A:TYR:HE2   | 1:12:A:LEU:HG  | 1        | 0.17          |
| (1,303) | 1:8:A:TYR:HD1   | 1:24:A:PRO:HB3 | 1        | 0.17          |
| (1,303) | 1:8:A:TYR:HD2   | 1:24:A:PRO:HB3 | 1        | 0.17          |
| (1,303) | 1:8:A:TYR:HD1   | 1:24:A:PRO:HB3 | 6        | 0.17          |
| (1,303) | 1:8:A:TYR:HD2   | 1:24:A:PRO:HB3 | 6        | 0.17          |
| (1,303) | 1:8:A:TYR:HD1   | 1:24:A:PRO:HB3 | 7        | 0.17          |
| (1,303) | 1:8:A:TYR:HD2   | 1:24:A:PRO:HB3 | 7        | 0.17          |
| (1,303) | 1:8:A:TYR:HD1   | 1:24:A:PRO:HB3 | 8        | 0.17          |
| (1,303) | 1:8:A:TYR:HD2   | 1:24:A:PRO:HB3 | 8        | 0.17          |
| (1,270) | 1:10:A:GLN:HE22 | 1:10:A:GLN:HG2 | 10       | 0.17          |
| (1,270) | 1:10:A:GLN:HE22 | 1:10:A:GLN:HG3 | 10       | 0.17          |
| (1,218) | 1:21:A:ARG:HB3  | 1:21:A:ARG:HG2 | 8        | 0.17          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,218) | 1:21:A:ARG:HB3  | 1:21:A:ARG:HG3  | 8        | 0.17          |
| (1,179) | 1:17:A:PRO:HB3  | 1:17:A:PRO:HD2  | 7        | 0.17          |
| (1,157) | 1:14:A:ASP:H    | 1:14:A:ASP:HB3  | 5        | 0.17          |
| (1,1)   | 1:2:A:GLU:HA    | 1:3:A:GLU:H     | 1        | 0.17          |
| (3,93)  | 1:10:A:GLN:HA   | 1:13:A:LYS:H    | 4        | 0.16          |
| (3,80)  | 1:4:A:ALA:HB1   | 1:7:A:LEU:HD11  | 1        | 0.16          |
| (3,80)  | 1:4:A:ALA:HB1   | 1:7:A:LEU:HD12  | 1        | 0.16          |
| (3,80)  | 1:4:A:ALA:HB1   | 1:7:A:LEU:HD13  | 1        | 0.16          |
| (3,80)  | 1:4:A:ALA:HB2   | 1:7:A:LEU:HD11  | 1        | 0.16          |
| (3,80)  | 1:4:A:ALA:HB2   | 1:7:A:LEU:HD12  | 1        | 0.16          |
| (3,80)  | 1:4:A:ALA:HB2   | 1:7:A:LEU:HD13  | 1        | 0.16          |
| (3,80)  | 1:4:A:ALA:HB3   | 1:7:A:LEU:HD11  | 1        | 0.16          |
| (3,80)  | 1:4:A:ALA:HB3   | 1:7:A:LEU:HD12  | 1        | 0.16          |
| (3,80)  | 1:4:A:ALA:HB3   | 1:7:A:LEU:HD13  | 1        | 0.16          |
| (3,77)  | 1:3:A:GLU:HG2   | 1:7:A:LEU:HD11  | 5        | 0.16          |
| (3,77)  | 1:3:A:GLU:HG2   | 1:7:A:LEU:HD12  | 5        | 0.16          |
| (3,77)  | 1:3:A:GLU:HG2   | 1:7:A:LEU:HD13  | 5        | 0.16          |
| (3,77)  | 1:3:A:GLU:HG3   | 1:7:A:LEU:HD11  | 5        | 0.16          |
| (3,77)  | 1:3:A:GLU:HG3   | 1:7:A:LEU:HD12  | 5        | 0.16          |
| (3,77)  | 1:3:A:GLU:HG3   | 1:7:A:LEU:HD13  | 5        | 0.16          |
| (3,71)  | 1:12:A:LEU:HD11 | 1:17:A:PRO:HD2  | 8        | 0.16          |
| (3,71)  | 1:12:A:LEU:HD12 | 1:17:A:PRO:HD2  | 8        | 0.16          |
| (3,71)  | 1:12:A:LEU:HD13 | 1:17:A:PRO:HD2  | 8        | 0.16          |
| (3,58)  | 1:13:A:LYS:HD2  | 1:14:A:ASP:H    | 2        | 0.16          |
| (3,58)  | 1:13:A:LYS:HD3  | 1:14:A:ASP:H    | 2        | 0.16          |
| (3,40)  | 1:11:A:TRP:HA   | 1:11:A:TRP:HE3  | 7        | 0.16          |
| (3,31)  | 1:8:A:TYR:HE1   | 1:12:A:LEU:HD21 | 1        | 0.16          |
| (3,31)  | 1:8:A:TYR:HE1   | 1:12:A:LEU:HD22 | 1        | 0.16          |
| (3,31)  | 1:8:A:TYR:HE1   | 1:12:A:LEU:HD23 | 1        | 0.16          |
| (3,31)  | 1:8:A:TYR:HE2   | 1:12:A:LEU:HD21 | 1        | 0.16          |
| (3,31)  | 1:8:A:TYR:HE2   | 1:12:A:LEU:HD22 | 1        | 0.16          |
| (3,31)  | 1:8:A:TYR:HE2   | 1:12:A:LEU:HD23 | 1        | 0.16          |
| (3,28)  | 1:4:A:ALA:HB1   | 1:8:A:TYR:HE1   | 2        | 0.16          |
| (3,28)  | 1:4:A:ALA:HB1   | 1:8:A:TYR:HE2   | 2        | 0.16          |
| (3,28)  | 1:4:A:ALA:HB2   | 1:8:A:TYR:HE1   | 2        | 0.16          |
| (3,28)  | 1:4:A:ALA:HB2   | 1:8:A:TYR:HE2   | 2        | 0.16          |
| (3,28)  | 1:4:A:ALA:HB3   | 1:8:A:TYR:HE1   | 2        | 0.16          |
| (3,28)  | 1:4:A:ALA:HB3   | 1:8:A:TYR:HE2   | 2        | 0.16          |
| (3,11)  | 1:12:A:LEU:HA   | 1:12:A:LEU:HD11 | 1        | 0.16          |
| (3,11)  | 1:12:A:LEU:HA   | 1:12:A:LEU:HD12 | 1        | 0.16          |
| (3,11)  | 1:12:A:LEU:HA   | 1:12:A:LEU:HD13 | 1        | 0.16          |
| (3,11)  | 1:12:A:LEU:HA   | 1:12:A:LEU:HD11 | 10       | 0.16          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (3,11)  | 1:12:A:LEU:HA   | 1:12:A:LEU:HD12 | 10       | 0.16          |
| (3,11)  | 1:12:A:LEU:HA   | 1:12:A:LEU:HD13 | 10       | 0.16          |
| (3,8)   | 1:8:A:TYR:HA    | 1:9:A:ILE:H     | 9        | 0.16          |
| (2,475) | 1:7:A:LEU:HD21  | 1:10:A:GLN:HG2  | 9        | 0.16          |
| (2,475) | 1:7:A:LEU:HD22  | 1:10:A:GLN:HG2  | 9        | 0.16          |
| (2,475) | 1:7:A:LEU:HD23  | 1:10:A:GLN:HG2  | 9        | 0.16          |
| (2,475) | 1:7:A:LEU:HD21  | 1:10:A:GLN:HG3  | 9        | 0.16          |
| (2,475) | 1:7:A:LEU:HD22  | 1:10:A:GLN:HG3  | 9        | 0.16          |
| (2,475) | 1:7:A:LEU:HD23  | 1:10:A:GLN:HG3  | 9        | 0.16          |
| (2,461) | 1:5:A:VAL:HG11  | 1:8:A:TYR:HB2   | 9        | 0.16          |
| (2,461) | 1:5:A:VAL:HG12  | 1:8:A:TYR:HB2   | 9        | 0.16          |
| (2,461) | 1:5:A:VAL:HG13  | 1:8:A:TYR:HB2   | 9        | 0.16          |
| (2,385) | 1:9:A:ILE:HG21  | 1:10:A:GLN:H    | 6        | 0.16          |
| (2,385) | 1:9:A:ILE:HG22  | 1:10:A:GLN:H    | 6        | 0.16          |
| (2,385) | 1:9:A:ILE:HG23  | 1:10:A:GLN:H    | 6        | 0.16          |
| (2,378) | 1:11:A:TRP:H    | 1:24:A:PRO:HG2  | 8        | 0.16          |
| (2,251) | 1:10:A:GLN:HE22 | 1:10:A:GLN:HG2  | 4        | 0.16          |
| (2,251) | 1:10:A:GLN:HE22 | 1:10:A:GLN:HG3  | 4        | 0.16          |
| (2,201) | 1:21:A:ARG:HB3  | 1:21:A:ARG:HG2  | 2        | 0.16          |
| (2,201) | 1:21:A:ARG:HB3  | 1:21:A:ARG:HG3  | 2        | 0.16          |
| (2,201) | 1:21:A:ARG:HB3  | 1:21:A:ARG:HG2  | 4        | 0.16          |
| (2,201) | 1:21:A:ARG:HB3  | 1:21:A:ARG:HG3  | 4        | 0.16          |
| (2,201) | 1:21:A:ARG:HB3  | 1:21:A:ARG:HG2  | 5        | 0.16          |
| (2,201) | 1:21:A:ARG:HB3  | 1:21:A:ARG:HG3  | 5        | 0.16          |
| (2,168) | 1:17:A:PRO:HB3  | 1:17:A:PRO:HG2  | 7        | 0.16          |
| (2,168) | 1:17:A:PRO:HB3  | 1:17:A:PRO:HG3  | 7        | 0.16          |
| (2,1)   | 1:2:A:GLU:HA    | 1:3:A:GLU:H     | 4        | 0.16          |
| (1,601) | 1:10:A:GLN:HA   | 1:13:A:LYS:H    | 4        | 0.16          |
| (1,558) | 1:4:A:ALA:HB1   | 1:7:A:LEU:HD11  | 1        | 0.16          |
| (1,558) | 1:4:A:ALA:HB1   | 1:7:A:LEU:HD12  | 1        | 0.16          |
| (1,558) | 1:4:A:ALA:HB1   | 1:7:A:LEU:HD13  | 1        | 0.16          |
| (1,558) | 1:4:A:ALA:HB2   | 1:7:A:LEU:HD11  | 1        | 0.16          |
| (1,558) | 1:4:A:ALA:HB2   | 1:7:A:LEU:HD12  | 1        | 0.16          |
| (1,558) | 1:4:A:ALA:HB2   | 1:7:A:LEU:HD13  | 1        | 0.16          |
| (1,558) | 1:4:A:ALA:HB3   | 1:7:A:LEU:HD11  | 1        | 0.16          |
| (1,558) | 1:4:A:ALA:HB3   | 1:7:A:LEU:HD12  | 1        | 0.16          |
| (1,558) | 1:4:A:ALA:HB3   | 1:7:A:LEU:HD13  | 1        | 0.16          |
| (1,552) | 1:3:A:GLU:HG2   | 1:7:A:LEU:HD11  | 5        | 0.16          |
| (1,552) | 1:3:A:GLU:HG2   | 1:7:A:LEU:HD12  | 5        | 0.16          |
| (1,552) | 1:3:A:GLU:HG2   | 1:7:A:LEU:HD13  | 5        | 0.16          |
| (1,552) | 1:3:A:GLU:HG3   | 1:7:A:LEU:HD11  | 5        | 0.16          |
| (1,552) | 1:3:A:GLU:HG3   | 1:7:A:LEU:HD12  | 5        | 0.16          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,552) | 1:3:A:GLU:HG3   | 1:7:A:LEU:HD13  | 5        | 0.16          |
| (1,551) | 1:7:A:LEU:HD21  | 1:10:A:GLN:HG2  | 9        | 0.16          |
| (1,551) | 1:7:A:LEU:HD22  | 1:10:A:GLN:HG2  | 9        | 0.16          |
| (1,551) | 1:7:A:LEU:HD23  | 1:10:A:GLN:HG2  | 9        | 0.16          |
| (1,551) | 1:7:A:LEU:HD21  | 1:10:A:GLN:HG3  | 9        | 0.16          |
| (1,551) | 1:7:A:LEU:HD22  | 1:10:A:GLN:HG3  | 9        | 0.16          |
| (1,551) | 1:7:A:LEU:HD23  | 1:10:A:GLN:HG3  | 9        | 0.16          |
| (1,532) | 1:5:A:VAL:HG11  | 1:8:A:TYR:HB2   | 9        | 0.16          |
| (1,532) | 1:5:A:VAL:HG12  | 1:8:A:TYR:HB2   | 9        | 0.16          |
| (1,532) | 1:5:A:VAL:HG13  | 1:8:A:TYR:HB2   | 9        | 0.16          |
| (1,529) | 1:12:A:LEU:HD11 | 1:17:A:PRO:HD2  | 8        | 0.16          |
| (1,529) | 1:12:A:LEU:HD12 | 1:17:A:PRO:HD2  | 8        | 0.16          |
| (1,529) | 1:12:A:LEU:HD13 | 1:17:A:PRO:HD2  | 8        | 0.16          |
| (1,445) | 1:9:A:ILE:HG21  | 1:10:A:GLN:H    | 6        | 0.16          |
| (1,445) | 1:9:A:ILE:HG22  | 1:10:A:GLN:H    | 6        | 0.16          |
| (1,445) | 1:9:A:ILE:HG23  | 1:10:A:GLN:H    | 6        | 0.16          |
| (1,437) | 1:13:A:LYS:HD2  | 1:14:A:ASP:H    | 2        | 0.16          |
| (1,437) | 1:13:A:LYS:HD3  | 1:14:A:ASP:H    | 2        | 0.16          |
| (1,434) | 1:11:A:TRP:H    | 1:24:A:PRO:HG2  | 8        | 0.16          |
| (1,357) | 1:11:A:TRP:HA   | 1:11:A:TRP:HE3  | 7        | 0.16          |
| (1,321) | 1:8:A:TYR:HE1   | 1:12:A:LEU:HD21 | 1        | 0.16          |
| (1,321) | 1:8:A:TYR:HE1   | 1:12:A:LEU:HD22 | 1        | 0.16          |
| (1,321) | 1:8:A:TYR:HE1   | 1:12:A:LEU:HD23 | 1        | 0.16          |
| (1,321) | 1:8:A:TYR:HE2   | 1:12:A:LEU:HD21 | 1        | 0.16          |
| (1,321) | 1:8:A:TYR:HE2   | 1:12:A:LEU:HD22 | 1        | 0.16          |
| (1,321) | 1:8:A:TYR:HE2   | 1:12:A:LEU:HD23 | 1        | 0.16          |
| (1,315) | 1:4:A:ALA:HB1   | 1:8:A:TYR:HE1   | 2        | 0.16          |
| (1,315) | 1:4:A:ALA:HB1   | 1:8:A:TYR:HE2   | 2        | 0.16          |
| (1,315) | 1:4:A:ALA:HB2   | 1:8:A:TYR:HE1   | 2        | 0.16          |
| (1,315) | 1:4:A:ALA:HB2   | 1:8:A:TYR:HE2   | 2        | 0.16          |
| (1,315) | 1:4:A:ALA:HB3   | 1:8:A:TYR:HE1   | 2        | 0.16          |
| (1,315) | 1:4:A:ALA:HB3   | 1:8:A:TYR:HE2   | 2        | 0.16          |
| (1,270) | 1:10:A:GLN:HE22 | 1:10:A:GLN:HG2  | 4        | 0.16          |
| (1,270) | 1:10:A:GLN:HE22 | 1:10:A:GLN:HG3  | 4        | 0.16          |
| (1,218) | 1:21:A:ARG:HB3  | 1:21:A:ARG:HG2  | 2        | 0.16          |
| (1,218) | 1:21:A:ARG:HB3  | 1:21:A:ARG:HG3  | 2        | 0.16          |
| (1,218) | 1:21:A:ARG:HB3  | 1:21:A:ARG:HG2  | 4        | 0.16          |
| (1,218) | 1:21:A:ARG:HB3  | 1:21:A:ARG:HG3  | 4        | 0.16          |
| (1,218) | 1:21:A:ARG:HB3  | 1:21:A:ARG:HG2  | 5        | 0.16          |
| (1,218) | 1:21:A:ARG:HB3  | 1:21:A:ARG:HG3  | 5        | 0.16          |
| (1,183) | 1:17:A:PRO:HB3  | 1:17:A:PRO:HG2  | 7        | 0.16          |
