



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 12:22 PM UTC

PDB ID : 9GDT / pdb\_00009gdt  
BMRB ID : 34944  
Title : Trp-cage fortified Tc5b-Exenatide chimera with disulfide bond cyclization (Ex-4-Tc5bCC) at 299K  
Authors : Horvath, D.  
Deposited on : 2024-08-06

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

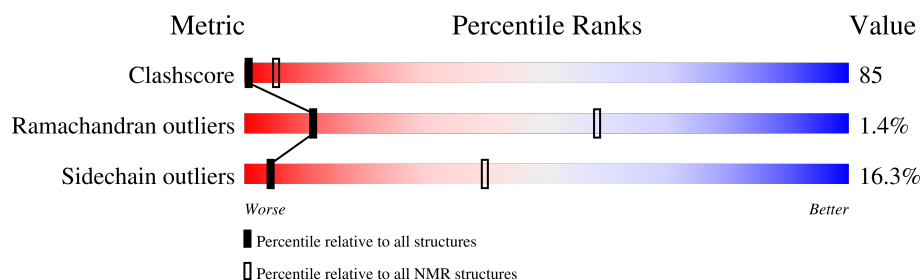
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 51%.

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>32%</div> <div>48%</div> <div>8%</div> <div>12%</div> </div> |

## 2 Ensemble composition and analysis

This entry contains 10 models. Model 10 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:4-A:25 (22)         | 0.28              | 10           |

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

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

There is only 1 type of molecule in this entry. The entry contains 384 atoms, of which 187 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Trp-cage fortified Tc5b-Exenatide chimera (Ex-4-Tc5bSS).

| Mol | Chain | Residues | Atoms |     |     |    |    |   | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---|-------|
| 1   | A     | 25       | Total | C   | H   | N  | O  | S | 0     |
|     |       |          | 384   | 123 | 187 | 34 | 38 | 2 |       |

## 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: Trp-cage fortified Tc5b-Exenatide chimera (Ex-4-Tc5bSS)



### 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: Trp-cage fortified Tc5b-Exenatide chimera (Ex-4-Tc5bSS)



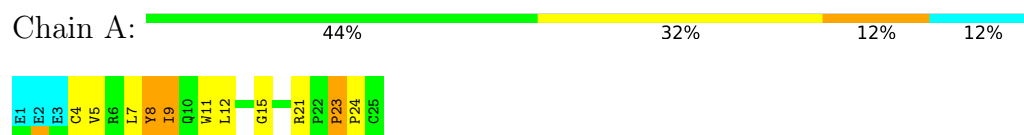
#### 4.2.2 Score per residue for model 2

- Molecule 1: Trp-cage fortified Tc5b-Exenatide chimera (Ex-4-Tc5bSS)



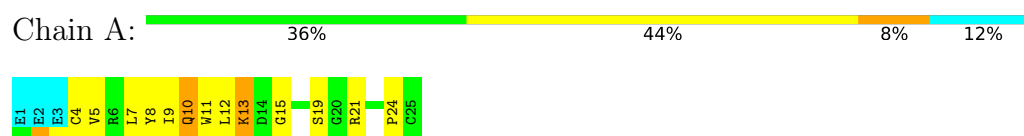
### 4.2.3 Score per residue for model 3

- Molecule 1: Trp-cage fortified Tc5b-Exenatide chimera (Ex-4-Tc5bSS)



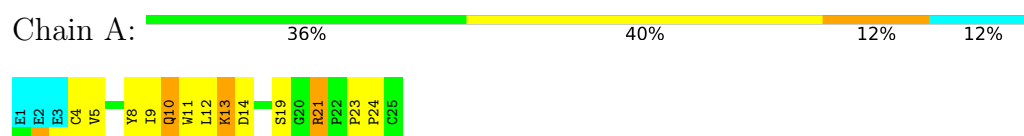
### 4.2.4 Score per residue for model 4

- Molecule 1: Trp-cage fortified Tc5b-Exenatide chimera (Ex-4-Tc5bSS)



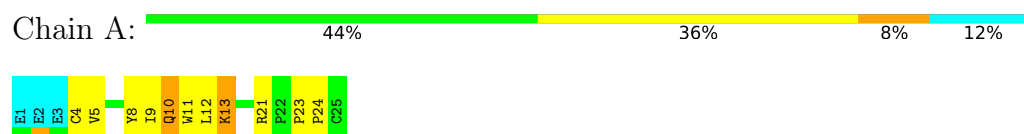
### 4.2.5 Score per residue for model 5

- Molecule 1: Trp-cage fortified Tc5b-Exenatide chimera (Ex-4-Tc5bSS)



### 4.2.6 Score per residue for model 6

- Molecule 1: Trp-cage fortified Tc5b-Exenatide chimera (Ex-4-Tc5bSS)



### 4.2.7 Score per residue for model 7

- Molecule 1: Trp-cage fortified Tc5b-Exenatide chimera (Ex-4-Tc5bSS)



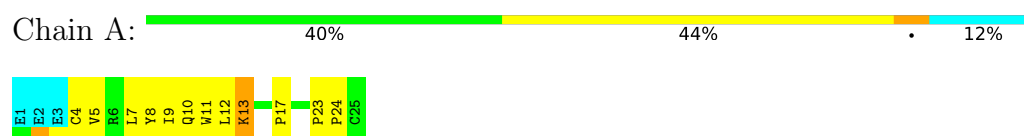
### 4.2.8 Score per residue for model 8

- Molecule 1: Trp-cage fortified Tc5b-Exenatide chimera (Ex-4-Tc5bSS)



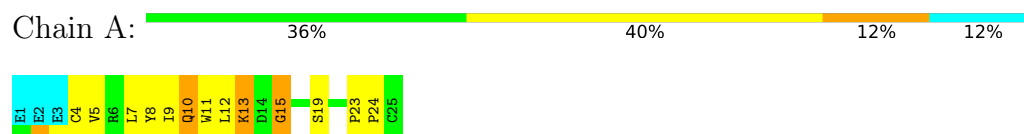
### 4.2.9 Score per residue for model 9

- Molecule 1: Trp-cage fortified Tc5b-Exenatide chimera (Ex-4-Tc5bSS)



### 4.2.10 Score per residue for model 10 (medoid)

- Molecule 1: Trp-cage fortified Tc5b-Exenatide chimera (Ex-4-Tc5bSS)



## 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                       | 167            |
| Number of shifts mapped to atoms             | 167            |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 51%            |

## 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     | 1.23±0.06    | 0±1/176 ( 0.2± 0.5%) | 1.18±0.06   | 0±1/238 ( 0.1± 0.3%) |
| All | All   | 1.23         | 3/1760 ( 0.2%)       | 1.18        | 2/2380 ( 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     | 8   | TYR  | C-N   | -6.27 | 1.26        | 1.33     | 3      | 1     |
| 1   | A     | 9   | ILE  | N-CA  | -5.87 | 1.38        | 1.46     | 3      | 1     |
| 1   | A     | 9   | ILE  | CA-CB | -5.33 | 1.47        | 1.54     | 3      | 1     |

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

| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|--------|------|-------------|----------|--------|-------|
|     |       |     |      |        |      |             |          | Worst  | Total |
| 1   | A     | 23  | PRO  | CA-C-N | 5.47 | 125.12      | 119.05   | 3      | 1     |
| 1   | A     | 23  | PRO  | C-N-CA | 5.47 | 125.12      | 119.05   | 3      | 1     |

There are no chirality outliers.

There are no planarity outliers.

### 6.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1   | A     | 170   | 167      | 167      | 29±4    |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| All | All   | 1700  | 1670     | 1670     | 288     |

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 85.