| (1,183) | 1:17:A:PRO:HB3  | 1:17:A:PRO:HG3  | 7        | 0.16          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,119) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD11 | 1        | 0.16          |
| (1,119) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD12 | 1        | 0.16          |
| (1,119) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD13 | 1        | 0.16          |
| (1,119) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD11 | 10       | 0.16          |
| (1,119) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD12 | 10       | 0.16          |
| (1,119) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD13 | 10       | 0.16          |
| (1,81)  | 1:8:A:TYR:HA    | 1:9:A:ILE:H     | 9        | 0.16          |
| (1,1)   | 1:2:A:GLU:HA    | 1:3:A:GLU:H     | 4        | 0.16          |
| (3,93)  | 1:10:A:GLN:HA   | 1:13:A:LYS:H    | 5        | 0.15          |
| (3,84)  | 1:3:A:GLU:HA    | 1:7:A:LEU:H     | 5        | 0.15          |
| (3,84)  | 1:3:A:GLU:HA    | 1:7:A:LEU:H     | 8        | 0.15          |
| (3,71)  | 1:12:A:LEU:HD11 | 1:17:A:PRO:HD2  | 1        | 0.15          |
| (3,71)  | 1:12:A:LEU:HD12 | 1:17:A:PRO:HD2  | 1        | 0.15          |
| (3,71)  | 1:12:A:LEU:HD13 | 1:17:A:PRO:HD2  | 1        | 0.15          |
| (3,71)  | 1:12:A:LEU:HD11 | 1:17:A:PRO:HD2  | 9        | 0.15          |
| (3,71)  | 1:12:A:LEU:HD12 | 1:17:A:PRO:HD2  | 9        | 0.15          |
| (3,71)  | 1:12:A:LEU:HD13 | 1:17:A:PRO:HD2  | 9        | 0.15          |
| (3,71)  | 1:12:A:LEU:HD11 | 1:17:A:PRO:HD2  | 10       | 0.15          |
| (3,71)  | 1:12:A:LEU:HD12 | 1:17:A:PRO:HD2  | 10       | 0.15          |
| (3,71)  | 1:12:A:LEU:HD13 | 1:17:A:PRO:HD2  | 10       | 0.15          |
| (3,64)  | 1:6:A:ARG:HA    | 1:10:A:GLN:HB2  | 2        | 0.15          |
| (3,63)  | 1:5:A:VAL:HA    | 1:8:A:TYR:HB2   | 5        | 0.15          |
| (3,63)  | 1:5:A:VAL:HA    | 1:8:A:TYR:HB2   | 6        | 0.15          |
| (3,63)  | 1:5:A:VAL:HA    | 1:8:A:TYR:HB2   | 8        | 0.15          |
| (3,41)  | 1:4:A:ALA:H     | 1:5:A:VAL:H     | 8        | 0.15          |
| (3,11)  | 1:12:A:LEU:HA   | 1:12:A:LEU:HD11 | 4        | 0.15          |
| (3,11)  | 1:12:A:LEU:HA   | 1:12:A:LEU:HD12 | 4        | 0.15          |
| (3,11)  | 1:12:A:LEU:HA   | 1:12:A:LEU:HD13 | 4        | 0.15          |
| (3,11)  | 1:12:A:LEU:HA   | 1:12:A:LEU:HD11 | 6        | 0.15          |
| (3,11)  | 1:12:A:LEU:HA   | 1:12:A:LEU:HD12 | 6        | 0.15          |
| (3,11)  | 1:12:A:LEU:HA   | 1:12:A:LEU:HD13 | 6        | 0.15          |
| (3,11)  | 1:12:A:LEU:HA   | 1:12:A:LEU:HD11 | 7        | 0.15          |
| (3,11)  | 1:12:A:LEU:HA   | 1:12:A:LEU:HD12 | 7        | 0.15          |
| (3,11)  | 1:12:A:LEU:HA   | 1:12:A:LEU:HD13 | 7        | 0.15          |
| (3,11)  | 1:12:A:LEU:HA   | 1:12:A:LEU:HD11 | 8        | 0.15          |
| (3,11)  | 1:12:A:LEU:HA   | 1:12:A:LEU:HD12 | 8        | 0.15          |
| (3,11)  | 1:12:A:LEU:HA   | 1:12:A:LEU:HD13 | 8        | 0.15          |
| (3,8)   | 1:8:A:TYR:HA    | 1:9:A:ILE:H     | 10       | 0.15          |
| (2,471) | 1:5:A:VAL:HG11  | 1:9:A:ILE:HG13  | 1        | 0.15          |
| (2,471) | 1:5:A:VAL:HG12  | 1:9:A:ILE:HG13  | 1        | 0.15          |
| (2,471) | 1:5:A:VAL:HG13  | 1:9:A:ILE:HG13  | 1        | 0.15          |
| (2,441) | 1:23:A:PRO:HB3  | 1:24:A:PRO:HD3  | 7        | 0.15          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (2,423) | 1:22:A:PRO:HB2  | 1:23:A:PRO:HD2 | 6        | 0.15          |
| (2,423) | 1:22:A:PRO:HB2  | 1:23:A:PRO:HD3 | 6        | 0.15          |
| (2,385) | 1:9:A:ILE:HG21  | 1:10:A:GLN:H   | 7        | 0.15          |
| (2,385) | 1:9:A:ILE:HG22  | 1:10:A:GLN:H   | 7        | 0.15          |
| (2,385) | 1:9:A:ILE:HG23  | 1:10:A:GLN:H   | 7        | 0.15          |
| (2,360) | 1:5:A:VAL:HG21  | 1:7:A:LEU:H    | 5        | 0.15          |
| (2,360) | 1:5:A:VAL:HG22  | 1:7:A:LEU:H    | 5        | 0.15          |
| (2,360) | 1:5:A:VAL:HG23  | 1:7:A:LEU:H    | 5        | 0.15          |
| (2,360) | 1:5:A:VAL:HG21  | 1:7:A:LEU:H    | 7        | 0.15          |
| (2,360) | 1:5:A:VAL:HG22  | 1:7:A:LEU:H    | 7        | 0.15          |
| (2,360) | 1:5:A:VAL:HG23  | 1:7:A:LEU:H    | 7        | 0.15          |
| (2,360) | 1:5:A:VAL:HG21  | 1:7:A:LEU:H    | 8        | 0.15          |
| (2,360) | 1:5:A:VAL:HG22  | 1:7:A:LEU:H    | 8        | 0.15          |
| (2,360) | 1:5:A:VAL:HG23  | 1:7:A:LEU:H    | 8        | 0.15          |
| (2,280) | 1:8:A:TYR:HD1   | 1:24:A:PRO:HB3 | 4        | 0.15          |
| (2,280) | 1:8:A:TYR:HD2   | 1:24:A:PRO:HB3 | 4        | 0.15          |
| (2,270) | 1:5:A:VAL:HA    | 1:8:A:TYR:HE1  | 8        | 0.15          |
| (2,270) | 1:5:A:VAL:HA    | 1:8:A:TYR:HE2  | 8        | 0.15          |
| (2,201) | 1:21:A:ARG:HB3  | 1:21:A:ARG:HG2 | 3        | 0.15          |
| (2,201) | 1:21:A:ARG:HB3  | 1:21:A:ARG:HG3 | 3        | 0.15          |
| (2,201) | 1:21:A:ARG:HB3  | 1:21:A:ARG:HG2 | 9        | 0.15          |
| (2,201) | 1:21:A:ARG:HB3  | 1:21:A:ARG:HG3 | 9        | 0.15          |
| (2,168) | 1:17:A:PRO:HB3  | 1:17:A:PRO:HG2 | 5        | 0.15          |
| (2,168) | 1:17:A:PRO:HB3  | 1:17:A:PRO:HG3 | 5        | 0.15          |
| (1,601) | 1:10:A:GLN:HA   | 1:13:A:LYS:H   | 5        | 0.15          |
| (1,569) | 1:3:A:GLU:HA    | 1:7:A:LEU:H    | 5        | 0.15          |
| (1,569) | 1:3:A:GLU:HA    | 1:7:A:LEU:H    | 8        | 0.15          |
| (1,547) | 1:5:A:VAL:HG11  | 1:9:A:ILE:HG13 | 1        | 0.15          |
| (1,547) | 1:5:A:VAL:HG12  | 1:9:A:ILE:HG13 | 1        | 0.15          |
| (1,547) | 1:5:A:VAL:HG13  | 1:9:A:ILE:HG13 | 1        | 0.15          |
| (1,529) | 1:12:A:LEU:HD11 | 1:17:A:PRO:HD2 | 1        | 0.15          |
| (1,529) | 1:12:A:LEU:HD12 | 1:17:A:PRO:HD2 | 1        | 0.15          |
| (1,529) | 1:12:A:LEU:HD13 | 1:17:A:PRO:HD2 | 1        | 0.15          |
| (1,529) | 1:12:A:LEU:HD11 | 1:17:A:PRO:HD2 | 9        | 0.15          |
| (1,529) | 1:12:A:LEU:HD12 | 1:17:A:PRO:HD2 | 9        | 0.15          |
| (1,529) | 1:12:A:LEU:HD13 | 1:17:A:PRO:HD2 | 9        | 0.15          |
| (1,529) | 1:12:A:LEU:HD11 | 1:17:A:PRO:HD2 | 10       | 0.15          |
| (1,529) | 1:12:A:LEU:HD12 | 1:17:A:PRO:HD2 | 10       | 0.15          |
| (1,529) | 1:12:A:LEU:HD13 | 1:17:A:PRO:HD2 | 10       | 0.15          |
| (1,508) | 1:23:A:PRO:HB3  | 1:24:A:PRO:HD3 | 7        | 0.15          |
| (1,488) | 1:22:A:PRO:HB2  | 1:23:A:PRO:HD2 | 6        | 0.15          |
| (1,488) | 1:22:A:PRO:HB2  | 1:23:A:PRO:HD3 | 6        | 0.15          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,480) | 1:6:A:ARG:HA   | 1:10:A:GLN:HB2  | 2        | 0.15          |
| (1,474) | 1:5:A:VAL:HA   | 1:8:A:TYR:HB2   | 5        | 0.15          |
| (1,474) | 1:5:A:VAL:HA   | 1:8:A:TYR:HB2   | 6        | 0.15          |
| (1,474) | 1:5:A:VAL:HA   | 1:8:A:TYR:HB2   | 8        | 0.15          |
| (1,445) | 1:9:A:ILE:HG21 | 1:10:A:GLN:H    | 7        | 0.15          |
| (1,445) | 1:9:A:ILE:HG22 | 1:10:A:GLN:H    | 7        | 0.15          |
| (1,445) | 1:9:A:ILE:HG23 | 1:10:A:GLN:H    | 7        | 0.15          |
| (1,411) | 1:5:A:VAL:HG21 | 1:7:A:LEU:H     | 5        | 0.15          |
| (1,411) | 1:5:A:VAL:HG22 | 1:7:A:LEU:H     | 5        | 0.15          |
| (1,411) | 1:5:A:VAL:HG23 | 1:7:A:LEU:H     | 5        | 0.15          |
| (1,411) | 1:5:A:VAL:HG21 | 1:7:A:LEU:H     | 7        | 0.15          |
| (1,411) | 1:5:A:VAL:HG22 | 1:7:A:LEU:H     | 7        | 0.15          |
| (1,411) | 1:5:A:VAL:HG23 | 1:7:A:LEU:H     | 7        | 0.15          |
| (1,411) | 1:5:A:VAL:HG21 | 1:7:A:LEU:H     | 8        | 0.15          |
| (1,411) | 1:5:A:VAL:HG22 | 1:7:A:LEU:H     | 8        | 0.15          |
| (1,411) | 1:5:A:VAL:HG23 | 1:7:A:LEU:H     | 8        | 0.15          |
| (1,370) | 1:4:A:ALA:H    | 1:5:A:VAL:H     | 8        | 0.15          |
| (1,303) | 1:8:A:TYR:HD1  | 1:24:A:PRO:HB3  | 4        | 0.15          |
| (1,303) | 1:8:A:TYR:HD2  | 1:24:A:PRO:HB3  | 4        | 0.15          |
| (1,290) | 1:5:A:VAL:HA   | 1:8:A:TYR:HE1   | 8        | 0.15          |
| (1,290) | 1:5:A:VAL:HA   | 1:8:A:TYR:HE2   | 8        | 0.15          |
| (1,218) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HG2  | 3        | 0.15          |
| (1,218) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HG3  | 3        | 0.15          |
| (1,218) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HG2  | 9        | 0.15          |
| (1,218) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HG3  | 9        | 0.15          |
| (1,183) | 1:17:A:PRO:HB3 | 1:17:A:PRO:HG2  | 5        | 0.15          |
| (1,183) | 1:17:A:PRO:HB3 | 1:17:A:PRO:HG3  | 5        | 0.15          |
| (1,119) | 1:12:A:LEU:HA  | 1:12:A:LEU:HD11 | 4        | 0.15          |
| (1,119) | 1:12:A:LEU:HA  | 1:12:A:LEU:HD12 | 4        | 0.15          |
| (1,119) | 1:12:A:LEU:HA  | 1:12:A:LEU:HD13 | 4        | 0.15          |
| (1,119) | 1:12:A:LEU:HA  | 1:12:A:LEU:HD11 | 6        | 0.15          |
| (1,119) | 1:12:A:LEU:HA  | 1:12:A:LEU:HD12 | 6        | 0.15          |
| (1,119) | 1:12:A:LEU:HA  | 1:12:A:LEU:HD13 | 6        | 0.15          |
| (1,119) | 1:12:A:LEU:HA  | 1:12:A:LEU:HD11 | 7        | 0.15          |
| (1,119) | 1:12:A:LEU:HA  | 1:12:A:LEU:HD12 | 7        | 0.15          |
| (1,119) | 1:12:A:LEU:HA  | 1:12:A:LEU:HD13 | 7        | 0.15          |
| (1,119) | 1:12:A:LEU:HA  | 1:12:A:LEU:HD11 | 8        | 0.15          |
| (1,119) | 1:12:A:LEU:HA  | 1:12:A:LEU:HD12 | 8        | 0.15          |
| (1,119) | 1:12:A:LEU:HA  | 1:12:A:LEU:HD13 | 8        | 0.15          |
| (1,81)  | 1:8:A:TYR:HA   | 1:9:A:ILE:H     | 10       | 0.15          |
| (3,93)  | 1:10:A:GLN:HA  | 1:13:A:LYS:H    | 6        | 0.14          |
| (3,93)  | 1:10:A:GLN:HA  | 1:13:A:LYS:H    | 7        | 0.14          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (3,71)  | 1:12:A:LEU:HD11 | 1:17:A:PRO:HD2  | 7        | 0.14          |
| (3,71)  | 1:12:A:LEU:HD12 | 1:17:A:PRO:HD2  | 7        | 0.14          |
| (3,71)  | 1:12:A:LEU:HD13 | 1:17:A:PRO:HD2  | 7        | 0.14          |
| (3,64)  | 1:6:A:ARG:HA    | 1:10:A:GLN:HB2  | 6        | 0.14          |
| (3,63)  | 1:5:A:VAL:HA    | 1:8:A:TYR:HB2   | 2        | 0.14          |
| (3,63)  | 1:5:A:VAL:HA    | 1:8:A:TYR:HB2   | 7        | 0.14          |
| (3,45)  | 1:11:A:TRP:HH2  | 1:11:A:TRP:HZ3  | 1        | 0.14          |
| (3,45)  | 1:11:A:TRP:HH2  | 1:11:A:TRP:HZ3  | 4        | 0.14          |