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

| Atom-1         | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|----------------|-----------------|----------|-------------|--------|-------|
|                |                 |          |             | Worst  | Total |
| 1:A:9:ILE:HG12 | 1:A:12:LEU:HD12 | 0.89     | 1.45        | 3      | 1     |
| 1:A:8:TYR:CZ   | 1:A:12:LEU:HD11 | 0.84     | 2.08        | 3      | 3     |
| 1:A:8:TYR:O    | 1:A:11:TRP:HB3  | 0.79     | 1.76        | 3      | 10    |
| 1:A:11:TRP:HE3 | 1:A:12:LEU:HD22 | 0.76     | 1.41        | 4      | 9     |
| 1:A:11:TRP:CE3 | 1:A:12:LEU:HD22 | 0.73     | 2.18        | 8      | 9     |
| 1:A:9:ILE:HA   | 1:A:12:LEU:HD23 | 0.72     | 1.61        | 2      | 9     |
| 1:A:11:TRP:CZ3 | 1:A:23:PRO:HB3  | 0.70     | 2.22        | 1      | 8     |
| 1:A:8:TYR:CE2  | 1:A:12:LEU:HD11 | 0.68     | 2.24        | 3      | 1     |
| 1:A:8:TYR:C    | 1:A:12:LEU:HD23 | 0.68     | 2.12        | 6      | 9     |
| 1:A:9:ILE:O    | 1:A:13:LYS:HD3  | 0.67     | 1.90        | 6      | 7     |
| 1:A:8:TYR:CE2  | 1:A:12:LEU:HD21 | 0.66     | 2.26        | 10     | 8     |
| 1:A:9:ILE:HA   | 1:A:12:LEU:HB2  | 0.62     | 1.71        | 9      | 10    |
| 1:A:8:TYR:CZ   | 1:A:12:LEU:HD21 | 0.62     | 2.30        | 8      | 9     |
| 1:A:9:ILE:CA   | 1:A:12:LEU:HD23 | 0.62     | 2.25        | 2      | 9     |
| 1:A:8:TYR:CE1  | 1:A:12:LEU:HD21 | 0.61     | 2.30        | 5      | 8     |
| 1:A:8:TYR:O    | 1:A:12:LEU:HG   | 0.61     | 1.96        | 3      | 1     |
| 1:A:5:VAL:HA   | 1:A:8:TYR:HB3   | 0.60     | 1.72        | 3      | 7     |
| 1:A:8:TYR:O    | 1:A:12:LEU:HD23 | 0.59     | 1.98        | 10     | 9     |
| 1:A:8:TYR:CD1  | 1:A:12:LEU:HD21 | 0.58     | 2.33        | 6      | 6     |
| 1:A:9:ILE:CG1  | 1:A:12:LEU:HD12 | 0.58     | 2.26        | 3      | 1     |
| 1:A:11:TRP:CE3 | 1:A:23:PRO:HB3  | 0.57     | 2.34        | 5      | 4     |
| 1:A:10:GLN:HA  | 1:A:13:LYS:CE   | 0.56     | 2.31        | 9      | 5     |
| 1:A:9:ILE:HG22 | 1:A:13:LYS:HD2  | 0.54     | 1.79        | 2      | 2     |
| 1:A:11:TRP:CZ2 | 1:A:23:PRO:HD3  | 0.54     | 2.38        | 5      | 3     |
| 1:A:8:TYR:HA   | 1:A:24:PRO:CG   | 0.53     | 2.33        | 10     | 10    |
| 1:A:8:TYR:CD2  | 1:A:12:LEU:HD21 | 0.53     | 2.38        | 4      | 8     |
| 1:A:11:TRP:CH2 | 1:A:23:PRO:HB3  | 0.53     | 2.39        | 10     | 4     |
| 1:A:11:TRP:HE3 | 1:A:12:LEU:CD2  | 0.52     | 2.16        | 8      | 9     |
| 1:A:14:ASP:OD2 | 1:A:19:SER:HB2  | 0.51     | 2.06        | 5      | 3     |
| 1:A:8:TYR:HA   | 1:A:24:PRO:HG2  | 0.50     | 1.83        | 6      | 9     |
| 1:A:4:CYS:SG   | 1:A:5:VAL:HG23  | 0.50     | 2.47        | 3      | 1     |
| 1:A:8:TYR:O    | 1:A:11:TRP:N    | 0.50     | 2.44        | 2      | 7     |
| 1:A:9:ILE:HA   | 1:A:12:LEU:HD12 | 0.50     | 1.81        | 3      | 1     |
| 1:A:9:ILE:HA   | 1:A:12:LEU:CD2  | 0.49     | 2.35        | 8      | 9     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:9:ILE:HA    | 1:A:12:LEU:CB   | 0.49     | 2.37        | 8      | 6     |
| 1:A:5:VAL:CG1   | 1:A:9:ILE:HD12  | 0.48     | 2.37        | 6      | 8     |
| 1:A:9:ILE:HG12  | 1:A:12:LEU:CD1  | 0.48     | 2.31        | 3      | 1     |
| 1:A:11:TRP:HE1  | 1:A:21:ARG:C    | 0.48     | 2.17        | 2      | 5     |
| 1:A:11:TRP:CZ3  | 1:A:12:LEU:CD2  | 0.48     | 2.97        | 3      | 1     |
| 1:A:9:ILE:N     | 1:A:12:LEU:HD23 | 0.47     | 2.24        | 5      | 4     |
| 1:A:10:GLN:HA   | 1:A:13:LYS:HE3  | 0.47     | 1.86        | 10     | 3     |
| 1:A:10:GLN:CD   | 1:A:13:LYS:HE2  | 0.47     | 2.34        | 4      | 1     |
| 1:A:8:TYR:CG    | 1:A:12:LEU:HD21 | 0.46     | 2.45        | 5      | 5     |
| 1:A:11:TRP:CE3  | 1:A:12:LEU:CD2  | 0.46     | 2.96        | 10     | 4     |
| 1:A:8:TYR:CE2   | 1:A:12:LEU:CD2  | 0.46     | 2.99        | 9      | 1     |
| 1:A:15:GLY:HA3  | 1:A:19:SER:HA   | 0.45     | 1.88        | 4      | 4     |
| 1:A:7:LEU:O     | 1:A:24:PRO:HG2  | 0.45     | 2.12        | 3      | 1     |
| 1:A:4:CYS:SG    | 1:A:5:VAL:N     | 0.45     | 2.89        | 3      | 1     |
| 1:A:5:VAL:O     | 1:A:9:ILE:N     | 0.44     | 2.42        | 6      | 1     |
| 1:A:9:ILE:HA    | 1:A:12:LEU:CG   | 0.44     | 2.43        | 8      | 2     |
| 1:A:8:TYR:CD2   | 1:A:12:LEU:CD2  | 0.43     | 3.01        | 9      | 2     |
| 1:A:10:GLN:HE21 | 1:A:13:LYS:HE3  | 0.43     | 1.74        | 10     | 3     |
| 1:A:12:LEU:HD22 | 1:A:12:LEU:N    | 0.43     | 2.28        | 1      | 4     |
| 1:A:10:GLN:CD   | 1:A:10:GLN:C    | 0.43     | 2.86        | 10     | 1     |
| 1:A:9:ILE:HG22  | 1:A:13:LYS:CD   | 0.43     | 2.43        | 1      | 1     |
| 1:A:5:VAL:HG13  | 1:A:9:ILE:CD1   | 0.42     | 2.44        | 2      | 4     |
| 1:A:15:GLY:HA3  | 1:A:19:SER:CA   | 0.42     | 2.45        | 7      | 4     |
| 1:A:7:LEU:O     | 1:A:10:GLN:HB3  | 0.42     | 2.15        | 9      | 2     |
| 1:A:8:TYR:OH    | 1:A:12:LEU:HD11 | 0.42     | 2.14        | 9      | 1     |
| 1:A:8:TYR:O     | 1:A:12:LEU:CD2  | 0.41     | 2.68        | 2      | 2     |
| 1:A:10:GLN:C    | 1:A:10:GLN:CD   | 0.41     | 2.88        | 8      | 1     |
| 1:A:11:TRP:CH2  | 1:A:17:PRO:HD3  | 0.41     | 2.50        | 9      | 1     |
| 1:A:10:GLN:HA   | 1:A:13:LYS:HE2  | 0.41     | 1.92        | 7      | 1     |
| 1:A:8:TYR:C     | 1:A:12:LEU:CD2  | 0.41     | 2.91        | 6      | 2     |
| 1:A:8:TYR:O     | 1:A:11:TRP:CB   | 0.40     | 2.70        | 6      | 2     |

## 6.3 Torsion angles ⓘ

### 6.3.1 Protein backbone ⓘ

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

| Mol | Chain | Analysed      | Favoured     | Allowed    | Outliers   | Percentiles |    |
|-----|-------|---------------|--------------|------------|------------|-------------|----|
| 1   | A     | 21/25 (84%)   | 19±1 (92±3%) | 1±1 (7±4%) | 0±0 (1±2%) | 11          | 58 |
| All | All   | 210/250 (84%) | 193 (92%)    | 14 (7%)    | 3 (1%)     | 11          | 58 |

All 1 unique Ramachandran outliers are listed below.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 15  | GLY  | 3              |

### 6.3.2 Protein sidechains ⓘ

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

| Mol | Chain | Analysed      | Rotameric    | Outliers    | Percentiles |    |
|-----|-------|---------------|--------------|-------------|-------------|----|
| 1   | A     | 19/22 (86%)   | 16±1 (84±6%) | 3±1 (16±6%) | 4           | 40 |
| All | All   | 190/220 (86%) | 159 (84%)    | 31 (16%)    | 4           | 40 |

All 5 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     | 4   | CYS  | 9              |
| 1   | A     | 10  | GLN  | 8              |
| 1   | A     | 13  | LYS  | 8              |
| 1   | A     | 21  | ARG  | 4              |
| 1   | A     | 6   | ARG  | 2              |

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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 51% for the well-defined parts and 51% for the entire structure.

### 7.1 Chemical shift list 2

File name: working\_cs.cif

Chemical shift list name: *nef\_chemical\_shift\_list\_ShiftList\_299K\_20160428*

#### 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                  | 167 |
| Number of shifts mapped to atoms        | 167 |
| 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 51%, i.e. 150 atoms were assigned a chemical shift out of a possible 292. 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  | 43/105 (41%)  | 43/43 (100%)   | 0/44 (0%)       | 0/18 (0%)       |
| Sidechain | 97/166 (58%)  | 97/108 (90%)   | 0/50 (0%)       | 0/8 (0%)        |
| Aromatic  | 10/21 (48%)   | 10/10 (100%)   | 0/10 (0%)       | 0/1 (0%)        |
| Overall   | 150/292 (51%) | 150/161 (93%)  | 0/104 (0%)      | 0/27 (0%)       |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 51%, i.e. 166 atoms were assigned a chemical shift out of a possible 328. 0 out of 3 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total         | $^1\text{H}$  | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|---------------|---------------|-----------------|-----------------|
| Backbone  | 47/120 (39%)  | 47/49 (96%)   | 0/50 (0%)       | 0/21 (0%)       |
| Sidechain | 109/187 (58%) | 109/120 (91%) | 0/59 (0%)       | 0/8 (0%)        |
| Aromatic  | 10/21 (48%)   | 10/10 (100%)  | 0/10 (0%)       | 0/1 (0%)        |
| Overall   | 166/328 (51%) | 166/179 (93%) | 0/119 (0%)      | 0/30 (0%)       |

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

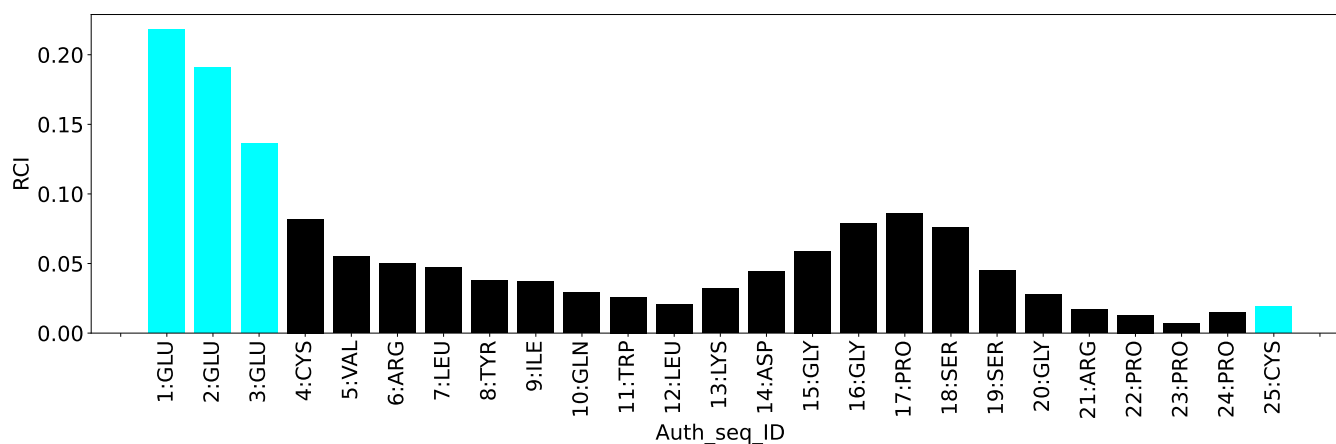
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

| List Id | Chain | Res | Type | Atom | Shift, <i>ppm</i> | Expected range, <i>ppm</i> | Z-score |
|---------|-------|-----|------|------|-------------------|----------------------------|---------|
| 2       | A     | 16  | GLY  | HA2  | 0.65              | 2.15 – 5.77                | -9.1    |
| 2       | A     | 23  | PRO  | HA   | 2.24              | 2.78 – 6.00                | -6.7    |

### 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                                | 737   |
| Intra-residue ( $ i-j =0$ )                              | 321   |
| Sequential ( $ i-j =1$ )                                 | 147   |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 161   |
| Long range ( $ i-j \geq 5$ )                             | 108   |
| 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                         | 29.5  |
| Number of long range restraints per residue <sup>1</sup> | 4.3   |

<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)  | 54.9                                   | 0.2     |
| 0.2-0.5 (Medium) | 102.8                                  | 0.5     |
| >0.5 (Large)     | 98.5                                   | 2.39    |

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

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

## 9 Distance violation analysis ⓘ

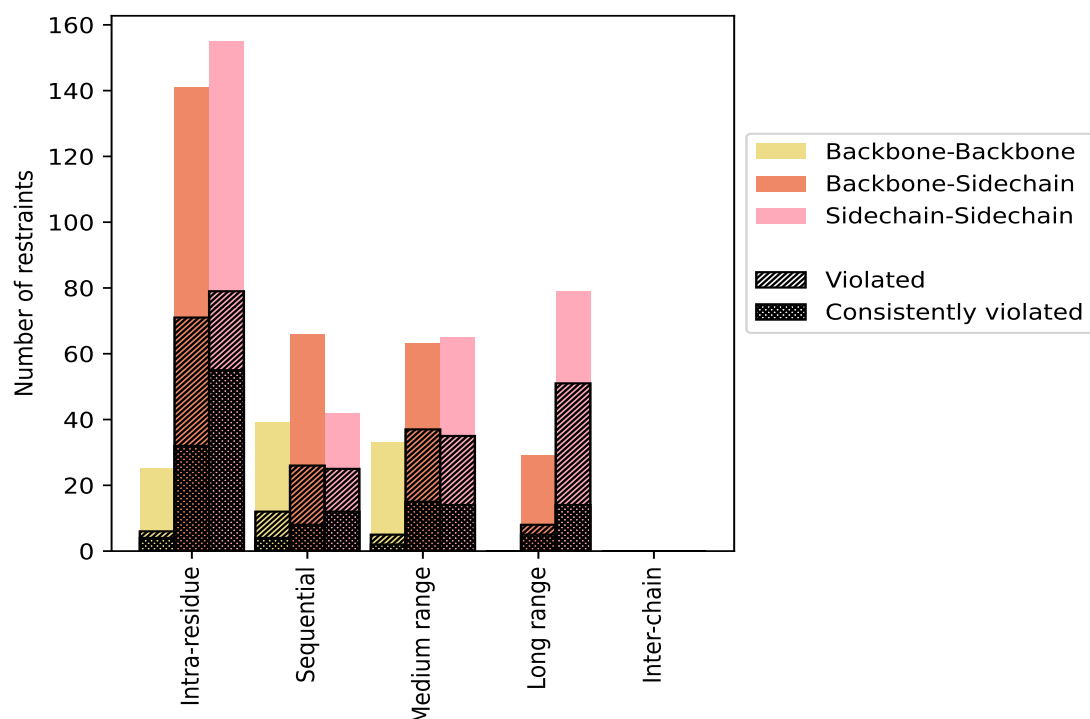
### 9.1 Summary of distance violations ⓘ

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

| Restraints type                                                             | Count      | % <sup>1</sup> | Violated <sup>3</sup> |                |                | Consistently Violated <sup>4</sup> |                |                |
|-----------------------------------------------------------------------------|------------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
|                                                                             |            |                | Count                 | % <sup>2</sup> | % <sup>1</sup> | Count                              | % <sup>2</sup> | % <sup>1</sup> |
| <b>Intra-residue (<math> i-j =0</math>)</b>                                 | <b>321</b> | <b>43.6</b>    | <b>156</b>            | <b>48.6</b>    | <b>21.2</b>    | <b>91</b>                          | <b>28.3</b>    | <b>12.3</b>    |
| Backbone-Backbone                                                           | 25         | 3.4            | 6                     | 24.0           | 0.8            | 4                                  | 16.0           | 0.5            |
| Backbone-Sidechain                                                          | 141        | 19.1           | 71                    | 50.4           | 9.6            | 32                                 | 22.7           | 4.3            |
| Sidechain-Sidechain                                                         | 155        | 21.0           | 79                    | 51.0           | 10.7           | 55                                 | 35.5           | 7.5            |
| <b>Sequential (<math> i-j =1</math>)</b>                                    | <b>147</b> | <b>19.9</b>    | <b>63</b>             | <b>42.9</b>    | <b>8.5</b>     | <b>24</b>                          | <b>16.3</b>    | <b>3.3</b>     |
| Backbone-Backbone                                                           | 39         | 5.3            | 12                    | 30.8           | 1.6            | 4                                  | 10.3           | 0.5            |
| Backbone-Sidechain                                                          | 66         | 9.0            | 26                    | 39.4           | 3.5            | 8                                  | 12.1           | 1.1            |
| Sidechain-Sidechain                                                         | 42         | 5.7            | 25                    | 59.5           | 3.4            | 12                                 | 28.6           | 1.6            |
| <b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b> | <b>161</b> | <b>21.8</b>    | <b>77</b>             | <b>47.8</b>    | <b>10.4</b>    | <b>31</b>                          | <b>19.3</b>    | <b>4.2</b>     |
| Backbone-Backbone                                                           | 33         | 4.5            | 5                     | 15.2           | 0.7            | 2                                  | 6.1            | 0.3            |
| Backbone-Sidechain                                                          | 63         | 8.5            | 37                    | 58.7           | 5.0            | 15                                 | 23.8           | 2.0            |
| Sidechain-Sidechain                                                         | 65         | 8.8            | 35                    | 53.8           | 4.7            | 14                                 | 21.5           | 1.9            |
| <b>Long range (<math> i-j \geq 5</math>)</b>                                | <b>108</b> | <b>14.7</b>    | <b>59</b>             | <b>54.6</b>    | <b>8.0</b>     | <b>19</b>                          | <b>17.6</b>    | <b>2.6</b>     |
| Backbone-Backbone                                                           | 0          | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 29         | 3.9            | 8                     | 27.6           | 1.1            | 5                                  | 17.2           | 0.7            |
| Sidechain-Sidechain                                                         | 79         | 10.7           | 51                    | 64.6           | 6.9            | 14                                 | 17.7           | 1.9            |
| <b>Inter-chain</b>                                                          | <b>0</b>   | <b>0.0</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| Backbone-Backbone                                                           | 0          | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 0          | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 0          | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| <b>Hydrogen bond</b>                                                        | <b>0</b>   | <b>0.0</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| <b>Disulfide bond</b>                                                       | <b>0</b>   | <b>0.0</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| <b>Total</b>                                                                | <b>737</b> | <b>100.0</b>   | <b>355</b>            | <b>48.2</b>    | <b>48.2</b>    | <b>165</b>                         | <b>22.4</b>    | <b>22.4</b>    |
| Backbone-Backbone                                                           | 97         | 13.2           | 23                    | 23.7           | 3.1            | 10                                 | 10.3           | 1.4            |
| Backbone-Sidechain                                                          | 299        | 40.6           | 142                   | 47.5           | 19.3           | 60                                 | 20.1           | 8.1            |
| Sidechain-Sidechain                                                         | 341        | 46.3           | 190                   | 55.7           | 25.8           | 95                                 | 27.9           | 12.9           |