| (3,45)  | 1:11:A:TRP:HH2  | 1:11:A:TRP:HZ3  | 8        | 0.14          |
| (3,45)  | 1:11:A:TRP:HH2  | 1:11:A:TRP:HZ3  | 9        | 0.14          |
| (3,41)  | 1:4:A:ALA:H     | 1:5:A:VAL:H     | 2        | 0.14          |
| (3,41)  | 1:4:A:ALA:H     | 1:5:A:VAL:H     | 5        | 0.14          |
| (3,11)  | 1:12:A:LEU:HA   | 1:12:A:LEU:HD11 | 2        | 0.14          |
| (3,11)  | 1:12:A:LEU:HA   | 1:12:A:LEU:HD12 | 2        | 0.14          |
| (3,11)  | 1:12:A:LEU:HA   | 1:12:A:LEU:HD13 | 2        | 0.14          |
| (3,11)  | 1:12:A:LEU:HA   | 1:12:A:LEU:HD11 | 3        | 0.14          |
| (3,11)  | 1:12:A:LEU:HA   | 1:12:A:LEU:HD12 | 3        | 0.14          |
| (3,11)  | 1:12:A:LEU:HA   | 1:12:A:LEU:HD13 | 3        | 0.14          |
| (3,11)  | 1:12:A:LEU:HA   | 1:12:A:LEU:HD11 | 5        | 0.14          |
| (3,11)  | 1:12:A:LEU:HA   | 1:12:A:LEU:HD12 | 5        | 0.14          |
| (3,11)  | 1:12:A:LEU:HA   | 1:12:A:LEU:HD13 | 5        | 0.14          |
| (3,8)   | 1:8:A:TYR:HA    | 1:9:A:ILE:H     | 2        | 0.14          |
| (3,8)   | 1:8:A:TYR:HA    | 1:9:A:ILE:H     | 4        | 0.14          |
| (2,461) | 1:5:A:VAL:HG11  | 1:8:A:TYR:HB2   | 10       | 0.14          |
| (2,461) | 1:5:A:VAL:HG12  | 1:8:A:TYR:HB2   | 10       | 0.14          |
| (2,461) | 1:5:A:VAL:HG13  | 1:8:A:TYR:HB2   | 10       | 0.14          |
| (2,459) | 1:9:A:ILE:HA    | 1:12:A:LEU:HD21 | 10       | 0.14          |
| (2,459) | 1:9:A:ILE:HA    | 1:12:A:LEU:HD22 | 10       | 0.14          |
| (2,459) | 1:9:A:ILE:HA    | 1:12:A:LEU:HD23 | 10       | 0.14          |
| (2,456) | 1:5:A:VAL:HA    | 1:9:A:ILE:HD11  | 9        | 0.14          |
| (2,456) | 1:5:A:VAL:HA    | 1:9:A:ILE:HD12  | 9        | 0.14          |
| (2,456) | 1:5:A:VAL:HA    | 1:9:A:ILE:HD13  | 9        | 0.14          |
| (2,456) | 1:5:A:VAL:HA    | 1:9:A:ILE:HD11  | 10       | 0.14          |
| (2,456) | 1:5:A:VAL:HA    | 1:9:A:ILE:HD12  | 10       | 0.14          |
| (2,456) | 1:5:A:VAL:HA    | 1:9:A:ILE:HD13  | 10       | 0.14          |
| (2,426) | 1:21:A:ARG:HG2  | 1:22:A:PRO:HD3  | 9        | 0.14          |
| (2,426) | 1:21:A:ARG:HG3  | 1:22:A:PRO:HD3  | 9        | 0.14          |
| (2,423) | 1:22:A:PRO:HB2  | 1:23:A:PRO:HD2  | 1        | 0.14          |
| (2,423) | 1:22:A:PRO:HB2  | 1:23:A:PRO:HD3  | 1        | 0.14          |
| (2,414) | 1:14:A:ASP:HB2  | 1:19:A:SER:HB2  | 2        | 0.14          |
| (2,414) | 1:14:A:ASP:HB2  | 1:19:A:SER:HB2  | 7        | 0.14          |
| (2,385) | 1:9:A:ILE:HG21  | 1:10:A:GLN:H    | 5        | 0.14          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,385) | 1:9:A:ILE:HG22  | 1:10:A:GLN:H    | 5        | 0.14          |
| (2,385) | 1:9:A:ILE:HG23  | 1:10:A:GLN:H    | 5        | 0.14          |
| (2,385) | 1:9:A:ILE:HG21  | 1:10:A:GLN:H    | 8        | 0.14          |
| (2,385) | 1:9:A:ILE:HG22  | 1:10:A:GLN:H    | 8        | 0.14          |
| (2,385) | 1:9:A:ILE:HG23  | 1:10:A:GLN:H    | 8        | 0.14          |
| (2,270) | 1:5:A:VAL:HA    | 1:8:A:TYR:HE1   | 1        | 0.14          |
| (2,270) | 1:5:A:VAL:HA    | 1:8:A:TYR:HE2   | 1        | 0.14          |
| (2,270) | 1:5:A:VAL:HA    | 1:8:A:TYR:HE1   | 7        | 0.14          |
| (2,270) | 1:5:A:VAL:HA    | 1:8:A:TYR:HE2   | 7        | 0.14          |
| (2,168) | 1:17:A:PRO:HB3  | 1:17:A:PRO:HG2  | 2        | 0.14          |
| (2,168) | 1:17:A:PRO:HB3  | 1:17:A:PRO:HG3  | 2        | 0.14          |
| (2,168) | 1:17:A:PRO:HB3  | 1:17:A:PRO:HG2  | 3        | 0.14          |
| (2,168) | 1:17:A:PRO:HB3  | 1:17:A:PRO:HG3  | 3        | 0.14          |
| (2,168) | 1:17:A:PRO:HB3  | 1:17:A:PRO:HG2  | 4        | 0.14          |
| (2,168) | 1:17:A:PRO:HB3  | 1:17:A:PRO:HG3  | 4        | 0.14          |
| (2,168) | 1:17:A:PRO:HB3  | 1:17:A:PRO:HG2  | 6        | 0.14          |
| (2,168) | 1:17:A:PRO:HB3  | 1:17:A:PRO:HG3  | 6        | 0.14          |
| (2,168) | 1:17:A:PRO:HB3  | 1:17:A:PRO:HG2  | 8        | 0.14          |
| (2,168) | 1:17:A:PRO:HB3  | 1:17:A:PRO:HG3  | 8        | 0.14          |
| (2,168) | 1:17:A:PRO:HB3  | 1:17:A:PRO:HG2  | 10       | 0.14          |
| (2,168) | 1:17:A:PRO:HB3  | 1:17:A:PRO:HG3  | 10       | 0.14          |
| (2,13)  | 1:3:A:GLU:H     | 1:3:A:GLU:HG2   | 4        | 0.14          |
| (2,13)  | 1:3:A:GLU:H     | 1:3:A:GLU:HG3   | 4        | 0.14          |
| (1,601) | 1:10:A:GLN:HA   | 1:13:A:LYS:H    | 6        | 0.14          |
| (1,601) | 1:10:A:GLN:HA   | 1:13:A:LYS:H    | 7        | 0.14          |
| (1,532) | 1:5:A:VAL:HG11  | 1:8:A:TYR:HB2   | 10       | 0.14          |
| (1,532) | 1:5:A:VAL:HG12  | 1:8:A:TYR:HB2   | 10       | 0.14          |
| (1,532) | 1:5:A:VAL:HG13  | 1:8:A:TYR:HB2   | 10       | 0.14          |
| (1,530) | 1:9:A:ILE:HA    | 1:12:A:LEU:HD21 | 10       | 0.14          |
| (1,530) | 1:9:A:ILE:HA    | 1:12:A:LEU:HD22 | 10       | 0.14          |
| (1,530) | 1:9:A:ILE:HA    | 1:12:A:LEU:HD23 | 10       | 0.14          |
| (1,529) | 1:12:A:LEU:HD11 | 1:17:A:PRO:HD2  | 7        | 0.14          |
| (1,529) | 1:12:A:LEU:HD12 | 1:17:A:PRO:HD2  | 7        | 0.14          |
| (1,529) | 1:12:A:LEU:HD13 | 1:17:A:PRO:HD2  | 7        | 0.14          |
| (1,526) | 1:5:A:VAL:HA    | 1:9:A:ILE:HD11  | 9        | 0.14          |
| (1,526) | 1:5:A:VAL:HA    | 1:9:A:ILE:HD12  | 9        | 0.14          |
| (1,526) | 1:5:A:VAL:HA    | 1:9:A:ILE:HD13  | 9        | 0.14          |
| (1,526) | 1:5:A:VAL:HA    | 1:9:A:ILE:HD11  | 10       | 0.14          |
| (1,526) | 1:5:A:VAL:HA    | 1:9:A:ILE:HD12  | 10       | 0.14          |
| (1,526) | 1:5:A:VAL:HA    | 1:9:A:ILE:HD13  | 10       | 0.14          |
| (1,493) | 1:21:A:ARG:HG2  | 1:22:A:PRO:HD3  | 9        | 0.14          |
| (1,493) | 1:21:A:ARG:HG3  | 1:22:A:PRO:HD3  | 9        | 0.14          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,488) | 1:22:A:PRO:HB2 | 1:23:A:PRO:HD2  | 1        | 0.14          |
| (1,488) | 1:22:A:PRO:HB2 | 1:23:A:PRO:HD3  | 1        | 0.14          |
| (1,480) | 1:6:A:ARG:HA   | 1:10:A:GLN:HB2  | 6        | 0.14          |
| (1,477) | 1:14:A:ASP:HB2 | 1:19:A:SER:HB2  | 2        | 0.14          |
| (1,477) | 1:14:A:ASP:HB2 | 1:19:A:SER:HB2  | 7        | 0.14          |
| (1,474) | 1:5:A:VAL:HA   | 1:8:A:TYR:HB2   | 2        | 0.14          |
| (1,474) | 1:5:A:VAL:HA   | 1:8:A:TYR:HB2   | 7        | 0.14          |
| (1,445) | 1:9:A:ILE:HG21 | 1:10:A:GLN:H    | 5        | 0.14          |
| (1,445) | 1:9:A:ILE:HG22 | 1:10:A:GLN:H    | 5        | 0.14          |
| (1,445) | 1:9:A:ILE:HG23 | 1:10:A:GLN:H    | 5        | 0.14          |
| (1,445) | 1:9:A:ILE:HG21 | 1:10:A:GLN:H    | 8        | 0.14          |
| (1,445) | 1:9:A:ILE:HG22 | 1:10:A:GLN:H    | 8        | 0.14          |
| (1,445) | 1:9:A:ILE:HG23 | 1:10:A:GLN:H    | 8        | 0.14          |
| (1,383) | 1:11:A:TRP:HH2 | 1:11:A:TRP:HZ3  | 1        | 0.14          |
| (1,383) | 1:11:A:TRP:HH2 | 1:11:A:TRP:HZ3  | 4        | 0.14          |
| (1,383) | 1:11:A:TRP:HH2 | 1:11:A:TRP:HZ3  | 8        | 0.14          |
| (1,383) | 1:11:A:TRP:HH2 | 1:11:A:TRP:HZ3  | 9        | 0.14          |
| (1,370) | 1:4:A:ALA:H    | 1:5:A:VAL:H     | 2        | 0.14          |
| (1,370) | 1:4:A:ALA:H    | 1:5:A:VAL:H     | 5        | 0.14          |
| (1,290) | 1:5:A:VAL:HA   | 1:8:A:TYR:HE1   | 1        | 0.14          |
| (1,290) | 1:5:A:VAL:HA   | 1:8:A:TYR:HE2   | 1        | 0.14          |
| (1,290) | 1:5:A:VAL:HA   | 1:8:A:TYR:HE1   | 7        | 0.14          |
| (1,290) | 1:5:A:VAL:HA   | 1:8:A:TYR:HE2   | 7        | 0.14          |
| (1,183) | 1:17:A:PRO:HB3 | 1:17:A:PRO:HG2  | 2        | 0.14          |
| (1,183) | 1:17:A:PRO:HB3 | 1:17:A:PRO:HG3  | 2        | 0.14          |
| (1,183) | 1:17:A:PRO:HB3 | 1:17:A:PRO:HG2  | 3        | 0.14          |
| (1,183) | 1:17:A:PRO:HB3 | 1:17:A:PRO:HG3  | 3        | 0.14          |
| (1,183) | 1:17:A:PRO:HB3 | 1:17:A:PRO:HG2  | 4        | 0.14          |
| (1,183) | 1:17:A:PRO:HB3 | 1:17:A:PRO:HG3  | 4        | 0.14          |
| (1,183) | 1:17:A:PRO:HB3 | 1:17:A:PRO:HG2  | 6        | 0.14          |
| (1,183) | 1:17:A:PRO:HB3 | 1:17:A:PRO:HG3  | 6        | 0.14          |
| (1,183) | 1:17:A:PRO:HB3 | 1:17:A:PRO:HG2  | 8        | 0.14          |
| (1,183) | 1:17:A:PRO:HB3 | 1:17:A:PRO:HG3  | 8        | 0.14          |
| (1,183) | 1:17:A:PRO:HB3 | 1:17:A:PRO:HG2  | 10       | 0.14          |
| (1,183) | 1:17:A:PRO:HB3 | 1:17:A:PRO:HG3  | 10       | 0.14          |
| (1,119) | 1:12:A:LEU:HA  | 1:12:A:LEU:HD11 | 2        | 0.14          |
| (1,119) | 1:12:A:LEU:HA  | 1:12:A:LEU:HD12 | 2        | 0.14          |
| (1,119) | 1:12:A:LEU:HA  | 1:12:A:LEU:HD13 | 2        | 0.14          |
| (1,119) | 1:12:A:LEU:HA  | 1:12:A:LEU:HD11 | 3        | 0.14          |
| (1,119) | 1:12:A:LEU:HA  | 1:12:A:LEU:HD12 | 3        | 0.14          |
| (1,119) | 1:12:A:LEU:HA  | 1:12:A:LEU:HD13 | 3        | 0.14          |
| (1,119) | 1:12:A:LEU:HA  | 1:12:A:LEU:HD11 | 5        | 0.14          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,119) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD12 | 5        | 0.14          |
| (1,119) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD13 | 5        | 0.14          |
| (1,81)  | 1:8:A:TYR:HA    | 1:9:A:ILE:H     | 2        | 0.14          |
| (1,81)  | 1:8:A:TYR:HA    | 1:9:A:ILE:H     | 4        | 0.14          |
| (1,13)  | 1:3:A:GLU:H     | 1:3:A:GLU:HG2   | 4        | 0.14          |
| (1,13)  | 1:3:A:GLU:H     | 1:3:A:GLU:HG3   | 4        | 0.14          |
| (3,84)  | 1:3:A:GLU:HA    | 1:7:A:LEU:H     | 6        | 0.13          |
| (3,77)  | 1:3:A:GLU:HG2   | 1:7:A:LEU:HD11  | 4        | 0.13          |
| (3,77)  | 1:3:A:GLU:HG2   | 1:7:A:LEU:HD12  | 4        | 0.13          |
| (3,77)  | 1:3:A:GLU:HG2   | 1:7:A:LEU:HD13  | 4        | 0.13          |
| (3,77)  | 1:3:A:GLU:HG3   | 1:7:A:LEU:HD11  | 4        | 0.13          |
| (3,77)  | 1:3:A:GLU:HG3   | 1:7:A:LEU:HD12  | 4        | 0.13          |
| (3,77)  | 1:3:A:GLU:HG3   | 1:7:A:LEU:HD13  | 4        | 0.13          |
| (3,77)  | 1:3:A:GLU:HG2   | 1:7:A:LEU:HD11  | 7        | 0.13          |
| (3,77)  | 1:3:A:GLU:HG2   | 1:7:A:LEU:HD12  | 7        | 0.13          |
| (3,77)  | 1:3:A:GLU:HG2   | 1:7:A:LEU:HD13  | 7        | 0.13          |
| (3,77)  | 1:3:A:GLU:HG3   | 1:7:A:LEU:HD11  | 7        | 0.13          |
| (3,77)  | 1:3:A:GLU:HG3   | 1:7:A:LEU:HD12  | 7        | 0.13          |
| (3,77)  | 1:3:A:GLU:HG3   | 1:7:A:LEU:HD13  | 7        | 0.13          |
| (3,77)  | 1:3:A:GLU:HG2   | 1:7:A:LEU:HD11  | 8        | 0.13          |