<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

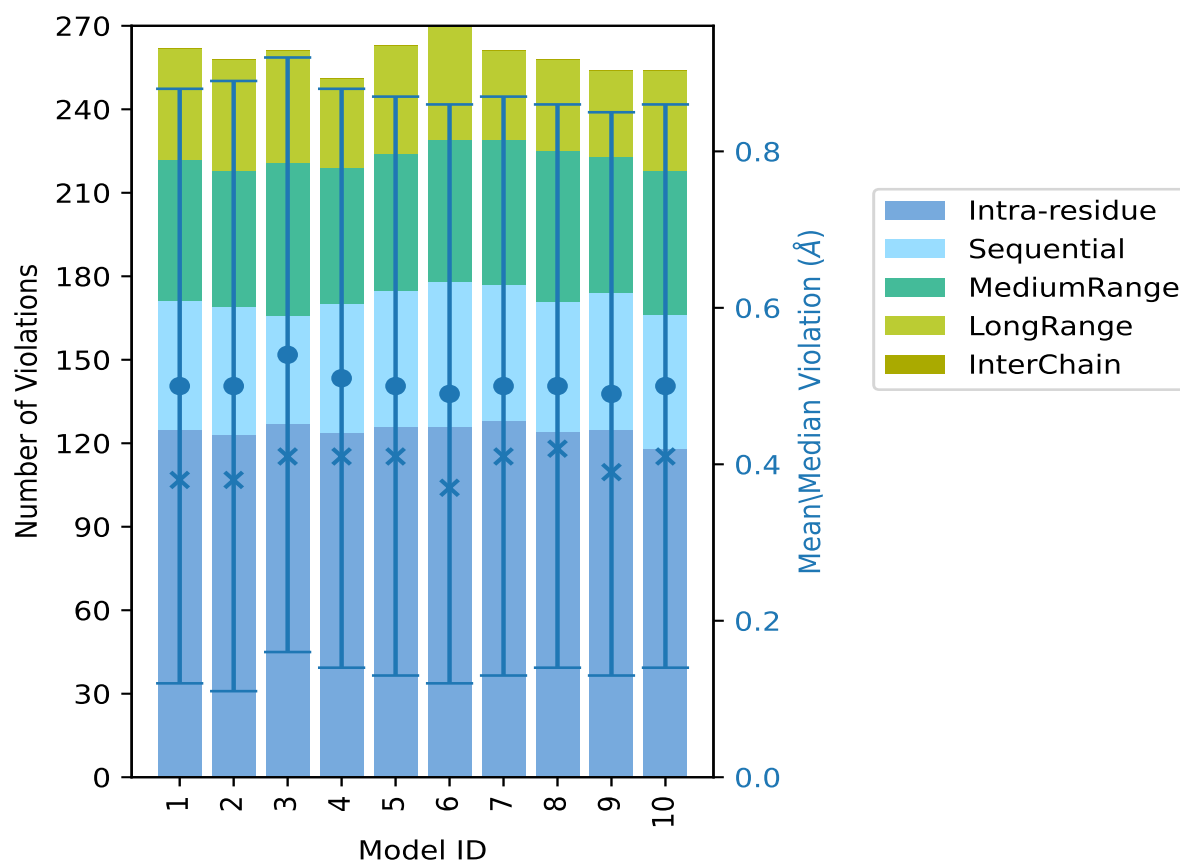
## 9.2 Distance violation statistics for each model [i](#)

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        | 125                  | 46              | 51              | 40              | 0               | 262   | 0.5      | 2.1     | 0.38                | 0.38       |
| 2        | 123                  | 46              | 49              | 40              | 0               | 258   | 0.5      | 2.25    | 0.39                | 0.38       |
| 3        | 127                  | 39              | 55              | 40              | 0               | 261   | 0.54     | 2.16    | 0.38                | 0.41       |
| 4        | 124                  | 46              | 49              | 32              | 0               | 251   | 0.51     | 2.35    | 0.37                | 0.41       |
| 5        | 126                  | 49              | 49              | 39              | 0               | 263   | 0.5      | 2.11    | 0.37                | 0.41       |
| 6        | 126                  | 52              | 51              | 41              | 0               | 270   | 0.49     | 2.15    | 0.37                | 0.37       |
| 7        | 128                  | 49              | 52              | 32              | 0               | 261   | 0.5      | 2.39    | 0.37                | 0.41       |
| 8        | 124                  | 47              | 54              | 33              | 0               | 258   | 0.5      | 2.19    | 0.36                | 0.42       |
| 9        | 125                  | 49              | 49              | 31              | 0               | 254   | 0.49     | 2.0     | 0.36                | 0.39       |
| 10       | 118                  | 48              | 52              | 36              | 0               | 254   | 0.5      | 2.15    | 0.36                | 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, 382(IR:165, SQ:84, MR:84, LR:49, 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>       | %    |
| 14                            | 9               | 15              | 8               | 0               | 46    | 1                        | 10.0 |
| 5                             | 0               | 3               | 4               | 0               | 12    | 2                        | 20.0 |
| 6                             | 2               | 2               | 1               | 0               | 11    | 3                        | 30.0 |

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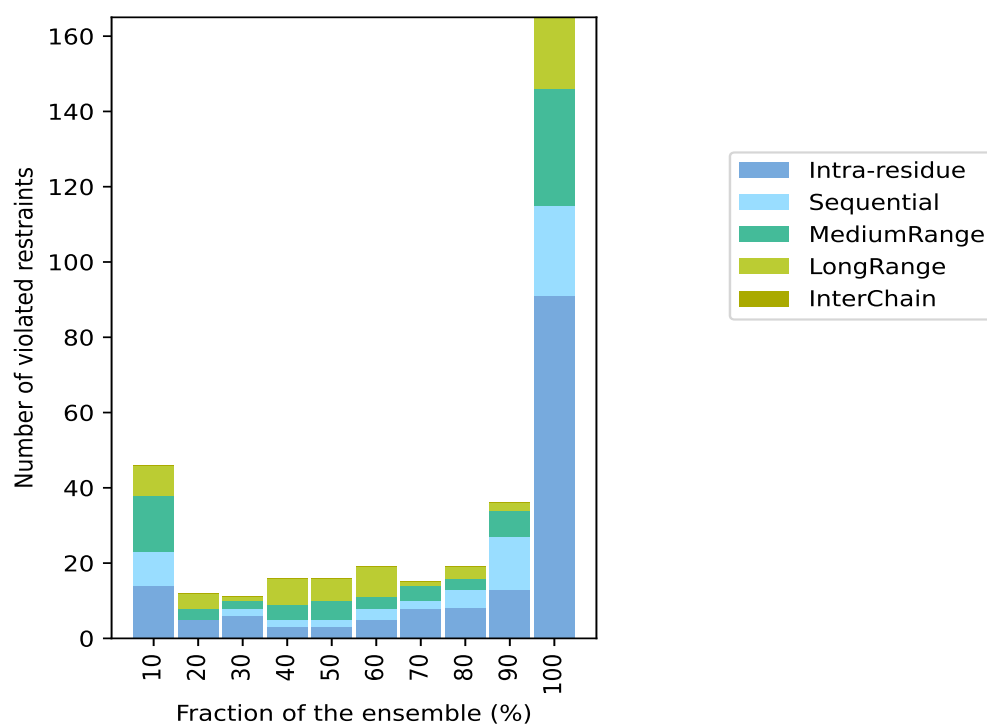
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| Number of violated restraints |                 |                 |                 |                 |       | Fraction of the ensemble |       |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|-------|
| 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>       | %     |
| 3                             | 2               | 4               | 7               | 0               | 16    | 4                        | 40.0  |
| 3                             | 2               | 5               | 6               | 0               | 16    | 5                        | 50.0  |
| 5                             | 3               | 3               | 8               | 0               | 19    | 6                        | 60.0  |
| 8                             | 2               | 4               | 1               | 0               | 15    | 7                        | 70.0  |
| 8                             | 5               | 3               | 3               | 0               | 19    | 8                        | 80.0  |
| 13                            | 14              | 7               | 2               | 0               | 36    | 9                        | 90.0  |
| 91                            | 24              | 31              | 19              | 0               | 165   | 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 ⓘ

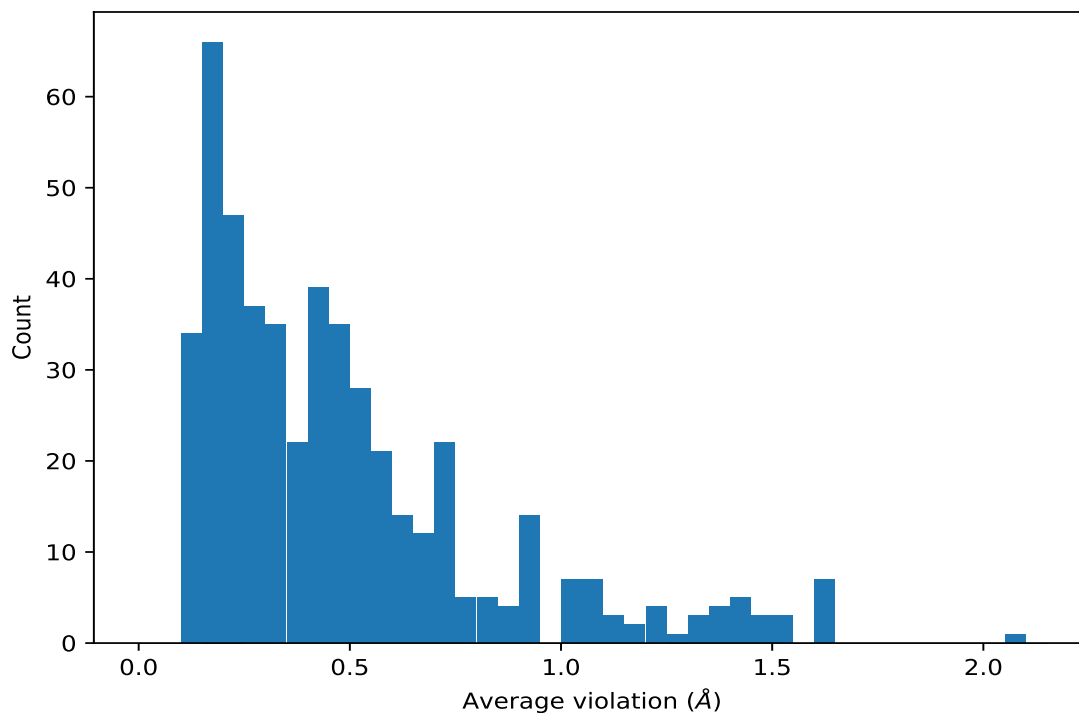


## 9.4 Most violated distance restraints in the ensemble ⓘ

### 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) |
|---------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,727) | 1:22:A:PRO:HB3 | 1:23:A:PRO:HG3  | 10                  | 2.09     | 0.21                | 2.16       |
| (1,696) | 1:5:A:VAL:HG21 | 1:9:A:ILE:HB    | 10                  | 1.62     | 0.05                | 1.62       |
| (1,696) | 1:5:A:VAL:HG22 | 1:9:A:ILE:HB    | 10                  | 1.62     | 0.05                | 1.62       |
| (1,696) | 1:5:A:VAL:HG23 | 1:9:A:ILE:HB    | 10                  | 1.62     | 0.05                | 1.62       |
| (1,681) | 1:11:A:TRP:HB3 | 1:12:A:LEU:HD21 | 10                  | 1.61     | 0.53                | 1.52       |
| (1,681) | 1:11:A:TRP:HB3 | 1:12:A:LEU:HD22 | 10                  | 1.61     | 0.53                | 1.52       |
| (1,681) | 1:11:A:TRP:HB3 | 1:12:A:LEU:HD23 | 10                  | 1.61     | 0.53                | 1.52       |
| (1,729) | 1:2:A:GLU:HG2  | 1:6:A:ARG:HG3   | 10                  | 1.6      | 0.34                | 1.74       |
| (1,680) | 1:11:A:TRP:HB3 | 1:12:A:LEU:HD21 | 10                  | 1.52     | 0.53                | 1.43       |
| (1,680) | 1:11:A:TRP:HB3 | 1:12:A:LEU:HD22 | 10                  | 1.52     | 0.53                | 1.43       |
| (1,680) | 1:11:A:TRP:HB3 | 1:12:A:LEU:HD23 | 10                  | 1.52     | 0.53                | 1.43       |
| (1,216) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD21 | 10                  | 1.47     | 0.14                | 1.51       |
| (1,216) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD22 | 10                  | 1.47     | 0.14                | 1.51       |
| (1,216) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD23 | 10                  | 1.47     | 0.14                | 1.51       |
| (1,109) | 1:9:A:ILE:HB   | 1:11:A:TRP:H    | 10                  | 1.44     | 0.25                | 1.51       |

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| Key     | Atom-1         | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,713) | 1:5:A:VAL:HG21 | 1:9:A:ILE:HG12  | 10                  | 1.42     | 0.02                | 1.42       |
| (1,713) | 1:5:A:VAL:HG22 | 1:9:A:ILE:HG12  | 10                  | 1.42     | 0.02                | 1.42       |
| (1,713) | 1:5:A:VAL:HG23 | 1:9:A:ILE:HG12  | 10                  | 1.42     | 0.02                | 1.42       |
| (1,661) | 1:17:A:PRO:HB3 | 1:18:A:SER:HB3  | 10                  | 1.4      | 0.51                | 1.65       |
| (1,687) | 1:2:A:GLU:HG3  | 1:5:A:VAL:HG11  | 10                  | 1.38     | 0.04                | 1.39       |
| (1,687) | 1:2:A:GLU:HG3  | 1:5:A:VAL:HG12  | 10                  | 1.38     | 0.04                | 1.39       |
| (1,687) | 1:2:A:GLU:HG3  | 1:5:A:VAL:HG13  | 10                  | 1.38     | 0.04                | 1.39       |
| (1,726) | 1:22:A:PRO:HB2 | 1:23:A:PRO:HG2  | 10                  | 1.36     | 0.14                | 1.31       |
| (1,568) | 1:8:A:TYR:HA   | 1:24:A:PRO:HD2  | 10                  | 1.34     | 0.13                | 1.36       |
| (1,547) | 1:13:A:LYS:HD2 | 1:13:A:LYS:HE2  | 10                  | 1.33     | 0.02                | 1.33       |
| (1,547) | 1:13:A:LYS:HD2 | 1:13:A:LYS:HE3  | 10                  | 1.33     | 0.02                | 1.33       |
| (1,473) | 1:22:A:PRO:HA  | 1:22:A:PRO:HD3  | 10                  | 1.24     | 0.05                | 1.21       |
| (1,504) | 1:11:A:TRP:HD1 | 1:23:A:PRO:HD3  | 10                  | 1.23     | 0.12                | 1.27       |
| (1,645) | 1:19:A:SER:HB2 | 1:19:A:SER:HG   | 10                  | 1.23     | 0.01                | 1.23       |
| (1,669) | 1:9:A:ILE:HA   | 1:12:A:LEU:HB2  | 10                  | 1.19     | 0.01                | 1.19       |
| (1,50)  | 1:2:A:GLU:HG2  | 1:6:A:ARG:H     | 10                  | 1.15     | 0.08                | 1.15       |
| (1,561) | 1:8:A:TYR:HA   | 1:24:A:PRO:HG2  | 10                  | 1.13     | 0.01                | 1.13       |
| (1,240) | 1:8:A:TYR:HD1  | 1:9:A:ILE:HG13  | 10                  | 1.11     | 0.17                | 1.17       |
| (1,240) | 1:8:A:TYR:HD2  | 1:9:A:ILE:HG13  | 10                  | 1.11     | 0.17                | 1.17       |
| (1,548) | 1:13:A:LYS:HE2 | 1:13:A:LYS:HG2  | 10                  | 1.05     | 0.12                | 1.02       |
| (1,548) | 1:13:A:LYS:HE2 | 1:13:A:LYS:HG3  | 10                  | 1.05     | 0.12                | 1.02       |
| (1,548) | 1:13:A:LYS:HE3 | 1:13:A:LYS:HG2  | 10                  | 1.05     | 0.12                | 1.02       |
| (1,548) | 1:13:A:LYS:HE3 | 1:13:A:LYS:HG3  | 10                  | 1.05     | 0.12                | 1.02       |
| (1,257) | 1:24:A:PRO:HD2 | 1:25:A:CYS:H    | 10                  | 1.04     | 0.15                | 1.04       |
| (1,543) | 1:2:A:GLU:HG2  | 1:9:A:ILE:HD11  | 10                  | 1.02     | 0.11                | 1.06       |
| (1,543) | 1:2:A:GLU:HG2  | 1:9:A:ILE:HD12  | 10                  | 1.02     | 0.11                | 1.06       |
| (1,543) | 1:2:A:GLU:HG2  | 1:9:A:ILE:HD13  | 10                  | 1.02     | 0.11                | 1.06       |
| (1,557) | 1:9:A:ILE:HA   | 1:12:A:LEU:HG   | 10                  | 1.02     | 0.12                | 1.06       |
| (1,189) | 1:8:A:TYR:HD1  | 1:24:A:PRO:HD2  | 10                  | 1.0      | 0.11                | 0.97       |
| (1,189) | 1:8:A:TYR:HD2  | 1:24:A:PRO:HD2  | 10                  | 1.0      | 0.11                | 0.97       |
| (1,553) | 1:11:A:TRP:HB2 | 1:24:A:PRO:HD3  | 10                  | 0.93     | 0.21                | 0.83       |
| (1,407) | 1:12:A:LEU:HA  | 1:12:A:LEU:HD21 | 10                  | 0.93     | 0.18                | 0.97       |
| (1,407) | 1:12:A:LEU:HA  | 1:12:A:LEU:HD22 | 10                  | 0.93     | 0.18                | 0.97       |
| (1,407) | 1:12:A:LEU:HA  | 1:12:A:LEU:HD23 | 10                  | 0.93     | 0.18                | 0.97       |
| (1,236) | 1:11:A:TRP:HH2 | 1:22:A:PRO:HB2  | 10                  | 0.91     | 0.24                | 0.97       |
| (1,176) | 1:11:A:TRP:HB2 | 1:11:A:TRP:HZ3  | 10                  | 0.89     | 0.04                | 0.91       |
| (1,129) | 1:10:A:GLN:HA  | 1:10:A:GLN:HE21 | 10                  | 0.88     | 0.29                | 0.95       |
| (1,649) | 1:15:A:GLY:HA2 | 1:19:A:SER:HB3  | 10                  | 0.86     | 0.07                | 0.84       |
| (1,441) | 1:17:A:PRO:HB2 | 1:17:A:PRO:HD2  | 10                  | 0.85     | 0.02                | 0.86       |
| (1,215) | 1:11:A:TRP:HZ3 | 1:12:A:LEU:HD21 | 10                  | 0.82     | 0.42                | 1.03       |
| (1,215) | 1:11:A:TRP:HZ3 | 1:12:A:LEU:HD22 | 10                  | 0.82     | 0.42                | 1.03       |
| (1,215) | 1:11:A:TRP:HZ3 | 1:12:A:LEU:HD23 | 10                  | 0.82     | 0.42                | 1.03       |