| (3,77)  | 1:3:A:GLU:HG2   | 1:7:A:LEU:HD12  | 8        | 0.13          |
| (3,77)  | 1:3:A:GLU:HG2   | 1:7:A:LEU:HD13  | 8        | 0.13          |
| (3,77)  | 1:3:A:GLU:HG3   | 1:7:A:LEU:HD11  | 8        | 0.13          |
| (3,77)  | 1:3:A:GLU:HG3   | 1:7:A:LEU:HD12  | 8        | 0.13          |
| (3,77)  | 1:3:A:GLU:HG3   | 1:7:A:LEU:HD13  | 8        | 0.13          |
| (3,73)  | 1:2:A:GLU:HG2   | 1:5:A:VAL:HG21  | 1        | 0.13          |
| (3,73)  | 1:2:A:GLU:HG2   | 1:5:A:VAL:HG22  | 1        | 0.13          |
| (3,73)  | 1:2:A:GLU:HG2   | 1:5:A:VAL:HG23  | 1        | 0.13          |
| (3,73)  | 1:2:A:GLU:HG3   | 1:5:A:VAL:HG21  | 1        | 0.13          |
| (3,73)  | 1:2:A:GLU:HG3   | 1:5:A:VAL:HG22  | 1        | 0.13          |
| (3,73)  | 1:2:A:GLU:HG3   | 1:5:A:VAL:HG23  | 1        | 0.13          |
| (3,73)  | 1:2:A:GLU:HG2   | 1:5:A:VAL:HG21  | 3        | 0.13          |
| (3,73)  | 1:2:A:GLU:HG2   | 1:5:A:VAL:HG22  | 3        | 0.13          |
| (3,73)  | 1:2:A:GLU:HG2   | 1:5:A:VAL:HG23  | 3        | 0.13          |
| (3,73)  | 1:2:A:GLU:HG3   | 1:5:A:VAL:HG21  | 3        | 0.13          |
| (3,73)  | 1:2:A:GLU:HG3   | 1:5:A:VAL:HG22  | 3        | 0.13          |
| (3,73)  | 1:2:A:GLU:HG3   | 1:5:A:VAL:HG23  | 3        | 0.13          |
| (3,71)  | 1:12:A:LEU:HD11 | 1:17:A:PRO:HD2  | 3        | 0.13          |
| (3,71)  | 1:12:A:LEU:HD12 | 1:17:A:PRO:HD2  | 3        | 0.13          |
| (3,71)  | 1:12:A:LEU:HD13 | 1:17:A:PRO:HD2  | 3        | 0.13          |
| (3,70)  | 1:6:A:ARG:HA    | 1:9:A:ILE:HG21  | 1        | 0.13          |
| (3,70)  | 1:6:A:ARG:HA    | 1:9:A:ILE:HG22  | 1        | 0.13          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (3,70)  | 1:6:A:ARG:HA   | 1:9:A:ILE:HG23 | 1        | 0.13          |
| (3,63)  | 1:5:A:VAL:HA   | 1:8:A:TYR:HB2  | 1        | 0.13          |
| (3,63)  | 1:5:A:VAL:HA   | 1:8:A:TYR:HB2  | 3        | 0.13          |
| (3,63)  | 1:5:A:VAL:HA   | 1:8:A:TYR:HB2  | 4        | 0.13          |
| (3,63)  | 1:5:A:VAL:HA   | 1:8:A:TYR:HB2  | 9        | 0.13          |
| (3,63)  | 1:5:A:VAL:HA   | 1:8:A:TYR:HB2  | 10       | 0.13          |
| (3,45)  | 1:11:A:TRP:HH2 | 1:11:A:TRP:HZ3 | 2        | 0.13          |
| (3,45)  | 1:11:A:TRP:HH2 | 1:11:A:TRP:HZ3 | 3        | 0.13          |
| (3,45)  | 1:11:A:TRP:HH2 | 1:11:A:TRP:HZ3 | 5        | 0.13          |
| (3,45)  | 1:11:A:TRP:HH2 | 1:11:A:TRP:HZ3 | 6        | 0.13          |
| (3,45)  | 1:11:A:TRP:HH2 | 1:11:A:TRP:HZ3 | 7        | 0.13          |
| (3,45)  | 1:11:A:TRP:HH2 | 1:11:A:TRP:HZ3 | 10       | 0.13          |
| (3,41)  | 1:4:A:ALA:H    | 1:5:A:VAL:H    | 7        | 0.13          |
| (3,40)  | 1:11:A:TRP:HA  | 1:11:A:TRP:HE3 | 6        | 0.13          |
| (3,28)  | 1:4:A:ALA:HB1  | 1:8:A:TYR:HE1  | 6        | 0.13          |
| (3,28)  | 1:4:A:ALA:HB1  | 1:8:A:TYR:HE2  | 6        | 0.13          |
| (3,28)  | 1:4:A:ALA:HB2  | 1:8:A:TYR:HE1  | 6        | 0.13          |
| (3,28)  | 1:4:A:ALA:HB2  | 1:8:A:TYR:HE2  | 6        | 0.13          |
| (3,28)  | 1:4:A:ALA:HB3  | 1:8:A:TYR:HE1  | 6        | 0.13          |
| (3,28)  | 1:4:A:ALA:HB3  | 1:8:A:TYR:HE2  | 6        | 0.13          |
| (3,20)  | 1:8:A:TYR:HA   | 1:8:A:TYR:HE1  | 10       | 0.13          |
| (3,20)  | 1:8:A:TYR:HA   | 1:8:A:TYR:HE2  | 10       | 0.13          |
| (3,8)   | 1:8:A:TYR:HA   | 1:9:A:ILE:H    | 1        | 0.13          |
| (3,8)   | 1:8:A:TYR:HA   | 1:9:A:ILE:H    | 3        | 0.13          |
| (3,8)   | 1:8:A:TYR:HA   | 1:9:A:ILE:H    | 7        | 0.13          |
| (3,8)   | 1:8:A:TYR:HA   | 1:9:A:ILE:H    | 8        | 0.13          |
| (3,7)   | 1:7:A:LEU:H    | 1:7:A:LEU:HG   | 9        | 0.13          |
| (3,7)   | 1:7:A:LEU:H    | 1:7:A:LEU:HG   | 10       | 0.13          |
| (2,474) | 1:9:A:ILE:HD11 | 1:13:A:LYS:HE3 | 8        | 0.13          |
| (2,474) | 1:9:A:ILE:HD12 | 1:13:A:LYS:HE3 | 8        | 0.13          |
| (2,474) | 1:9:A:ILE:HD13 | 1:13:A:LYS:HE3 | 8        | 0.13          |
| (2,471) | 1:5:A:VAL:HG11 | 1:9:A:ILE:HG13 | 4        | 0.13          |
| (2,471) | 1:5:A:VAL:HG12 | 1:9:A:ILE:HG13 | 4        | 0.13          |
| (2,471) | 1:5:A:VAL:HG13 | 1:9:A:ILE:HG13 | 4        | 0.13          |
| (2,471) | 1:5:A:VAL:HG11 | 1:9:A:ILE:HG13 | 5        | 0.13          |
| (2,471) | 1:5:A:VAL:HG12 | 1:9:A:ILE:HG13 | 5        | 0.13          |
| (2,471) | 1:5:A:VAL:HG13 | 1:9:A:ILE:HG13 | 5        | 0.13          |
| (2,470) | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG11 | 1        | 0.13          |
| (2,470) | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG12 | 1        | 0.13          |
| (2,470) | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG13 | 1        | 0.13          |
| (2,470) | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG11 | 1        | 0.13          |
| (2,470) | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG12 | 1        | 0.13          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (2,470) | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG13 | 1        | 0.13          |
| (2,470) | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG11 | 1        | 0.13          |
| (2,470) | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG12 | 1        | 0.13          |
| (2,470) | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG13 | 1        | 0.13          |
| (2,470) | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG11 | 3        | 0.13          |
| (2,470) | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG12 | 3        | 0.13          |
| (2,470) | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG13 | 3        | 0.13          |
| (2,470) | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG11 | 3        | 0.13          |
| (2,470) | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG12 | 3        | 0.13          |
| (2,470) | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG13 | 3        | 0.13          |
| (2,470) | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG11 | 3        | 0.13          |
| (2,470) | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG12 | 3        | 0.13          |
| (2,470) | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG13 | 3        | 0.13          |
| (2,456) | 1:5:A:VAL:HA   | 1:9:A:ILE:HD11 | 6        | 0.13          |
| (2,456) | 1:5:A:VAL:HA   | 1:9:A:ILE:HD12 | 6        | 0.13          |
| (2,456) | 1:5:A:VAL:HA   | 1:9:A:ILE:HD13 | 6        | 0.13          |
| (2,426) | 1:21:A:ARG:HG2 | 1:22:A:PRO:HD3 | 4        | 0.13          |
| (2,426) | 1:21:A:ARG:HG3 | 1:22:A:PRO:HD3 | 4        | 0.13          |
| (2,423) | 1:22:A:PRO:HB2 | 1:23:A:PRO:HD2 | 2        | 0.13          |
| (2,423) | 1:22:A:PRO:HB2 | 1:23:A:PRO:HD3 | 2        | 0.13          |
| (2,385) | 1:9:A:ILE:HG21 | 1:10:A:GLN:H   | 2        | 0.13          |
| (2,385) | 1:9:A:ILE:HG22 | 1:10:A:GLN:H   | 2        | 0.13          |
| (2,385) | 1:9:A:ILE:HG23 | 1:10:A:GLN:H   | 2        | 0.13          |
| (2,385) | 1:9:A:ILE:HG21 | 1:10:A:GLN:H   | 3        | 0.13          |
| (2,385) | 1:9:A:ILE:HG22 | 1:10:A:GLN:H   | 3        | 0.13          |
| (2,385) | 1:9:A:ILE:HG23 | 1:10:A:GLN:H   | 3        | 0.13          |
| (2,385) | 1:9:A:ILE:HG21 | 1:10:A:GLN:H   | 4        | 0.13          |
| (2,385) | 1:9:A:ILE:HG22 | 1:10:A:GLN:H   | 4        | 0.13          |
| (2,385) | 1:9:A:ILE:HG23 | 1:10:A:GLN:H   | 4        | 0.13          |
| (2,312) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HA  | 2        | 0.13          |
| (2,283) | 1:11:A:TRP:HD1 | 1:21:A:ARG:HB3 | 3        | 0.13          |
| (2,278) | 1:11:A:TRP:HD1 | 1:23:A:PRO:HA  | 5        | 0.13          |
| (2,257) | 1:11:A:TRP:HE1 | 1:21:A:ARG:HG2 | 1        | 0.13          |
| (2,257) | 1:11:A:TRP:HE1 | 1:21:A:ARG:HG3 | 1        | 0.13          |
| (2,168) | 1:17:A:PRO:HB3 | 1:17:A:PRO:HG2 | 1        | 0.13          |
| (2,168) | 1:17:A:PRO:HB3 | 1:17:A:PRO:HG3 | 1        | 0.13          |
| (2,168) | 1:17:A:PRO:HB3 | 1:17:A:PRO:HG2 | 9        | 0.13          |
| (2,168) | 1:17:A:PRO:HB3 | 1:17:A:PRO:HG3 | 9        | 0.13          |
| (2,49)  | 1:6:A:ARG:H    | 1:6:A:ARG:HG2  | 6        | 0.13          |
| (2,1)   | 1:2:A:GLU:HA   | 1:3:A:GLU:H    | 2        | 0.13          |
| (2,1)   | 1:2:A:GLU:HA   | 1:3:A:GLU:H    | 5        | 0.13          |
| (2,1)   | 1:2:A:GLU:HA   | 1:3:A:GLU:H    | 9        | 0.13          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,569) | 1:3:A:GLU:HA   | 1:7:A:LEU:H    | 6        | 0.13          |
| (1,552) | 1:3:A:GLU:HG2  | 1:7:A:LEU:HD11 | 4        | 0.13          |
| (1,552) | 1:3:A:GLU:HG2  | 1:7:A:LEU:HD12 | 4        | 0.13          |
| (1,552) | 1:3:A:GLU:HG2  | 1:7:A:LEU:HD13 | 4        | 0.13          |
| (1,552) | 1:3:A:GLU:HG3  | 1:7:A:LEU:HD11 | 4        | 0.13          |
| (1,552) | 1:3:A:GLU:HG3  | 1:7:A:LEU:HD12 | 4        | 0.13          |
| (1,552) | 1:3:A:GLU:HG3  | 1:7:A:LEU:HD13 | 4        | 0.13          |
| (1,552) | 1:3:A:GLU:HG2  | 1:7:A:LEU:HD11 | 7        | 0.13          |
| (1,552) | 1:3:A:GLU:HG2  | 1:7:A:LEU:HD12 | 7        | 0.13          |
| (1,552) | 1:3:A:GLU:HG2  | 1:7:A:LEU:HD13 | 7        | 0.13          |
| (1,552) | 1:3:A:GLU:HG3  | 1:7:A:LEU:HD11 | 7        | 0.13          |
| (1,552) | 1:3:A:GLU:HG3  | 1:7:A:LEU:HD12 | 7        | 0.13          |
| (1,552) | 1:3:A:GLU:HG3  | 1:7:A:LEU:HD13 | 7        | 0.13          |
| (1,552) | 1:3:A:GLU:HG2  | 1:7:A:LEU:HD11 | 8        | 0.13          |
| (1,552) | 1:3:A:GLU:HG2  | 1:7:A:LEU:HD12 | 8        | 0.13          |
| (1,552) | 1:3:A:GLU:HG2  | 1:7:A:LEU:HD13 | 8        | 0.13          |
| (1,552) | 1:3:A:GLU:HG3  | 1:7:A:LEU:HD11 | 8        | 0.13          |
| (1,552) | 1:3:A:GLU:HG3  | 1:7:A:LEU:HD12 | 8        | 0.13          |
| (1,552) | 1:3:A:GLU:HG3  | 1:7:A:LEU:HD13 | 8        | 0.13          |
| (1,550) | 1:9:A:ILE:HD11 | 1:13:A:LYS:HE3 | 8        | 0.13          |
| (1,550) | 1:9:A:ILE:HD12 | 1:13:A:LYS:HE3 | 8        | 0.13          |
| (1,550) | 1:9:A:ILE:HD13 | 1:13:A:LYS:HE3 | 8        | 0.13          |
| (1,547) | 1:5:A:VAL:HG11 | 1:9:A:ILE:HG13 | 4        | 0.13          |
| (1,547) | 1:5:A:VAL:HG12 | 1:9:A:ILE:HG13 | 4        | 0.13          |
| (1,547) | 1:5:A:VAL:HG13 | 1:9:A:ILE:HG13 | 4        | 0.13          |
| (1,547) | 1:5:A:VAL:HG11 | 1:9:A:ILE:HG13 | 5        | 0.13          |
| (1,547) | 1:5:A:VAL:HG12 | 1:9:A:ILE:HG13 | 5        | 0.13          |
| (1,547) | 1:5:A:VAL:HG13 | 1:9:A:ILE:HG13 | 5        | 0.13          |