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| Key     | Atom-1         | Atom-2         | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|----------------|----------------|---------------------|----------|---------------------|------------|
| (1,517) | 1:23:A:PRO:HB3 | 1:23:A:PRO:HG3 | 10                  | 0.8      | 0.04                | 0.78       |
| (1,121) | 1:2:A:GLU:HB2  | 1:5:A:VAL:H    | 10                  | 0.79     | 0.12                | 0.78       |
| (1,722) | 1:9:A:ILE:HG12 | 1:12:A:LEU:HB3 | 10                  | 0.77     | 0.11                | 0.74       |
| (1,476) | 1:22:A:PRO:HA  | 1:22:A:PRO:HG3 | 10                  | 0.73     | 0.18                | 0.74       |
| (1,427) | 1:13:A:LYS:HB2 | 1:13:A:LYS:HG2 | 10                  | 0.73     | 0.0                 | 0.73       |
| (1,427) | 1:13:A:LYS:HB2 | 1:13:A:LYS:HG3 | 10                  | 0.73     | 0.0                 | 0.73       |
| (1,427) | 1:13:A:LYS:HB3 | 1:13:A:LYS:HG2 | 10                  | 0.73     | 0.0                 | 0.73       |
| (1,427) | 1:13:A:LYS:HB3 | 1:13:A:LYS:HG3 | 10                  | 0.73     | 0.0                 | 0.73       |
| (1,322) | 1:11:A:TRP:HB3 | 1:11:A:TRP:HE3 | 10                  | 0.72     | 0.01                | 0.72       |
| (1,701) | 1:5:A:VAL:HG11 | 1:9:A:ILE:HG13 | 10                  | 0.71     | 0.05                | 0.7        |
| (1,701) | 1:5:A:VAL:HG12 | 1:9:A:ILE:HG13 | 10                  | 0.71     | 0.05                | 0.7        |
| (1,701) | 1:5:A:VAL:HG13 | 1:9:A:ILE:HG13 | 10                  | 0.71     | 0.05                | 0.7        |
| (1,662) | 1:17:A:PRO:HB3 | 1:18:A:SER:HB2 | 10                  | 0.7      | 0.27                | 0.68       |
| (1,198) | 1:11:A:TRP:HZ3 | 1:23:A:PRO:HB3 | 10                  | 0.69     | 0.14                | 0.69       |
| (1,644) | 1:22:A:PRO:HA  | 1:23:A:PRO:HD2 | 10                  | 0.69     | 0.18                | 0.76       |
| (1,468) | 1:21:A:ARG:HD3 | 1:21:A:ARG:HG2 | 10                  | 0.68     | 0.07                | 0.66       |
| (1,468) | 1:21:A:ARG:HD3 | 1:21:A:ARG:HG3 | 10                  | 0.68     | 0.07                | 0.66       |
| (1,732) | 1:2:A:GLU:HG3  | 1:6:A:ARG:HB3  | 10                  | 0.68     | 0.11                | 0.62       |
| (1,401) | 1:11:A:TRP:HA  | 1:11:A:TRP:HB2 | 10                  | 0.65     | 0.04                | 0.66       |
| (1,721) | 1:9:A:ILE:HG13 | 1:12:A:LEU:HB2 | 10                  | 0.64     | 0.08                | 0.62       |
| (1,282) | 1:15:A:GLY:H   | 1:16:A:GLY:H   | 10                  | 0.64     | 0.04                | 0.62       |
| (1,439) | 1:17:A:PRO:HA  | 1:17:A:PRO:HB3 | 10                  | 0.62     | 0.01                | 0.62       |
| (1,574) | 1:5:A:VAL:HA   | 1:8:A:TYR:HB2  | 10                  | 0.62     | 0.04                | 0.6        |
| (1,574) | 1:5:A:VAL:HA   | 1:8:A:TYR:HB3  | 10                  | 0.62     | 0.04                | 0.6        |
| (1,571) | 1:14:A:ASP:HB3 | 1:19:A:SER:HB2 | 10                  | 0.61     | 0.18                | 0.59       |
| (1,201) | 1:8:A:TYR:HE1  | 1:23:A:PRO:HB3 | 10                  | 0.6      | 0.08                | 0.6        |
| (1,201) | 1:8:A:TYR:HE2  | 1:23:A:PRO:HB3 | 10                  | 0.6      | 0.08                | 0.6        |
| (1,472) | 1:22:A:PRO:HA  | 1:22:A:PRO:HD2 | 10                  | 0.59     | 0.06                | 0.62       |
| (1,433) | 1:15:A:GLY:HA2 | 1:15:A:GLY:HA3 | 10                  | 0.58     | 0.01                | 0.57       |
| (1,593) | 1:11:A:TRP:HA  | 1:14:A:ASP:HB3 | 10                  | 0.58     | 0.25                | 0.66       |
| (1,349) | 1:6:A:ARG:HA   | 1:6:A:ARG:HG2  | 10                  | 0.58     | 0.06                | 0.57       |
| (1,570) | 1:16:A:GLY:HA3 | 1:17:A:PRO:HD2 | 10                  | 0.57     | 0.04                | 0.58       |
| (1,598) | 1:1:A:GLU:HA   | 1:1:A:GLU:HB3  | 10                  | 0.57     | 0.22                | 0.66       |
| (1,160) | 1:11:A:TRP:HZ2 | 1:22:A:PRO:HA  | 10                  | 0.57     | 0.16                | 0.48       |
| (1,461) | 1:21:A:ARG:HA  | 1:21:A:ARG:HG2 | 10                  | 0.56     | 0.31                | 0.35       |
| (1,461) | 1:21:A:ARG:HA  | 1:21:A:ARG:HG3 | 10                  | 0.56     | 0.31                | 0.35       |
| (1,530) | 1:24:A:PRO:HD2 | 1:24:A:PRO:HG2 | 10                  | 0.55     | 0.01                | 0.55       |
| (1,270) | 1:8:A:TYR:HD1  | 1:25:A:CYS:H   | 10                  | 0.55     | 0.07                | 0.52       |
| (1,270) | 1:8:A:TYR:HD2  | 1:25:A:CYS:H   | 10                  | 0.55     | 0.07                | 0.52       |
| (1,507) | 1:23:A:PRO:HD2 | 1:23:A:PRO:HG2 | 10                  | 0.54     | 0.03                | 0.53       |
| (1,353) | 1:6:A:ARG:HB3  | 1:6:A:ARG:HD3  | 10                  | 0.54     | 0.14                | 0.58       |
| (1,378) | 1:9:A:ILE:HA   | 1:9:A:ILE:HG12 | 10                  | 0.54     | 0.03                | 0.54       |

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| Key     | Atom-1         | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,212) | 1:8:A:TYR:HD1  | 1:9:A:ILE:HG21  | 10                  | 0.54     | 0.13                | 0.5        |
| (1,212) | 1:8:A:TYR:HD1  | 1:9:A:ILE:HG22  | 10                  | 0.54     | 0.13                | 0.5        |
| (1,212) | 1:8:A:TYR:HD1  | 1:9:A:ILE:HG23  | 10                  | 0.54     | 0.13                | 0.5        |
| (1,212) | 1:8:A:TYR:HD2  | 1:9:A:ILE:HG21  | 10                  | 0.54     | 0.13                | 0.5        |
| (1,212) | 1:8:A:TYR:HD2  | 1:9:A:ILE:HG22  | 10                  | 0.54     | 0.13                | 0.5        |
| (1,212) | 1:8:A:TYR:HD2  | 1:9:A:ILE:HG23  | 10                  | 0.54     | 0.13                | 0.5        |
| (1,675) | 1:12:A:LEU:HA  | 1:12:A:LEU:HD21 | 10                  | 0.53     | 0.18                | 0.57       |
| (1,675) | 1:12:A:LEU:HA  | 1:12:A:LEU:HD22 | 10                  | 0.53     | 0.18                | 0.57       |
| (1,675) | 1:12:A:LEU:HA  | 1:12:A:LEU:HD23 | 10                  | 0.53     | 0.18                | 0.57       |
| (1,616) | 1:14:A:ASP:HB3 | 1:16:A:GLY:H    | 10                  | 0.52     | 0.09                | 0.53       |
| (1,705) | 1:9:A:ILE:HG21 | 1:13:A:LYS:HD2  | 10                  | 0.52     | 0.35                | 0.38       |
| (1,705) | 1:9:A:ILE:HG22 | 1:13:A:LYS:HD2  | 10                  | 0.52     | 0.35                | 0.38       |
| (1,705) | 1:9:A:ILE:HG23 | 1:13:A:LYS:HD2  | 10                  | 0.52     | 0.35                | 0.38       |
| (1,564) | 1:4:A:CYS:HA   | 1:7:A:LEU:HB3   | 10                  | 0.51     | 0.09                | 0.51       |
| (1,431) | 1:14:A:ASP:HA  | 1:14:A:ASP:HB2  | 10                  | 0.51     | 0.05                | 0.51       |
| (1,185) | 1:11:A:TRP:HB3 | 1:11:A:TRP:HE3  | 10                  | 0.5      | 0.01                | 0.5        |
| (1,368) | 1:7:A:LEU:HA   | 1:7:A:LEU:HD11  | 10                  | 0.48     | 0.07                | 0.5        |
| (1,368) | 1:7:A:LEU:HA   | 1:7:A:LEU:HD12  | 10                  | 0.48     | 0.07                | 0.5        |
| (1,368) | 1:7:A:LEU:HA   | 1:7:A:LEU:HD13  | 10                  | 0.48     | 0.07                | 0.5        |
| (1,368) | 1:7:A:LEU:HA   | 1:7:A:LEU:HD21  | 10                  | 0.48     | 0.07                | 0.5        |
| (1,368) | 1:7:A:LEU:HA   | 1:7:A:LEU:HD22  | 10                  | 0.48     | 0.07                | 0.5        |
| (1,368) | 1:7:A:LEU:HA   | 1:7:A:LEU:HD23  | 10                  | 0.48     | 0.07                | 0.5        |
| (1,371) | 1:7:A:LEU:HB2  | 1:7:A:LEU:HG    | 10                  | 0.48     | 0.01                | 0.48       |
| (1,325) | 1:2:A:GLU:HA   | 1:2:A:GLU:HB2   | 10                  | 0.47     | 0.04                | 0.46       |
| (1,172) | 1:11:A:TRP:HZ2 | 1:23:A:PRO:HD3  | 10                  | 0.46     | 0.16                | 0.38       |
| (1,494) | 1:21:A:ARG:HA  | 1:22:A:PRO:HD3  | 10                  | 0.46     | 0.14                | 0.47       |
| (1,654) | 1:14:A:ASP:HB3 | 1:19:A:SER:HB3  | 10                  | 0.46     | 0.21                | 0.6        |
| (1,166) | 1:5:A:VAL:HA   | 1:8:A:TYR:HD1   | 10                  | 0.46     | 0.16                | 0.42       |
| (1,166) | 1:5:A:VAL:HA   | 1:8:A:TYR:HD2   | 10                  | 0.46     | 0.16                | 0.42       |
| (1,492) | 1:22:A:PRO:HB3 | 1:22:A:PRO:HG3  | 10                  | 0.45     | 0.01                | 0.46       |
| (1,699) | 1:6:A:ARG:HB3  | 1:7:A:LEU:HD11  | 10                  | 0.45     | 0.02                | 0.44       |
| (1,699) | 1:6:A:ARG:HB3  | 1:7:A:LEU:HD12  | 10                  | 0.45     | 0.02                | 0.44       |
| (1,699) | 1:6:A:ARG:HB3  | 1:7:A:LEU:HD13  | 10                  | 0.45     | 0.02                | 0.44       |
| (1,699) | 1:6:A:ARG:HB3  | 1:7:A:LEU:HD21  | 10                  | 0.45     | 0.02                | 0.44       |
| (1,699) | 1:6:A:ARG:HB3  | 1:7:A:LEU:HD22  | 10                  | 0.45     | 0.02                | 0.44       |
| (1,699) | 1:6:A:ARG:HB3  | 1:7:A:LEU:HD23  | 10                  | 0.45     | 0.02                | 0.44       |
| (1,626) | 1:14:A:ASP:HB3 | 1:15:A:GLY:H    | 10                  | 0.44     | 0.15                | 0.4        |
| (1,92)  | 1:19:A:SER:H   | 1:19:A:SER:HG   | 10                  | 0.44     | 0.04                | 0.42       |
| (1,415) | 1:12:A:LEU:HB3 | 1:12:A:LEU:HD11 | 10                  | 0.44     | 0.05                | 0.44       |
| (1,415) | 1:12:A:LEU:HB3 | 1:12:A:LEU:HD12 | 10                  | 0.44     | 0.05                | 0.44       |
| (1,415) | 1:12:A:LEU:HB3 | 1:12:A:LEU:HD13 | 10                  | 0.44     | 0.05                | 0.44       |
| (1,140) | 1:9:A:ILE:HA   | 1:12:A:LEU:H    | 10                  | 0.44     | 0.05                | 0.45       |