| (1,545) | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG11 | 1        | 0.13          |
| (1,545) | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG12 | 1        | 0.13          |
| (1,545) | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG13 | 1        | 0.13          |
| (1,545) | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG11 | 1        | 0.13          |
| (1,545) | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG12 | 1        | 0.13          |
| (1,545) | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG13 | 1        | 0.13          |
| (1,545) | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG11 | 1        | 0.13          |
| (1,545) | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG12 | 1        | 0.13          |
| (1,545) | 1:4:A:ALA:HB3  | 1:5:A:VAL:HG13 | 1        | 0.13          |
| (1,545) | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG11 | 3        | 0.13          |
| (1,545) | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG12 | 3        | 0.13          |
| (1,545) | 1:4:A:ALA:HB1  | 1:5:A:VAL:HG13 | 3        | 0.13          |
| (1,545) | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG11 | 3        | 0.13          |
| (1,545) | 1:4:A:ALA:HB2  | 1:5:A:VAL:HG12 | 3        | 0.13          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,545) | 1:4:A:ALA:HB2   | 1:5:A:VAL:HG13 | 3        | 0.13          |
| (1,545) | 1:4:A:ALA:HB3   | 1:5:A:VAL:HG11 | 3        | 0.13          |
| (1,545) | 1:4:A:ALA:HB3   | 1:5:A:VAL:HG12 | 3        | 0.13          |
| (1,545) | 1:4:A:ALA:HB3   | 1:5:A:VAL:HG13 | 3        | 0.13          |
| (1,539) | 1:2:A:GLU:HG2   | 1:5:A:VAL:HG21 | 1        | 0.13          |
| (1,539) | 1:2:A:GLU:HG2   | 1:5:A:VAL:HG22 | 1        | 0.13          |
| (1,539) | 1:2:A:GLU:HG2   | 1:5:A:VAL:HG23 | 1        | 0.13          |
| (1,539) | 1:2:A:GLU:HG3   | 1:5:A:VAL:HG21 | 1        | 0.13          |
| (1,539) | 1:2:A:GLU:HG3   | 1:5:A:VAL:HG22 | 1        | 0.13          |
| (1,539) | 1:2:A:GLU:HG3   | 1:5:A:VAL:HG23 | 1        | 0.13          |
| (1,539) | 1:2:A:GLU:HG2   | 1:5:A:VAL:HG21 | 3        | 0.13          |
| (1,539) | 1:2:A:GLU:HG2   | 1:5:A:VAL:HG22 | 3        | 0.13          |
| (1,539) | 1:2:A:GLU:HG2   | 1:5:A:VAL:HG23 | 3        | 0.13          |
| (1,539) | 1:2:A:GLU:HG3   | 1:5:A:VAL:HG21 | 3        | 0.13          |
| (1,539) | 1:2:A:GLU:HG3   | 1:5:A:VAL:HG22 | 3        | 0.13          |
| (1,539) | 1:2:A:GLU:HG3   | 1:5:A:VAL:HG23 | 3        | 0.13          |
| (1,529) | 1:12:A:LEU:HD11 | 1:17:A:PRO:HD2 | 3        | 0.13          |
| (1,529) | 1:12:A:LEU:HD12 | 1:17:A:PRO:HD2 | 3        | 0.13          |
| (1,529) | 1:12:A:LEU:HD13 | 1:17:A:PRO:HD2 | 3        | 0.13          |
| (1,526) | 1:5:A:VAL:HA    | 1:9:A:ILE:HD11 | 6        | 0.13          |
| (1,526) | 1:5:A:VAL:HA    | 1:9:A:ILE:HD12 | 6        | 0.13          |
| (1,526) | 1:5:A:VAL:HA    | 1:9:A:ILE:HD13 | 6        | 0.13          |
| (1,521) | 1:6:A:ARG:HA    | 1:9:A:ILE:HG21 | 1        | 0.13          |
| (1,521) | 1:6:A:ARG:HA    | 1:9:A:ILE:HG22 | 1        | 0.13          |
| (1,521) | 1:6:A:ARG:HA    | 1:9:A:ILE:HG23 | 1        | 0.13          |
| (1,493) | 1:21:A:ARG:HG2  | 1:22:A:PRO:HD3 | 4        | 0.13          |
| (1,493) | 1:21:A:ARG:HG3  | 1:22:A:PRO:HD3 | 4        | 0.13          |
| (1,488) | 1:22:A:PRO:HB2  | 1:23:A:PRO:HD2 | 2        | 0.13          |
| (1,488) | 1:22:A:PRO:HB2  | 1:23:A:PRO:HD3 | 2        | 0.13          |
| (1,474) | 1:5:A:VAL:HA    | 1:8:A:TYR:HB2  | 1        | 0.13          |
| (1,474) | 1:5:A:VAL:HA    | 1:8:A:TYR:HB2  | 3        | 0.13          |
| (1,474) | 1:5:A:VAL:HA    | 1:8:A:TYR:HB2  | 4        | 0.13          |
| (1,474) | 1:5:A:VAL:HA    | 1:8:A:TYR:HB2  | 9        | 0.13          |
| (1,474) | 1:5:A:VAL:HA    | 1:8:A:TYR:HB2  | 10       | 0.13          |
| (1,445) | 1:9:A:ILE:HG21  | 1:10:A:GLN:H   | 2        | 0.13          |
| (1,445) | 1:9:A:ILE:HG22  | 1:10:A:GLN:H   | 2        | 0.13          |
| (1,445) | 1:9:A:ILE:HG23  | 1:10:A:GLN:H   | 2        | 0.13          |
| (1,445) | 1:9:A:ILE:HG21  | 1:10:A:GLN:H   | 3        | 0.13          |
| (1,445) | 1:9:A:ILE:HG22  | 1:10:A:GLN:H   | 3        | 0.13          |
| (1,445) | 1:9:A:ILE:HG23  | 1:10:A:GLN:H   | 3        | 0.13          |
| (1,445) | 1:9:A:ILE:HG21  | 1:10:A:GLN:H   | 4        | 0.13          |
| (1,445) | 1:9:A:ILE:HG22  | 1:10:A:GLN:H   | 4        | 0.13          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,445) | 1:9:A:ILE:HG23 | 1:10:A:GLN:H   | 4        | 0.13          |
| (1,383) | 1:11:A:TRP:HH2 | 1:11:A:TRP:HZ3 | 2        | 0.13          |
| (1,383) | 1:11:A:TRP:HH2 | 1:11:A:TRP:HZ3 | 3        | 0.13          |
| (1,383) | 1:11:A:TRP:HH2 | 1:11:A:TRP:HZ3 | 5        | 0.13          |
| (1,383) | 1:11:A:TRP:HH2 | 1:11:A:TRP:HZ3 | 6        | 0.13          |
| (1,383) | 1:11:A:TRP:HH2 | 1:11:A:TRP:HZ3 | 7        | 0.13          |
| (1,383) | 1:11:A:TRP:HH2 | 1:11:A:TRP:HZ3 | 10       | 0.13          |
| (1,370) | 1:4:A:ALA:H    | 1:5:A:VAL:H    | 7        | 0.13          |
| (1,357) | 1:11:A:TRP:HA  | 1:11:A:TRP:HE3 | 6        | 0.13          |
| (1,349) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HA  | 2        | 0.13          |
| (1,315) | 1:4:A:ALA:HB1  | 1:8:A:TYR:HE1  | 6        | 0.13          |
| (1,315) | 1:4:A:ALA:HB1  | 1:8:A:TYR:HE2  | 6        | 0.13          |
| (1,315) | 1:4:A:ALA:HB2  | 1:8:A:TYR:HE1  | 6        | 0.13          |
| (1,315) | 1:4:A:ALA:HB2  | 1:8:A:TYR:HE2  | 6        | 0.13          |
| (1,315) | 1:4:A:ALA:HB3  | 1:8:A:TYR:HE1  | 6        | 0.13          |
| (1,315) | 1:4:A:ALA:HB3  | 1:8:A:TYR:HE2  | 6        | 0.13          |
| (1,306) | 1:11:A:TRP:HD1 | 1:21:A:ARG:HB3 | 3        | 0.13          |
| (1,301) | 1:11:A:TRP:HD1 | 1:23:A:PRO:HA  | 5        | 0.13          |
| (1,287) | 1:8:A:TYR:HA   | 1:8:A:TYR:HE1  | 10       | 0.13          |
| (1,287) | 1:8:A:TYR:HA   | 1:8:A:TYR:HE2  | 10       | 0.13          |
| (1,276) | 1:11:A:TRP:HE1 | 1:21:A:ARG:HG2 | 1        | 0.13          |
| (1,276) | 1:11:A:TRP:HE1 | 1:21:A:ARG:HG3 | 1        | 0.13          |
| (1,183) | 1:17:A:PRO:HB3 | 1:17:A:PRO:HG2 | 1        | 0.13          |
| (1,183) | 1:17:A:PRO:HB3 | 1:17:A:PRO:HG3 | 1        | 0.13          |
| (1,183) | 1:17:A:PRO:HB3 | 1:17:A:PRO:HG2 | 9        | 0.13          |
| (1,183) | 1:17:A:PRO:HB3 | 1:17:A:PRO:HG3 | 9        | 0.13          |
| (1,81)  | 1:8:A:TYR:HA   | 1:9:A:ILE:H    | 1        | 0.13          |
| (1,81)  | 1:8:A:TYR:HA   | 1:9:A:ILE:H    | 3        | 0.13          |
| (1,81)  | 1:8:A:TYR:HA   | 1:9:A:ILE:H    | 7        | 0.13          |
| (1,81)  | 1:8:A:TYR:HA   | 1:9:A:ILE:H    | 8        | 0.13          |
| (1,70)  | 1:7:A:LEU:H    | 1:7:A:LEU:HG   | 9        | 0.13          |
| (1,70)  | 1:7:A:LEU:H    | 1:7:A:LEU:HG   | 10       | 0.13          |
| (1,52)  | 1:6:A:ARG:H    | 1:6:A:ARG:HG2  | 6        | 0.13          |
| (1,1)   | 1:2:A:GLU:HA   | 1:3:A:GLU:H    | 2        | 0.13          |
| (1,1)   | 1:2:A:GLU:HA   | 1:3:A:GLU:H    | 5        | 0.13          |
| (1,1)   | 1:2:A:GLU:HA   | 1:3:A:GLU:H    | 9        | 0.13          |
| (3,84)  | 1:3:A:GLU:HA   | 1:7:A:LEU:H    | 7        | 0.12          |
| (3,70)  | 1:6:A:ARG:HA   | 1:9:A:ILE:HG21 | 3        | 0.12          |
| (3,70)  | 1:6:A:ARG:HA   | 1:9:A:ILE:HG22 | 3        | 0.12          |
| (3,70)  | 1:6:A:ARG:HA   | 1:9:A:ILE:HG23 | 3        | 0.12          |
| (3,28)  | 1:4:A:ALA:HB1  | 1:8:A:TYR:HE1  | 5        | 0.12          |
| (3,28)  | 1:4:A:ALA:HB1  | 1:8:A:TYR:HE2  | 5        | 0.12          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (3,28)  | 1:4:A:ALA:HB2  | 1:8:A:TYR:HE1  | 5        | 0.12          |
| (3,28)  | 1:4:A:ALA:HB2  | 1:8:A:TYR:HE2  | 5        | 0.12          |
| (3,28)  | 1:4:A:ALA:HB3  | 1:8:A:TYR:HE1  | 5        | 0.12          |
| (3,28)  | 1:4:A:ALA:HB3  | 1:8:A:TYR:HE2  | 5        | 0.12          |
| (3,24)  | 1:11:A:TRP:HD1 | 1:21:A:ARG:HG2 | 10       | 0.12          |
| (3,24)  | 1:11:A:TRP:HD1 | 1:21:A:ARG:HG3 | 10       | 0.12          |
| (3,8)   | 1:8:A:TYR:HA   | 1:9:A:ILE:H    | 5        | 0.12          |
| (3,8)   | 1:8:A:TYR:HA   | 1:9:A:ILE:H    | 6        | 0.12          |
| (2,471) | 1:5:A:VAL:HG11 | 1:9:A:ILE:HG13 | 2        | 0.12          |
| (2,471) | 1:5:A:VAL:HG12 | 1:9:A:ILE:HG13 | 2        | 0.12          |
| (2,471) | 1:5:A:VAL:HG13 | 1:9:A:ILE:HG13 | 2        | 0.12          |
| (2,471) | 1:5:A:VAL:HG11 | 1:9:A:ILE:HG13 | 3        | 0.12          |
| (2,471) | 1:5:A:VAL:HG12 | 1:9:A:ILE:HG13 | 3        | 0.12          |
| (2,471) | 1:5:A:VAL:HG13 | 1:9:A:ILE:HG13 | 3        | 0.12          |
| (2,471) | 1:5:A:VAL:HG11 | 1:9:A:ILE:HG13 | 6        | 0.12          |
| (2,471) | 1:5:A:VAL:HG12 | 1:9:A:ILE:HG13 | 6        | 0.12          |
| (2,471) | 1:5:A:VAL:HG13 | 1:9:A:ILE:HG13 | 6        | 0.12          |
| (2,467) | 1:2:A:GLU:HB3  | 1:5:A:VAL:HG11 | 1        | 0.12          |
| (2,467) | 1:2:A:GLU:HB3  | 1:5:A:VAL:HG12 | 1        | 0.12          |
| (2,467) | 1:2:A:GLU:HB3  | 1:5:A:VAL:HG13 | 1        | 0.12          |
| (2,467) | 1:2:A:GLU:HB3  | 1:5:A:VAL:HG11 | 3        | 0.12          |
| (2,467) | 1:2:A:GLU:HB3  | 1:5:A:VAL:HG12 | 3        | 0.12          |
| (2,467) | 1:2:A:GLU:HB3  | 1:5:A:VAL:HG13 | 3        | 0.12          |
| (2,463) | 1:7:A:LEU:HD11 | 1:8:A:TYR:HB2  | 1        | 0.12          |
| (2,463) | 1:7:A:LEU:HD12 | 1:8:A:TYR:HB2  | 1        | 0.12          |
| (2,463) | 1:7:A:LEU:HD13 | 1:8:A:TYR:HB2  | 1        | 0.12          |
| (2,463) | 1:7:A:LEU:HD11 | 1:8:A:TYR:HB2  | 4        | 0.12          |
| (2,463) | 1:7:A:LEU:HD12 | 1:8:A:TYR:HB2  | 4        | 0.12          |
| (2,463) | 1:7:A:LEU:HD13 | 1:8:A:TYR:HB2  | 4        | 0.12          |
| (2,456) | 1:5:A:VAL:HA   | 1:9:A:ILE:HD11 | 2        | 0.12          |
| (2,456) | 1:5:A:VAL:HA   | 1:9:A:ILE:HD12 | 2        | 0.12          |
| (2,456) | 1:5:A:VAL:HA   | 1:9:A:ILE:HD13 | 2        | 0.12          |
| (2,456) | 1:5:A:VAL:HA   | 1:9:A:ILE:HD11 | 4        | 0.12          |
| (2,456) | 1:5:A:VAL:HA   | 1:9:A:ILE:HD12 | 4        | 0.12          |
| (2,456) | 1:5:A:VAL:HA   | 1:9:A:ILE:HD13 | 4        | 0.12          |
| (2,456) | 1:5:A:VAL:HA   | 1:9:A:ILE:HD11 | 5        | 0.12          |
| (2,456) | 1:5:A:VAL:HA   | 1:9:A:ILE:HD12 | 5        | 0.12          |
| (2,456) | 1:5:A:VAL:HA   | 1:9:A:ILE:HD13 | 5        | 0.12          |