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| Key     | Atom-1         | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,99)  | 1:11:A:TRP:HE1 | 1:22:A:PRO:HA   | 10                  | 0.43     | 0.08                | 0.43       |
| (1,467) | 1:21:A:ARG:HD2 | 1:21:A:ARG:HG2  | 10                  | 0.43     | 0.04                | 0.42       |
| (1,467) | 1:21:A:ARG:HD2 | 1:21:A:ARG:HG3  | 10                  | 0.43     | 0.04                | 0.42       |
| (1,597) | 1:1:A:GLU:HA   | 1:1:A:GLU:HB2   | 10                  | 0.43     | 0.28                | 0.2        |
| (1,357) | 1:6:A:ARG:HD3  | 1:6:A:ARG:HG2   | 10                  | 0.42     | 0.03                | 0.42       |
| (1,605) | 1:8:A:TYR:HE1  | 1:11:A:TRP:HZ3  | 10                  | 0.42     | 0.21                | 0.48       |
| (1,605) | 1:8:A:TYR:HE2  | 1:11:A:TRP:HZ3  | 10                  | 0.42     | 0.21                | 0.48       |
| (1,474) | 1:22:A:PRO:HA  | 1:22:A:PRO:HB3  | 10                  | 0.42     | 0.03                | 0.44       |
| (1,631) | 1:5:A:VAL:HG11 | 1:8:A:TYR:HD1   | 10                  | 0.42     | 0.06                | 0.41       |
| (1,631) | 1:5:A:VAL:HG11 | 1:8:A:TYR:HD2   | 10                  | 0.42     | 0.06                | 0.41       |
| (1,631) | 1:5:A:VAL:HG12 | 1:8:A:TYR:HD1   | 10                  | 0.42     | 0.06                | 0.41       |
| (1,631) | 1:5:A:VAL:HG12 | 1:8:A:TYR:HD2   | 10                  | 0.42     | 0.06                | 0.41       |
| (1,631) | 1:5:A:VAL:HG13 | 1:8:A:TYR:HD1   | 10                  | 0.42     | 0.06                | 0.41       |
| (1,631) | 1:5:A:VAL:HG13 | 1:8:A:TYR:HD2   | 10                  | 0.42     | 0.06                | 0.41       |
| (1,369) | 1:7:A:LEU:HB3  | 1:7:A:LEU:HD11  | 10                  | 0.42     | 0.01                | 0.42       |
| (1,369) | 1:7:A:LEU:HB3  | 1:7:A:LEU:HD12  | 10                  | 0.42     | 0.01                | 0.42       |
| (1,369) | 1:7:A:LEU:HB3  | 1:7:A:LEU:HD13  | 10                  | 0.42     | 0.01                | 0.42       |
| (1,369) | 1:7:A:LEU:HB3  | 1:7:A:LEU:HD21  | 10                  | 0.42     | 0.01                | 0.42       |
| (1,369) | 1:7:A:LEU:HB3  | 1:7:A:LEU:HD22  | 10                  | 0.42     | 0.01                | 0.42       |
| (1,369) | 1:7:A:LEU:HB3  | 1:7:A:LEU:HD23  | 10                  | 0.42     | 0.01                | 0.42       |
| (1,579) | 1:4:A:CYS:HA   | 1:7:A:LEU:HB2   | 10                  | 0.41     | 0.09                | 0.4        |
| (1,640) | 1:11:A:TRP:HE3 | 1:24:A:PRO:HD2  | 10                  | 0.4      | 0.11                | 0.4        |
| (1,276) | 1:19:A:SER:H   | 1:20:A:GLY:H    | 10                  | 0.4      | 0.09                | 0.38       |
| (1,485) | 1:22:A:PRO:HD3 | 1:22:A:PRO:HG3  | 10                  | 0.39     | 0.01                | 0.39       |
| (1,622) | 1:2:A:GLU:HB3  | 1:5:A:VAL:H     | 10                  | 0.38     | 0.16                | 0.44       |
| (1,546) | 1:13:A:LYS:HD3 | 1:13:A:LYS:HE2  | 10                  | 0.38     | 0.07                | 0.42       |
| (1,546) | 1:13:A:LYS:HD3 | 1:13:A:LYS:HE3  | 10                  | 0.38     | 0.07                | 0.42       |
| (1,735) | 1:2:A:GLU:HB2  | 1:5:A:VAL:HB    | 10                  | 0.38     | 0.02                | 0.38       |
| (1,232) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HG   | 10                  | 0.37     | 0.16                | 0.48       |
| (1,365) | 1:7:A:LEU:HA   | 1:7:A:LEU:HB3   | 10                  | 0.37     | 0.01                | 0.37       |
| (1,483) | 1:22:A:PRO:HD2 | 1:22:A:PRO:HG2  | 10                  | 0.37     | 0.02                | 0.36       |
| (1,734) | 1:2:A:GLU:HG3  | 1:5:A:VAL:HB    | 10                  | 0.36     | 0.07                | 0.38       |
| (1,273) | 1:18:A:SER:H   | 1:19:A:SER:H    | 10                  | 0.36     | 0.07                | 0.38       |
| (1,10)  | 1:9:A:ILE:H    | 1:12:A:LEU:HD21 | 10                  | 0.35     | 0.09                | 0.34       |
| (1,10)  | 1:9:A:ILE:H    | 1:12:A:LEU:HD22 | 10                  | 0.35     | 0.09                | 0.34       |
| (1,10)  | 1:9:A:ILE:H    | 1:12:A:LEU:HD23 | 10                  | 0.35     | 0.09                | 0.34       |
| (1,488) | 1:22:A:PRO:HB2 | 1:22:A:PRO:HB3  | 10                  | 0.35     | 0.0                 | 0.35       |
| (1,518) | 1:23:A:PRO:HB2 | 1:23:A:PRO:HB3  | 10                  | 0.35     | 0.01                | 0.34       |
| (1,456) | 1:20:A:GLY:HA2 | 1:20:A:GLY:HA3  | 10                  | 0.34     | 0.0                 | 0.34       |
| (1,370) | 1:7:A:LEU:HD11 | 1:7:A:LEU:HG    | 10                  | 0.34     | 0.0                 | 0.34       |
| (1,370) | 1:7:A:LEU:HD12 | 1:7:A:LEU:HG    | 10                  | 0.34     | 0.0                 | 0.34       |
| (1,370) | 1:7:A:LEU:HD13 | 1:7:A:LEU:HG    | 10                  | 0.34     | 0.0                 | 0.34       |