| (2,456) | 1:5:A:VAL:HA   | 1:9:A:ILE:HD11 | 7        | 0.12          |
| (2,456) | 1:5:A:VAL:HA   | 1:9:A:ILE:HD12 | 7        | 0.12          |
| (2,456) | 1:5:A:VAL:HA   | 1:9:A:ILE:HD13 | 7        | 0.12          |
| (2,456) | 1:5:A:VAL:HA   | 1:9:A:ILE:HD11 | 8        | 0.12          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (2,456) | 1:5:A:VAL:HA   | 1:9:A:ILE:HD12  | 8        | 0.12          |
| (2,456) | 1:5:A:VAL:HA   | 1:9:A:ILE:HD13  | 8        | 0.12          |
| (2,441) | 1:23:A:PRO:HB3 | 1:24:A:PRO:HD3  | 9        | 0.12          |
| (2,426) | 1:21:A:ARG:HG2 | 1:22:A:PRO:HD3  | 3        | 0.12          |
| (2,426) | 1:21:A:ARG:HG3 | 1:22:A:PRO:HD3  | 3        | 0.12          |
| (2,426) | 1:21:A:ARG:HG2 | 1:22:A:PRO:HD3  | 7        | 0.12          |
| (2,426) | 1:21:A:ARG:HG3 | 1:22:A:PRO:HD3  | 7        | 0.12          |
| (2,423) | 1:22:A:PRO:HB2 | 1:23:A:PRO:HD2  | 5        | 0.12          |
| (2,423) | 1:22:A:PRO:HB2 | 1:23:A:PRO:HD3  | 5        | 0.12          |
| (2,386) | 1:23:A:PRO:HB3 | 1:25:A:SER:H    | 10       | 0.12          |
| (2,312) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HA   | 3        | 0.12          |
| (2,312) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HA   | 4        | 0.12          |
| (2,312) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HA   | 5        | 0.12          |
| (2,312) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HA   | 7        | 0.12          |
| (2,312) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HA   | 8        | 0.12          |
| (2,289) | 1:8:A:TYR:HD1  | 1:12:A:LEU:HD21 | 2        | 0.12          |
| (2,289) | 1:8:A:TYR:HD1  | 1:12:A:LEU:HD22 | 2        | 0.12          |
| (2,289) | 1:8:A:TYR:HD1  | 1:12:A:LEU:HD23 | 2        | 0.12          |
| (2,289) | 1:8:A:TYR:HD2  | 1:12:A:LEU:HD21 | 2        | 0.12          |
| (2,289) | 1:8:A:TYR:HD2  | 1:12:A:LEU:HD22 | 2        | 0.12          |
| (2,289) | 1:8:A:TYR:HD2  | 1:12:A:LEU:HD23 | 2        | 0.12          |
| (2,278) | 1:11:A:TRP:HD1 | 1:23:A:PRO:HA   | 2        | 0.12          |
| (2,278) | 1:11:A:TRP:HD1 | 1:23:A:PRO:HA   | 3        | 0.12          |
| (2,278) | 1:11:A:TRP:HD1 | 1:23:A:PRO:HA   | 6        | 0.12          |
| (2,270) | 1:5:A:VAL:HA   | 1:8:A:TYR:HE1   | 9        | 0.12          |
| (2,270) | 1:5:A:VAL:HA   | 1:8:A:TYR:HE2   | 9        | 0.12          |
| (2,270) | 1:5:A:VAL:HA   | 1:8:A:TYR:HE1   | 10       | 0.12          |
| (2,270) | 1:5:A:VAL:HA   | 1:8:A:TYR:HE2   | 10       | 0.12          |
| (2,94)  | 1:10:A:GLN:H   | 1:10:A:GLN:HG2  | 9        | 0.12          |
| (2,94)  | 1:10:A:GLN:H   | 1:10:A:GLN:HG3  | 9        | 0.12          |
| (2,1)   | 1:2:A:GLU:HA   | 1:3:A:GLU:H     | 6        | 0.12          |
| (2,1)   | 1:2:A:GLU:HA   | 1:3:A:GLU:H     | 8        | 0.12          |
| (2,1)   | 1:2:A:GLU:HA   | 1:3:A:GLU:H     | 10       | 0.12          |
| (1,569) | 1:3:A:GLU:HA   | 1:7:A:LEU:H     | 7        | 0.12          |
| (1,547) | 1:5:A:VAL:HG11 | 1:9:A:ILE:HG13  | 2        | 0.12          |
| (1,547) | 1:5:A:VAL:HG12 | 1:9:A:ILE:HG13  | 2        | 0.12          |
| (1,547) | 1:5:A:VAL:HG13 | 1:9:A:ILE:HG13  | 2        | 0.12          |
| (1,547) | 1:5:A:VAL:HG11 | 1:9:A:ILE:HG13  | 3        | 0.12          |
| (1,547) | 1:5:A:VAL:HG12 | 1:9:A:ILE:HG13  | 3        | 0.12          |
| (1,547) | 1:5:A:VAL:HG13 | 1:9:A:ILE:HG13  | 3        | 0.12          |
| (1,547) | 1:5:A:VAL:HG11 | 1:9:A:ILE:HG13  | 6        | 0.12          |
| (1,547) | 1:5:A:VAL:HG12 | 1:9:A:ILE:HG13  | 6        | 0.12          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,547) | 1:5:A:VAL:HG13 | 1:9:A:ILE:HG13 | 6        | 0.12          |
| (1,540) | 1:2:A:GLU:HB3  | 1:5:A:VAL:HG11 | 1        | 0.12          |
| (1,540) | 1:2:A:GLU:HB3  | 1:5:A:VAL:HG12 | 1        | 0.12          |
| (1,540) | 1:2:A:GLU:HB3  | 1:5:A:VAL:HG13 | 1        | 0.12          |
| (1,540) | 1:2:A:GLU:HB3  | 1:5:A:VAL:HG11 | 3        | 0.12          |
| (1,540) | 1:2:A:GLU:HB3  | 1:5:A:VAL:HG12 | 3        | 0.12          |
| (1,540) | 1:2:A:GLU:HB3  | 1:5:A:VAL:HG13 | 3        | 0.12          |
| (1,534) | 1:7:A:LEU:HD11 | 1:8:A:TYR:HB2  | 1        | 0.12          |
| (1,534) | 1:7:A:LEU:HD12 | 1:8:A:TYR:HB2  | 1        | 0.12          |
| (1,534) | 1:7:A:LEU:HD13 | 1:8:A:TYR:HB2  | 1        | 0.12          |
| (1,534) | 1:7:A:LEU:HD11 | 1:8:A:TYR:HB2  | 4        | 0.12          |
| (1,534) | 1:7:A:LEU:HD12 | 1:8:A:TYR:HB2  | 4        | 0.12          |
| (1,534) | 1:7:A:LEU:HD13 | 1:8:A:TYR:HB2  | 4        | 0.12          |
| (1,526) | 1:5:A:VAL:HA   | 1:9:A:ILE:HD11 | 2        | 0.12          |
| (1,526) | 1:5:A:VAL:HA   | 1:9:A:ILE:HD12 | 2        | 0.12          |
| (1,526) | 1:5:A:VAL:HA   | 1:9:A:ILE:HD13 | 2        | 0.12          |
| (1,526) | 1:5:A:VAL:HA   | 1:9:A:ILE:HD11 | 4        | 0.12          |
| (1,526) | 1:5:A:VAL:HA   | 1:9:A:ILE:HD12 | 4        | 0.12          |
| (1,526) | 1:5:A:VAL:HA   | 1:9:A:ILE:HD13 | 4        | 0.12          |
| (1,526) | 1:5:A:VAL:HA   | 1:9:A:ILE:HD11 | 5        | 0.12          |
| (1,526) | 1:5:A:VAL:HA   | 1:9:A:ILE:HD12 | 5        | 0.12          |
| (1,526) | 1:5:A:VAL:HA   | 1:9:A:ILE:HD13 | 5        | 0.12          |
| (1,526) | 1:5:A:VAL:HA   | 1:9:A:ILE:HD11 | 7        | 0.12          |
| (1,526) | 1:5:A:VAL:HA   | 1:9:A:ILE:HD12 | 7        | 0.12          |
| (1,526) | 1:5:A:VAL:HA   | 1:9:A:ILE:HD13 | 7        | 0.12          |
| (1,526) | 1:5:A:VAL:HA   | 1:9:A:ILE:HD11 | 8        | 0.12          |
| (1,526) | 1:5:A:VAL:HA   | 1:9:A:ILE:HD12 | 8        | 0.12          |
| (1,526) | 1:5:A:VAL:HA   | 1:9:A:ILE:HD13 | 8        | 0.12          |
| (1,521) | 1:6:A:ARG:HA   | 1:9:A:ILE:HG21 | 3        | 0.12          |
| (1,521) | 1:6:A:ARG:HA   | 1:9:A:ILE:HG22 | 3        | 0.12          |
| (1,521) | 1:6:A:ARG:HA   | 1:9:A:ILE:HG23 | 3        | 0.12          |
| (1,508) | 1:23:A:PRO:HB3 | 1:24:A:PRO:HD3 | 9        | 0.12          |
| (1,493) | 1:21:A:ARG:HG2 | 1:22:A:PRO:HD3 | 3        | 0.12          |
| (1,493) | 1:21:A:ARG:HG3 | 1:22:A:PRO:HD3 | 3        | 0.12          |
| (1,493) | 1:21:A:ARG:HG2 | 1:22:A:PRO:HD3 | 7        | 0.12          |
| (1,493) | 1:21:A:ARG:HG3 | 1:22:A:PRO:HD3 | 7        | 0.12          |
| (1,488) | 1:22:A:PRO:HB2 | 1:23:A:PRO:HD2 | 5        | 0.12          |
| (1,488) | 1:22:A:PRO:HB2 | 1:23:A:PRO:HD3 | 5        | 0.12          |
| (1,448) | 1:23:A:PRO:HB3 | 1:25:A:SER:H   | 10       | 0.12          |
| (1,349) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HA  | 3        | 0.12          |
| (1,349) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HA  | 4        | 0.12          |
| (1,349) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HA  | 5        | 0.12          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,349) | 1:11:A:TRP:HE3  | 1:12:A:LEU:HA   | 7        | 0.12          |
| (1,349) | 1:11:A:TRP:HE3  | 1:12:A:LEU:HA   | 8        | 0.12          |
| (1,319) | 1:8:A:TYR:HD1   | 1:12:A:LEU:HD21 | 2        | 0.12          |
| (1,319) | 1:8:A:TYR:HD1   | 1:12:A:LEU:HD22 | 2        | 0.12          |
| (1,319) | 1:8:A:TYR:HD1   | 1:12:A:LEU:HD23 | 2        | 0.12          |
| (1,319) | 1:8:A:TYR:HD2   | 1:12:A:LEU:HD21 | 2        | 0.12          |
| (1,319) | 1:8:A:TYR:HD2   | 1:12:A:LEU:HD22 | 2        | 0.12          |
| (1,319) | 1:8:A:TYR:HD2   | 1:12:A:LEU:HD23 | 2        | 0.12          |
| (1,315) | 1:4:A:ALA:HB1   | 1:8:A:TYR:HE1   | 5        | 0.12          |
| (1,315) | 1:4:A:ALA:HB1   | 1:8:A:TYR:HE2   | 5        | 0.12          |
| (1,315) | 1:4:A:ALA:HB2   | 1:8:A:TYR:HE1   | 5        | 0.12          |
| (1,315) | 1:4:A:ALA:HB2   | 1:8:A:TYR:HE2   | 5        | 0.12          |
| (1,315) | 1:4:A:ALA:HB3   | 1:8:A:TYR:HE1   | 5        | 0.12          |
| (1,315) | 1:4:A:ALA:HB3   | 1:8:A:TYR:HE2   | 5        | 0.12          |
| (1,308) | 1:11:A:TRP:HD1  | 1:21:A:ARG:HG2  | 10       | 0.12          |
| (1,308) | 1:11:A:TRP:HD1  | 1:21:A:ARG:HG3  | 10       | 0.12          |
| (1,301) | 1:11:A:TRP:HD1  | 1:23:A:PRO:HA   | 2        | 0.12          |
| (1,301) | 1:11:A:TRP:HD1  | 1:23:A:PRO:HA   | 3        | 0.12          |
| (1,301) | 1:11:A:TRP:HD1  | 1:23:A:PRO:HA   | 6        | 0.12          |
| (1,290) | 1:5:A:VAL:HA    | 1:8:A:TYR:HE1   | 9        | 0.12          |
| (1,290) | 1:5:A:VAL:HA    | 1:8:A:TYR:HE2   | 9        | 0.12          |
| (1,290) | 1:5:A:VAL:HA    | 1:8:A:TYR:HE1   | 10       | 0.12          |
| (1,290) | 1:5:A:VAL:HA    | 1:8:A:TYR:HE2   | 10       | 0.12          |
| (1,104) | 1:10:A:GLN:H    | 1:10:A:GLN:HG2  | 9        | 0.12          |
| (1,104) | 1:10:A:GLN:H    | 1:10:A:GLN:HG3  | 9        | 0.12          |
| (1,81)  | 1:8:A:TYR:HA    | 1:9:A:ILE:H     | 5        | 0.12          |
| (1,81)  | 1:8:A:TYR:HA    | 1:9:A:ILE:H     | 6        | 0.12          |
| (1,1)   | 1:2:A:GLU:HA    | 1:3:A:GLU:H     | 6        | 0.12          |
| (1,1)   | 1:2:A:GLU:HA    | 1:3:A:GLU:H     | 8        | 0.12          |
| (1,1)   | 1:2:A:GLU:HA    | 1:3:A:GLU:H     | 10       | 0.12          |
| (3,71)  | 1:12:A:LEU:HD11 | 1:17:A:PRO:HD2  | 4        | 0.11          |
| (3,71)  | 1:12:A:LEU:HD12 | 1:17:A:PRO:HD2  | 4        | 0.11          |
| (3,71)  | 1:12:A:LEU:HD13 | 1:17:A:PRO:HD2  | 4        | 0.11          |
| (3,70)  | 1:6:A:ARG:HA    | 1:9:A:ILE:HG21  | 2        | 0.11          |
| (3,70)  | 1:6:A:ARG:HA    | 1:9:A:ILE:HG22  | 2        | 0.11          |
| (3,70)  | 1:6:A:ARG:HA    | 1:9:A:ILE:HG23  | 2        | 0.11          |
| (3,70)  | 1:6:A:ARG:HA    | 1:9:A:ILE:HG21  | 8        | 0.11          |
| (3,70)  | 1:6:A:ARG:HA    | 1:9:A:ILE:HG22  | 8        | 0.11          |
| (3,70)  | 1:6:A:ARG:HA    | 1:9:A:ILE:HG23  | 8        | 0.11          |
| (3,41)  | 1:4:A:ALA:H     | 1:5:A:VAL:H     | 3        | 0.11          |
| (3,41)  | 1:4:A:ALA:H     | 1:5:A:VAL:H     | 6        | 0.11          |
| (2,507) | 1:12:A:LEU:HD11 | 1:17:A:PRO:HD3  | 8        | 0.11          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,507) | 1:12:A:LEU:HD12 | 1:17:A:PRO:HD3  | 8        | 0.11          |
| (2,507) | 1:12:A:LEU:HD13 | 1:17:A:PRO:HD3  | 8        | 0.11          |
| (2,475) | 1:7:A:LEU:HD21  | 1:10:A:GLN:HG2  | 10       | 0.11          |
| (2,475) | 1:7:A:LEU:HD22  | 1:10:A:GLN:HG2  | 10       | 0.11          |
| (2,475) | 1:7:A:LEU:HD23  | 1:10:A:GLN:HG2  | 10       | 0.11          |
| (2,475) | 1:7:A:LEU:HD21  | 1:10:A:GLN:HG3  | 10       | 0.11          |
| (2,475) | 1:7:A:LEU:HD22  | 1:10:A:GLN:HG3  | 10       | 0.11          |
| (2,475) | 1:7:A:LEU:HD23  | 1:10:A:GLN:HG3  | 10       | 0.11          |
| (2,474) | 1:9:A:ILE:HD11  | 1:13:A:LYS:HE3  | 3        | 0.11          |
| (2,474) | 1:9:A:ILE:HD12  | 1:13:A:LYS:HE3  | 3        | 0.11          |
| (2,474) | 1:9:A:ILE:HD13  | 1:13:A:LYS:HE3  | 3        | 0.11          |
| (2,474) | 1:9:A:ILE:HD11  | 1:13:A:LYS:HE3  | 4        | 0.11          |
| (2,474) | 1:9:A:ILE:HD12  | 1:13:A:LYS:HE3  | 4        | 0.11          |
| (2,474) | 1:9:A:ILE:HD13  | 1:13:A:LYS:HE3  | 4        | 0.11          |
| (2,474) | 1:9:A:ILE:HD11  | 1:13:A:LYS:HE3  | 6        | 0.11          |
| (2,474) | 1:9:A:ILE:HD12  | 1:13:A:LYS:HE3  | 6        | 0.11          |
| (2,474) | 1:9:A:ILE:HD13  | 1:13:A:LYS:HE3  | 6        | 0.11          |
| (2,471) | 1:5:A:VAL:HG11  | 1:9:A:ILE:HG13  | 7        | 0.11          |
| (2,471) | 1:5:A:VAL:HG12  | 1:9:A:ILE:HG13  | 7        | 0.11          |
| (2,471) | 1:5:A:VAL:HG13  | 1:9:A:ILE:HG13  | 7        | 0.11          |
| (2,470) | 1:4:A:ALA:HB1   | 1:5:A:VAL:HG11  | 2        | 0.11          |
| (2,470) | 1:4:A:ALA:HB1   | 1:5:A:VAL:HG12  | 2        | 0.11          |
| (2,470) | 1:4:A:ALA:HB1   | 1:5:A:VAL:HG13  | 2        | 0.11          |
| (2,470) | 1:4:A:ALA:HB2   | 1:5:A:VAL:HG11  | 2        | 0.11          |
| (2,470) | 1:4:A:ALA:HB2   | 1:5:A:VAL:HG12  | 2        | 0.11          |
| (2,470) | 1:4:A:ALA:HB2   | 1:5:A:VAL:HG13  | 2        | 0.11          |
| (2,470) | 1:4:A:ALA:HB3   | 1:5:A:VAL:HG11  | 2        | 0.11          |
| (2,470) | 1:4:A:ALA:HB3   | 1:5:A:VAL:HG12  | 2        | 0.11          |
| (2,470) | 1:4:A:ALA:HB3   | 1:5:A:VAL:HG13  | 2        | 0.11          |
| (2,467) | 1:2:A:GLU:HB3   | 1:5:A:VAL:HG11  | 2        | 0.11          |
| (2,467) | 1:2:A:GLU:HB3   | 1:5:A:VAL:HG12  | 2        | 0.11          |
| (2,467) | 1:2:A:GLU:HB3   | 1:5:A:VAL:HG13  | 2        | 0.11          |
| (2,467) | 1:2:A:GLU:HB3   | 1:5:A:VAL:HG11  | 7        | 0.11          |
| (2,467) | 1:2:A:GLU:HB3   | 1:5:A:VAL:HG12  | 7        | 0.11          |
| (2,467) | 1:2:A:GLU:HB3   | 1:5:A:VAL:HG13  | 7        | 0.11          |
| (2,459) | 1:9:A:ILE:HA    | 1:12:A:LEU:HD21 | 2        | 0.11          |
| (2,459) | 1:9:A:ILE:HA    | 1:12:A:LEU:HD22 | 2        | 0.11          |
| (2,459) | 1:9:A:ILE:HA    | 1:12:A:LEU:HD23 | 2        | 0.11          |
| (2,456) | 1:5:A:VAL:HA    | 1:9:A:ILE:HD11  | 1        | 0.11          |
| (2,456) | 1:5:A:VAL:HA    | 1:9:A:ILE:HD12  | 1        | 0.11          |
| (2,456) | 1:5:A:VAL:HA    | 1:9:A:ILE:HD13  | 1        | 0.11          |
| (2,456) | 1:5:A:VAL:HA    | 1:9:A:ILE:HD11  | 3        | 0.11          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,456) | 1:5:A:VAL:HA    | 1:9:A:ILE:HD12  | 3        | 0.11          |
| (2,456) | 1:5:A:VAL:HA    | 1:9:A:ILE:HD13  | 3        | 0.11          |
| (2,384) | 1:5:A:VAL:HG21  | 1:6:A:ARG:H     | 4        | 0.11          |
| (2,384) | 1:5:A:VAL:HG22  | 1:6:A:ARG:H     | 4        | 0.11          |
| (2,384) | 1:5:A:VAL:HG23  | 1:6:A:ARG:H     | 4        | 0.11          |
| (2,384) | 1:5:A:VAL:HG21  | 1:6:A:ARG:H     | 6        | 0.11          |
| (2,384) | 1:5:A:VAL:HG22  | 1:6:A:ARG:H     | 6        | 0.11          |
| (2,384) | 1:5:A:VAL:HG23  | 1:6:A:ARG:H     | 6        | 0.11          |
| (2,384) | 1:5:A:VAL:HG21  | 1:6:A:ARG:H     | 7        | 0.11          |
| (2,384) | 1:5:A:VAL:HG22  | 1:6:A:ARG:H     | 7        | 0.11          |
| (2,384) | 1:5:A:VAL:HG23  | 1:6:A:ARG:H     | 7        | 0.11          |
| (2,382) | 1:4:A:ALA:HB1   | 1:6:A:ARG:H     | 10       | 0.11          |
| (2,382) | 1:4:A:ALA:HB2   | 1:6:A:ARG:H     | 10       | 0.11          |
| (2,382) | 1:4:A:ALA:HB3   | 1:6:A:ARG:H     | 10       | 0.11          |
| (2,343) | 1:16:A:GLY:H    | 1:17:A:PRO:HD2  | 6        | 0.11          |
| (2,312) | 1:11:A:TRP:HE3  | 1:12:A:LEU:HA   | 1        | 0.11          |
| (2,312) | 1:11:A:TRP:HE3  | 1:12:A:LEU:HA   | 9        | 0.11          |
| (2,312) | 1:11:A:TRP:HE3  | 1:12:A:LEU:HA   | 10       | 0.11          |
| (2,308) | 1:11:A:TRP:HH2  | 1:16:A:GLY:HA2  | 3        | 0.11          |
| (2,308) | 1:11:A:TRP:HZ2  | 1:16:A:GLY:HA2  | 3        | 0.11          |
| (2,308) | 1:11:A:TRP:HH2  | 1:16:A:GLY:HA2  | 6        | 0.11          |
| (2,308) | 1:11:A:TRP:HZ2  | 1:16:A:GLY:HA2  | 6        | 0.11          |
| (2,308) | 1:11:A:TRP:HH2  | 1:16:A:GLY:HA2  | 10       | 0.11          |
| (2,308) | 1:11:A:TRP:HZ2  | 1:16:A:GLY:HA2  | 10       | 0.11          |
| (2,289) | 1:8:A:TYR:HD1   | 1:12:A:LEU:HD21 | 7        | 0.11          |
| (2,289) | 1:8:A:TYR:HD1   | 1:12:A:LEU:HD22 | 7        | 0.11          |
| (2,289) | 1:8:A:TYR:HD1   | 1:12:A:LEU:HD23 | 7        | 0.11          |
| (2,289) | 1:8:A:TYR:HD2   | 1:12:A:LEU:HD21 | 7        | 0.11          |
| (2,289) | 1:8:A:TYR:HD2   | 1:12:A:LEU:HD22 | 7        | 0.11          |
| (2,289) | 1:8:A:TYR:HD2   | 1:12:A:LEU:HD23 | 7        | 0.11          |
| (2,283) | 1:11:A:TRP:HD1  | 1:21:A:ARG:HB3  | 4        | 0.11          |
| (2,280) | 1:8:A:TYR:HD1   | 1:24:A:PRO:HB3  | 9        | 0.11          |
| (2,280) | 1:8:A:TYR:HD2   | 1:24:A:PRO:HB3  | 9        | 0.11          |
| (2,278) | 1:11:A:TRP:HD1  | 1:23:A:PRO:HA   | 1        | 0.11          |
| (2,278) | 1:11:A:TRP:HD1  | 1:23:A:PRO:HA   | 7        | 0.11          |
| (2,272) | 1:11:A:TRP:HD1  | 1:19:A:SER:HB3  | 1        | 0.11          |
| (2,257) | 1:11:A:TRP:HE1  | 1:21:A:ARG:HG2  | 6        | 0.11          |
| (2,257) | 1:11:A:TRP:HE1  | 1:21:A:ARG:HG3  | 6        | 0.11          |
| (1,598) | 1:12:A:LEU:HD11 | 1:17:A:PRO:HD3  | 8        | 0.11          |
| (1,598) | 1:12:A:LEU:HD12 | 1:17:A:PRO:HD3  | 8        | 0.11          |
| (1,598) | 1:12:A:LEU:HD13 | 1:17:A:PRO:HD3  | 8        | 0.11          |
| (1,551) | 1:7:A:LEU:HD21  | 1:10:A:GLN:HG2  | 10       | 0.11          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,551) | 1:7:A:LEU:HD22  | 1:10:A:GLN:HG2  | 10       | 0.11          |
| (1,551) | 1:7:A:LEU:HD23  | 1:10:A:GLN:HG2  | 10       | 0.11          |
| (1,551) | 1:7:A:LEU:HD21  | 1:10:A:GLN:HG3  | 10       | 0.11          |
| (1,551) | 1:7:A:LEU:HD22  | 1:10:A:GLN:HG3  | 10       | 0.11          |
| (1,551) | 1:7:A:LEU:HD23  | 1:10:A:GLN:HG3  | 10       | 0.11          |
| (1,550) | 1:9:A:ILE:HD11  | 1:13:A:LYS:HE3  | 3        | 0.11          |
| (1,550) | 1:9:A:ILE:HD12  | 1:13:A:LYS:HE3  | 3        | 0.11          |
| (1,550) | 1:9:A:ILE:HD13  | 1:13:A:LYS:HE3  | 3        | 0.11          |
| (1,550) | 1:9:A:ILE:HD11  | 1:13:A:LYS:HE3  | 4        | 0.11          |
| (1,550) | 1:9:A:ILE:HD12  | 1:13:A:LYS:HE3  | 4        | 0.11          |
| (1,550) | 1:9:A:ILE:HD13  | 1:13:A:LYS:HE3  | 4        | 0.11          |
| (1,550) | 1:9:A:ILE:HD11  | 1:13:A:LYS:HE3  | 6        | 0.11          |
| (1,550) | 1:9:A:ILE:HD12  | 1:13:A:LYS:HE3  | 6        | 0.11          |
| (1,550) | 1:9:A:ILE:HD13  | 1:13:A:LYS:HE3  | 6        | 0.11          |
| (1,547) | 1:5:A:VAL:HG11  | 1:9:A:ILE:HG13  | 7        | 0.11          |
| (1,547) | 1:5:A:VAL:HG12  | 1:9:A:ILE:HG13  | 7        | 0.11          |
| (1,547) | 1:5:A:VAL:HG13  | 1:9:A:ILE:HG13  | 7        | 0.11          |
| (1,545) | 1:4:A:ALA:HB1   | 1:5:A:VAL:HG11  | 2        | 0.11          |
| (1,545) | 1:4:A:ALA:HB1   | 1:5:A:VAL:HG12  | 2        | 0.11          |
| (1,545) | 1:4:A:ALA:HB1   | 1:5:A:VAL:HG13  | 2        | 0.11          |
| (1,545) | 1:4:A:ALA:HB2   | 1:5:A:VAL:HG11  | 2        | 0.11          |
| (1,545) | 1:4:A:ALA:HB2   | 1:5:A:VAL:HG12  | 2        | 0.11          |
| (1,545) | 1:4:A:ALA:HB2   | 1:5:A:VAL:HG13  | 2        | 0.11          |
| (1,545) | 1:4:A:ALA:HB3   | 1:5:A:VAL:HG11  | 2        | 0.11          |
| (1,545) | 1:4:A:ALA:HB3   | 1:5:A:VAL:HG12  | 2        | 0.11          |
| (1,545) | 1:4:A:ALA:HB3   | 1:5:A:VAL:HG13  | 2        | 0.11          |
| (1,540) | 1:2:A:GLU:HB3   | 1:5:A:VAL:HG11  | 2        | 0.11          |
| (1,540) | 1:2:A:GLU:HB3   | 1:5:A:VAL:HG12  | 2        | 0.11          |
| (1,540) | 1:2:A:GLU:HB3   | 1:5:A:VAL:HG13  | 2        | 0.11          |
| (1,540) | 1:2:A:GLU:HB3   | 1:5:A:VAL:HG11  | 7        | 0.11          |
| (1,540) | 1:2:A:GLU:HB3   | 1:5:A:VAL:HG12  | 7        | 0.11          |
| (1,540) | 1:2:A:GLU:HB3   | 1:5:A:VAL:HG13  | 7        | 0.11          |
| (1,530) | 1:9:A:ILE:HA    | 1:12:A:LEU:HD21 | 2        | 0.11          |
| (1,530) | 1:9:A:ILE:HA    | 1:12:A:LEU:HD22 | 2        | 0.11          |
| (1,530) | 1:9:A:ILE:HA    | 1:12:A:LEU:HD23 | 2        | 0.11          |
| (1,529) | 1:12:A:LEU:HD11 | 1:17:A:PRO:HD2  | 4        | 0.11          |
| (1,529) | 1:12:A:LEU:HD12 | 1:17:A:PRO:HD2  | 4        | 0.11          |
| (1,529) | 1:12:A:LEU:HD13 | 1:17:A:PRO:HD2  | 4        | 0.11          |
| (1,526) | 1:5:A:VAL:HA    | 1:9:A:ILE:HD11  | 1        | 0.11          |
| (1,526) | 1:5:A:VAL:HA    | 1:9:A:ILE:HD12  | 1        | 0.11          |
| (1,526) | 1:5:A:VAL:HA    | 1:9:A:ILE:HD13  | 1        | 0.11          |
| (1,526) | 1:5:A:VAL:HA    | 1:9:A:ILE:HD11  | 3        | 0.11          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,526) | 1:5:A:VAL:HA   | 1:9:A:ILE:HD12  | 3        | 0.11          |
| (1,526) | 1:5:A:VAL:HA   | 1:9:A:ILE:HD13  | 3        | 0.11          |
| (1,521) | 1:6:A:ARG:HA   | 1:9:A:ILE:HG21  | 2        | 0.11          |
| (1,521) | 1:6:A:ARG:HA   | 1:9:A:ILE:HG22  | 2        | 0.11          |
| (1,521) | 1:6:A:ARG:HA   | 1:9:A:ILE:HG23  | 2        | 0.11          |
| (1,521) | 1:6:A:ARG:HA   | 1:9:A:ILE:HG21  | 8        | 0.11          |
| (1,521) | 1:6:A:ARG:HA   | 1:9:A:ILE:HG22  | 8        | 0.11          |
| (1,521) | 1:6:A:ARG:HA   | 1:9:A:ILE:HG23  | 8        | 0.11          |
| (1,443) | 1:5:A:VAL:HG21 | 1:6:A:ARG:H     | 4        | 0.11          |
| (1,443) | 1:5:A:VAL:HG22 | 1:6:A:ARG:H     | 4        | 0.11          |
| (1,443) | 1:5:A:VAL:HG23 | 1:6:A:ARG:H     | 4        | 0.11          |
| (1,443) | 1:5:A:VAL:HG21 | 1:6:A:ARG:H     | 6        | 0.11          |
| (1,443) | 1:5:A:VAL:HG22 | 1:6:A:ARG:H     | 6        | 0.11          |
| (1,443) | 1:5:A:VAL:HG23 | 1:6:A:ARG:H     | 6        | 0.11          |
| (1,443) | 1:5:A:VAL:HG21 | 1:6:A:ARG:H     | 7        | 0.11          |
| (1,443) | 1:5:A:VAL:HG22 | 1:6:A:ARG:H     | 7        | 0.11          |
| (1,443) | 1:5:A:VAL:HG23 | 1:6:A:ARG:H     | 7        | 0.11          |
| (1,440) | 1:4:A:ALA:HB1  | 1:6:A:ARG:H     | 10       | 0.11          |
| (1,440) | 1:4:A:ALA:HB2  | 1:6:A:ARG:H     | 10       | 0.11          |
| (1,440) | 1:4:A:ALA:HB3  | 1:6:A:ARG:H     | 10       | 0.11          |
| (1,389) | 1:16:A:GLY:H   | 1:17:A:PRO:HD2  | 6        | 0.11          |
| (1,370) | 1:4:A:ALA:H    | 1:5:A:VAL:H     | 3        | 0.11          |
| (1,370) | 1:4:A:ALA:H    | 1:5:A:VAL:H     | 6        | 0.11          |
| (1,349) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HA   | 1        | 0.11          |
| (1,349) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HA   | 9        | 0.11          |
| (1,349) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HA   | 10       | 0.11          |
| (1,344) | 1:11:A:TRP:HH2 | 1:16:A:GLY:HA2  | 3        | 0.11          |
| (1,344) | 1:11:A:TRP:HZ2 | 1:16:A:GLY:HA2  | 3        | 0.11          |
| (1,344) | 1:11:A:TRP:HH2 | 1:16:A:GLY:HA2  | 6        | 0.11          |
| (1,344) | 1:11:A:TRP:HZ2 | 1:16:A:GLY:HA2  | 6        | 0.11          |
| (1,344) | 1:11:A:TRP:HH2 | 1:16:A:GLY:HA2  | 10       | 0.11          |
| (1,344) | 1:11:A:TRP:HZ2 | 1:16:A:GLY:HA2  | 10       | 0.11          |
| (1,319) | 1:8:A:TYR:HD1  | 1:12:A:LEU:HD21 | 7        | 0.11          |
| (1,319) | 1:8:A:TYR:HD1  | 1:12:A:LEU:HD22 | 7        | 0.11          |
| (1,319) | 1:8:A:TYR:HD1  | 1:12:A:LEU:HD23 | 7        | 0.11          |
| (1,319) | 1:8:A:TYR:HD2  | 1:12:A:LEU:HD21 | 7        | 0.11          |
| (1,319) | 1:8:A:TYR:HD2  | 1:12:A:LEU:HD22 | 7        | 0.11          |
| (1,319) | 1:8:A:TYR:HD2  | 1:12:A:LEU:HD23 | 7        | 0.11          |
| (1,306) | 1:11:A:TRP:HD1 | 1:21:A:ARG:HB3  | 4        | 0.11          |
| (1,303) | 1:8:A:TYR:HD1  | 1:24:A:PRO:HB3  | 9        | 0.11          |
| (1,303) | 1:8:A:TYR:HD2  | 1:24:A:PRO:HB3  | 9        | 0.11          |
| (1,301) | 1:11:A:TRP:HD1 | 1:23:A:PRO:HA   | 1        | 0.11          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,301) | 1:11:A:TRP:HD1  | 1:23:A:PRO:HA  | 7        | 0.11          |
| (1,293) | 1:11:A:TRP:HD1  | 1:19:A:SER:HB3 | 1        | 0.11          |
| (1,276) | 1:11:A:TRP:HE1  | 1:21:A:ARG:HG2 | 6        | 0.11          |
| (1,276) | 1:11:A:TRP:HE1  | 1:21:A:ARG:HG3 | 6        | 0.11          |
| (3,84)  | 1:3:A:GLU:HA    | 1:7:A:LEU:H    | 9        | 0.1           |
| (3,84)  | 1:3:A:GLU:HA    | 1:7:A:LEU:H    | 10       | 0.1           |
| (2,507) | 1:12:A:LEU:HD11 | 1:17:A:PRO:HD3 | 6        | 0.1           |
| (2,507) | 1:12:A:LEU:HD12 | 1:17:A:PRO:HD3 | 6        | 0.1           |
| (2,507) | 1:12:A:LEU:HD13 | 1:17:A:PRO:HD3 | 6        | 0.1           |
| (2,474) | 1:9:A:ILE:HD11  | 1:13:A:LYS:HE3 | 5        | 0.1           |
| (2,474) | 1:9:A:ILE:HD12  | 1:13:A:LYS:HE3 | 5        | 0.1           |
| (2,474) | 1:9:A:ILE:HD13  | 1:13:A:LYS:HE3 | 5        | 0.1           |
| (2,471) | 1:5:A:VAL:HG11  | 1:9:A:ILE:HG13 | 10       | 0.1           |
| (2,471) | 1:5:A:VAL:HG12  | 1:9:A:ILE:HG13 | 10       | 0.1           |
| (2,471) | 1:5:A:VAL:HG13  | 1:9:A:ILE:HG13 | 10       | 0.1           |
| (2,470) | 1:4:A:ALA:HB1   | 1:5:A:VAL:HG11 | 4        | 0.1           |
| (2,470) | 1:4:A:ALA:HB1   | 1:5:A:VAL:HG12 | 4        | 0.1           |
| (2,470) | 1:4:A:ALA:HB1   | 1:5:A:VAL:HG13 | 4        | 0.1           |
| (2,470) | 1:4:A:ALA:HB2   | 1:5:A:VAL:HG11 | 4        | 0.1           |
| (2,470) | 1:4:A:ALA:HB2   | 1:5:A:VAL:HG12 | 4        | 0.1           |
| (2,470) | 1:4:A:ALA:HB2   | 1:5:A:VAL:HG13 | 4        | 0.1           |
| (2,470) | 1:4:A:ALA:HB3   | 1:5:A:VAL:HG11 | 4        | 0.1           |
| (2,470) | 1:4:A:ALA:HB3   | 1:5:A:VAL:HG12 | 4        | 0.1           |
| (2,470) | 1:4:A:ALA:HB3   | 1:5:A:VAL:HG13 | 4        | 0.1           |
| (2,467) | 1:2:A:GLU:HB3   | 1:5:A:VAL:HG11 | 5        | 0.1           |
| (2,467) | 1:2:A:GLU:HB3   | 1:5:A:VAL:HG12 | 5        | 0.1           |
| (2,467) | 1:2:A:GLU:HB3   | 1:5:A:VAL:HG13 | 5        | 0.1           |
| (2,426) | 1:21:A:ARG:HG2  | 1:22:A:PRO:HD3 | 8        | 0.1           |
| (2,426) | 1:21:A:ARG:HG3  | 1:22:A:PRO:HD3 | 8        | 0.1           |
| (2,425) | 1:9:A:ILE:HA    | 1:12:A:LEU:HG  | 10       | 0.1           |
| (2,397) | 1:5:A:VAL:H     | 1:9:A:ILE:HD11 | 1        | 0.1           |
| (2,397) | 1:5:A:VAL:H     | 1:9:A:ILE:HD12 | 1        | 0.1           |
| (2,397) | 1:5:A:VAL:H     | 1:9:A:ILE:HD13 | 1        | 0.1           |
| (2,385) | 1:9:A:ILE:HG21  | 1:10:A:GLN:H   | 1        | 0.1           |
| (2,385) | 1:9:A:ILE:HG22  | 1:10:A:GLN:H   | 1        | 0.1           |
| (2,385) | 1:9:A:ILE:HG23  | 1:10:A:GLN:H   | 1        | 0.1           |
| (2,384) | 1:5:A:VAL:HG21  | 1:6:A:ARG:H    | 5        | 0.1           |
| (2,384) | 1:5:A:VAL:HG22  | 1:6:A:ARG:H    | 5        | 0.1           |
| (2,384) | 1:5:A:VAL:HG23  | 1:6:A:ARG:H    | 5        | 0.1           |
| (2,384) | 1:5:A:VAL:HG21  | 1:6:A:ARG:H    | 8        | 0.1           |
| (2,384) | 1:5:A:VAL:HG22  | 1:6:A:ARG:H    | 8        | 0.1           |
| (2,384) | 1:5:A:VAL:HG23  | 1:6:A:ARG:H    | 8        | 0.1           |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,382) | 1:4:A:ALA:HB1   | 1:6:A:ARG:H     | 9        | 0.1           |
| (2,382) | 1:4:A:ALA:HB2   | 1:6:A:ARG:H     | 9        | 0.1           |
| (2,382) | 1:4:A:ALA:HB3   | 1:6:A:ARG:H     | 9        | 0.1           |
| (2,381) | 1:11:A:TRP:H    | 1:12:A:LEU:HG   | 6        | 0.1           |
| (2,312) | 1:11:A:TRP:HE3  | 1:12:A:LEU:HA   | 6        | 0.1           |
| (2,289) | 1:8:A:TYR:HD1   | 1:12:A:LEU:HD21 | 5        | 0.1           |
| (2,289) | 1:8:A:TYR:HD1   | 1:12:A:LEU:HD22 | 5        | 0.1           |
| (2,289) | 1:8:A:TYR:HD1   | 1:12:A:LEU:HD23 | 5        | 0.1           |
| (2,289) | 1:8:A:TYR:HD2   | 1:12:A:LEU:HD21 | 5        | 0.1           |
| (2,289) | 1:8:A:TYR:HD2   | 1:12:A:LEU:HD22 | 5        | 0.1           |
| (2,289) | 1:8:A:TYR:HD2   | 1:12:A:LEU:HD23 | 5        | 0.1           |
| (2,278) | 1:11:A:TRP:HD1  | 1:23:A:PRO:HA   | 4        | 0.1           |
| (2,263) | 1:11:A:TRP:HE1  | 1:19:A:SER:HB2  | 10       | 0.1           |
| (2,129) | 1:13:A:LYS:HE2  | 1:13:A:LYS:HG2  | 7        | 0.1           |
| (2,64)  | 1:7:A:LEU:H     | 1:7:A:LEU:HB3   | 4        | 0.1           |
| (2,1)   | 1:2:A:GLU:HA    | 1:3:A:GLU:H     | 7        | 0.1           |
| (1,598) | 1:12:A:LEU:HD11 | 1:17:A:PRO:HD3  | 6        | 0.1           |
| (1,598) | 1:12:A:LEU:HD12 | 1:17:A:PRO:HD3  | 6        | 0.1           |
| (1,598) | 1:12:A:LEU:HD13 | 1:17:A:PRO:HD3  | 6        | 0.1           |
| (1,569) | 1:3:A:GLU:HA    | 1:7:A:LEU:H     | 9        | 0.1           |
| (1,569) | 1:3:A:GLU:HA    | 1:7:A:LEU:H     | 10       | 0.1           |
| (1,550) | 1:9:A:ILE:HD11  | 1:13:A:LYS:HE3  | 5        | 0.1           |
| (1,550) | 1:9:A:ILE:HD12  | 1:13:A:LYS:HE3  | 5        | 0.1           |
| (1,550) | 1:9:A:ILE:HD13  | 1:13:A:LYS:HE3  | 5        | 0.1           |
| (1,547) | 1:5:A:VAL:HG11  | 1:9:A:ILE:HG13  | 10       | 0.1           |
| (1,547) | 1:5:A:VAL:HG12  | 1:9:A:ILE:HG13  | 10       | 0.1           |
| (1,547) | 1:5:A:VAL:HG13  | 1:9:A:ILE:HG13  | 10       | 0.1           |
| (1,545) | 1:4:A:ALA:HB1   | 1:5:A:VAL:HG11  | 4        | 0.1           |
| (1,545) | 1:4:A:ALA:HB1   | 1:5:A:VAL:HG12  | 4        | 0.1           |
| (1,545) | 1:4:A:ALA:HB1   | 1:5:A:VAL:HG13  | 4        | 0.1           |
| (1,545) | 1:4:A:ALA:HB2   | 1:5:A:VAL:HG11  | 4        | 0.1           |
| (1,545) | 1:4:A:ALA:HB2   | 1:5:A:VAL:HG12  | 4        | 0.1           |
| (1,545) | 1:4:A:ALA:HB2   | 1:5:A:VAL:HG13  | 4        | 0.1           |
| (1,545) | 1:4:A:ALA:HB3   | 1:5:A:VAL:HG11  | 4        | 0.1           |
| (1,545) | 1:4:A:ALA:HB3   | 1:5:A:VAL:HG12  | 4        | 0.1           |
| (1,545) | 1:4:A:ALA:HB3   | 1:5:A:VAL:HG13  | 4        | 0.1           |
| (1,540) | 1:2:A:GLU:HB3   | 1:5:A:VAL:HG11  | 5        | 0.1           |
| (1,540) | 1:2:A:GLU:HB3   | 1:5:A:VAL:HG12  | 5        | 0.1           |
| (1,540) | 1:2:A:GLU:HB3   | 1:5:A:VAL:HG13  | 5        | 0.1           |
| (1,493) | 1:21:A:ARG:HG2  | 1:22:A:PRO:HD3  | 8        | 0.1           |
| (1,493) | 1:21:A:ARG:HG3  | 1:22:A:PRO:HD3  | 8        | 0.1           |
| (1,492) | 1:9:A:ILE:HA    | 1:12:A:LEU:HG   | 10       | 0.1           |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,459) | 1:5:A:VAL:H    | 1:9:A:ILE:HD11  | 1        | 0.1           |
| (1,459) | 1:5:A:VAL:H    | 1:9:A:ILE:HD12  | 1        | 0.1           |
| (1,459) | 1:5:A:VAL:H    | 1:9:A:ILE:HD13  | 1        | 0.1           |
| (1,445) | 1:9:A:ILE:HG21 | 1:10:A:GLN:H    | 1        | 0.1           |
| (1,445) | 1:9:A:ILE:HG22 | 1:10:A:GLN:H    | 1        | 0.1           |
| (1,445) | 1:9:A:ILE:HG23 | 1:10:A:GLN:H    | 1        | 0.1           |
| (1,443) | 1:5:A:VAL:HG21 | 1:6:A:ARG:H     | 5        | 0.1           |
| (1,443) | 1:5:A:VAL:HG22 | 1:6:A:ARG:H     | 5        | 0.1           |
| (1,443) | 1:5:A:VAL:HG23 | 1:6:A:ARG:H     | 5        | 0.1           |
| (1,443) | 1:5:A:VAL:HG21 | 1:6:A:ARG:H     | 8        | 0.1           |
| (1,443) | 1:5:A:VAL:HG22 | 1:6:A:ARG:H     | 8        | 0.1           |
| (1,443) | 1:5:A:VAL:HG23 | 1:6:A:ARG:H     | 8        | 0.1           |
| (1,440) | 1:4:A:ALA:HB1  | 1:6:A:ARG:H     | 9        | 0.1           |
| (1,440) | 1:4:A:ALA:HB2  | 1:6:A:ARG:H     | 9        | 0.1           |
| (1,440) | 1:4:A:ALA:HB3  | 1:6:A:ARG:H     | 9        | 0.1           |
| (1,439) | 1:11:A:TRP:H   | 1:12:A:LEU:HG   | 6        | 0.1           |
| (1,349) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HA   | 6        | 0.1           |
| (1,319) | 1:8:A:TYR:HD1  | 1:12:A:LEU:HD21 | 5        | 0.1           |
| (1,319) | 1:8:A:TYR:HD1  | 1:12:A:LEU:HD22 | 5        | 0.1           |
| (1,319) | 1:8:A:TYR:HD1  | 1:12:A:LEU:HD23 | 5        | 0.1           |
| (1,319) | 1:8:A:TYR:HD2  | 1:12:A:LEU:HD21 | 5        | 0.1           |
| (1,319) | 1:8:A:TYR:HD2  | 1:12:A:LEU:HD22 | 5        | 0.1           |
| (1,319) | 1:8:A:TYR:HD2  | 1:12:A:LEU:HD23 | 5        | 0.1           |
| (1,301) | 1:11:A:TRP:HD1 | 1:23:A:PRO:HA   | 4        | 0.1           |
| (1,282) | 1:11:A:TRP:HE1 | 1:19:A:SER:HB2  | 10       | 0.1           |
| (1,143) | 1:13:A:LYS:HE2 | 1:13:A:LYS:HG2  | 7        | 0.1           |
| (1,71)  | 1:7:A:LEU:H    | 1:7:A:LEU:HB3   | 4        | 0.1           |
| (1,1)   | 1:2:A:GLU:HA   | 1:3:A:GLU:H     | 7        | 0.1           |

## 10 Dihedral-angle violation analysis

No dihedral-angle restraints found