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| Key     | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,370) | 1:7:A:LEU:HD21  | 1:7:A:LEU:HG    | 10                  | 0.34     | 0.0                 | 0.34       |
| (1,370) | 1:7:A:LEU:HD22  | 1:7:A:LEU:HG    | 10                  | 0.34     | 0.0                 | 0.34       |
| (1,370) | 1:7:A:LEU:HD23  | 1:7:A:LEU:HG    | 10                  | 0.34     | 0.0                 | 0.34       |
| (1,542) | 1:7:A:LEU:HB2   | 1:24:A:PRO:HB3  | 10                  | 0.34     | 0.09                | 0.35       |
| (1,448) | 1:17:A:PRO:HB2  | 1:17:A:PRO:HB3  | 10                  | 0.34     | 0.01                | 0.34       |
| (1,411) | 1:12:A:LEU:HB2  | 1:12:A:LEU:HG   | 10                  | 0.33     | 0.04                | 0.34       |
| (1,576) | 1:22:A:PRO:HA   | 1:23:A:PRO:HD3  | 10                  | 0.33     | 0.1                 | 0.29       |
| (1,69)  | 1:18:A:SER:H    | 1:18:A:SER:HA   | 10                  | 0.33     | 0.02                | 0.32       |
| (1,173) | 1:11:A:TRP:HH2  | 1:17:A:PRO:HD3  | 10                  | 0.33     | 0.08                | 0.36       |
| (1,199) | 1:8:A:TYR:HD1   | 1:23:A:PRO:HB3  | 10                  | 0.33     | 0.13                | 0.32       |
| (1,199) | 1:8:A:TYR:HD2   | 1:23:A:PRO:HB3  | 10                  | 0.33     | 0.13                | 0.32       |
| (1,321) | 1:11:A:TRP:HB3  | 1:12:A:LEU:H    | 10                  | 0.32     | 0.14                | 0.26       |
| (1,403) | 1:11:A:TRP:HB2  | 1:11:A:TRP:HB3  | 10                  | 0.31     | 0.0                 | 0.31       |
| (1,40)  | 1:6:A:ARG:H     | 1:6:A:ARG:HB2   | 10                  | 0.31     | 0.03                | 0.3        |
| (1,498) | 1:23:A:PRO:HA   | 1:23:A:PRO:HB3  | 10                  | 0.31     | 0.02                | 0.31       |
| (1,280) | 1:4:A:CYS:H     | 1:5:A:VAL:H     | 10                  | 0.3      | 0.1                 | 0.32       |
| (1,506) | 1:23:A:PRO:HD3  | 1:23:A:PRO:HG3  | 10                  | 0.3      | 0.03                | 0.29       |
| (1,715) | 1:9:A:ILE:HG21  | 1:12:A:LEU:HB2  | 10                  | 0.29     | 0.05                | 0.3        |
| (1,715) | 1:9:A:ILE:HG22  | 1:12:A:LEU:HB2  | 10                  | 0.29     | 0.05                | 0.3        |
| (1,715) | 1:9:A:ILE:HG23  | 1:12:A:LEU:HB2  | 10                  | 0.29     | 0.05                | 0.3        |
| (1,443) | 1:17:A:PRO:HD2  | 1:17:A:PRO:HG2  | 10                  | 0.29     | 0.0                 | 0.29       |
| (1,443) | 1:17:A:PRO:HD2  | 1:17:A:PRO:HG3  | 10                  | 0.29     | 0.0                 | 0.29       |
| (1,359) | 1:6:A:ARG:HD2   | 1:6:A:ARG:HG3   | 10                  | 0.28     | 0.03                | 0.28       |
| (1,154) | 1:7:A:LEU:H     | 1:7:A:LEU:HB2   | 10                  | 0.27     | 0.02                | 0.27       |
| (1,445) | 1:17:A:PRO:HD3  | 1:17:A:PRO:HG2  | 10                  | 0.27     | 0.0                 | 0.27       |
| (1,445) | 1:17:A:PRO:HD3  | 1:17:A:PRO:HG3  | 10                  | 0.27     | 0.0                 | 0.27       |
| (1,410) | 1:12:A:LEU:HB2  | 1:12:A:LEU:HB3  | 10                  | 0.26     | 0.0                 | 0.26       |
| (1,301) | 1:12:A:LEU:H    | 1:12:A:LEU:HB2  | 10                  | 0.25     | 0.03                | 0.24       |
| (1,717) | 1:12:A:LEU:HD11 | 1:16:A:GLY:HA2  | 10                  | 0.25     | 0.13                | 0.2        |
| (1,717) | 1:12:A:LEU:HD12 | 1:16:A:GLY:HA2  | 10                  | 0.25     | 0.13                | 0.2        |
| (1,717) | 1:12:A:LEU:HD13 | 1:16:A:GLY:HA2  | 10                  | 0.25     | 0.13                | 0.2        |
| (1,412) | 1:12:A:LEU:HD21 | 1:12:A:LEU:HG   | 10                  | 0.25     | 0.02                | 0.26       |
| (1,412) | 1:12:A:LEU:HD22 | 1:12:A:LEU:HG   | 10                  | 0.25     | 0.02                | 0.26       |
| (1,412) | 1:12:A:LEU:HD23 | 1:12:A:LEU:HG   | 10                  | 0.25     | 0.02                | 0.26       |
| (1,434) | 1:16:A:GLY:HA2  | 1:16:A:GLY:HA3  | 10                  | 0.25     | 0.0                 | 0.25       |
| (1,526) | 1:24:A:PRO:HB3  | 1:24:A:PRO:HD2  | 10                  | 0.25     | 0.01                | 0.24       |
| (1,383) | 1:9:A:ILE:HG12  | 1:9:A:ILE:HG13  | 10                  | 0.24     | 0.0                 | 0.24       |
| (1,477) | 1:22:A:PRO:HA   | 1:22:A:PRO:HB2  | 10                  | 0.24     | 0.07                | 0.24       |
| (1,326) | 1:2:A:GLU:HA    | 1:2:A:GLU:HB3   | 10                  | 0.24     | 0.05                | 0.23       |
| (1,677) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD11 | 10                  | 0.24     | 0.07                | 0.22       |
| (1,677) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD12 | 10                  | 0.24     | 0.07                | 0.22       |
| (1,677) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD13 | 10                  | 0.24     | 0.07                | 0.22       |

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| Key     | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,404) | 1:12:A:LEU:HA   | 1:12:A:LEU:HB3  | 10                  | 0.23     | 0.01                | 0.23       |
| (1,736) | 1:23:A:PRO:HA   | 1:24:A:PRO:HD3  | 10                  | 0.23     | 0.07                | 0.2        |
| (1,522) | 1:24:A:PRO:HA   | 1:24:A:PRO:HD3  | 10                  | 0.23     | 0.05                | 0.22       |
| (1,364) | 1:6:A:ARG:HG2   | 1:6:A:ARG:HG3   | 10                  | 0.23     | 0.0                 | 0.23       |
| (1,600) | 1:1:A:GLU:HB3   | 1:1:A:GLU:HG2   | 10                  | 0.22     | 0.03                | 0.21       |
| (1,600) | 1:1:A:GLU:HB3   | 1:1:A:GLU:HG3   | 10                  | 0.22     | 0.03                | 0.21       |
| (1,455) | 1:19:A:SER:HB2  | 1:19:A:SER:HB3  | 10                  | 0.22     | 0.0                 | 0.22       |
| (1,385) | 1:9:A:ILE:HD11  | 1:9:A:ILE:HG13  | 10                  | 0.21     | 0.01                | 0.22       |
| (1,385) | 1:9:A:ILE:HD12  | 1:9:A:ILE:HG13  | 10                  | 0.21     | 0.01                | 0.22       |
| (1,385) | 1:9:A:ILE:HD13  | 1:9:A:ILE:HG13  | 10                  | 0.21     | 0.01                | 0.22       |
| (1,489) | 1:22:A:PRO:HB2  | 1:22:A:PRO:HG2  | 10                  | 0.2      | 0.02                | 0.21       |
| (1,333) | 1:2:A:GLU:HB2   | 1:2:A:GLU:HB3   | 10                  | 0.2      | 0.0                 | 0.2        |
| (1,331) | 1:2:A:GLU:HB2   | 1:2:A:GLU:HG3   | 10                  | 0.2      | 0.02                | 0.19       |
| (1,601) | 1:10:A:GLN:H    | 1:12:A:LEU:H    | 10                  | 0.19     | 0.04                | 0.2        |
| (1,418) | 1:12:A:LEU:HD11 | 1:12:A:LEU:HD21 | 10                  | 0.18     | 0.02                | 0.18       |
| (1,418) | 1:12:A:LEU:HD11 | 1:12:A:LEU:HD22 | 10                  | 0.18     | 0.02                | 0.18       |
| (1,418) | 1:12:A:LEU:HD11 | 1:12:A:LEU:HD23 | 10                  | 0.18     | 0.02                | 0.18       |
| (1,418) | 1:12:A:LEU:HD12 | 1:12:A:LEU:HD21 | 10                  | 0.18     | 0.02                | 0.18       |
| (1,418) | 1:12:A:LEU:HD12 | 1:12:A:LEU:HD22 | 10                  | 0.18     | 0.02                | 0.18       |
| (1,418) | 1:12:A:LEU:HD12 | 1:12:A:LEU:HD23 | 10                  | 0.18     | 0.02                | 0.18       |
| (1,418) | 1:12:A:LEU:HD13 | 1:12:A:LEU:HD21 | 10                  | 0.18     | 0.02                | 0.18       |
| (1,418) | 1:12:A:LEU:HD13 | 1:12:A:LEU:HD22 | 10                  | 0.18     | 0.02                | 0.18       |
| (1,418) | 1:12:A:LEU:HD13 | 1:12:A:LEU:HD23 | 10                  | 0.18     | 0.02                | 0.18       |
| (1,440) | 1:17:A:PRO:HD2  | 1:17:A:PRO:HD3  | 10                  | 0.18     | 0.0                 | 0.18       |
| (1,375) | 1:8:A:TYR:HA    | 1:8:A:TYR:HB2   | 10                  | 0.18     | 0.01                | 0.18       |
| (1,375) | 1:8:A:TYR:HA    | 1:8:A:TYR:HB3   | 10                  | 0.18     | 0.01                | 0.18       |
| (1,432) | 1:14:A:ASP:HB2  | 1:14:A:ASP:HB3  | 10                  | 0.18     | 0.0                 | 0.18       |
| (1,531) | 1:24:A:PRO:HB2  | 1:24:A:PRO:HB3  | 10                  | 0.17     | 0.01                | 0.17       |
| (1,540) | 1:25:A:CYS:HB2  | 1:25:A:CYS:HB3  | 10                  | 0.17     | 0.01                | 0.17       |
| (1,339) | 1:4:A:CYS:HB2   | 1:4:A:CYS:HB3   | 10                  | 0.17     | 0.01                | 0.16       |
| (1,180) | 1:11:A:TRP:HB2  | 1:11:A:TRP:HE3  | 10                  | 0.16     | 0.04                | 0.19       |
| (1,524) | 1:24:A:PRO:HD2  | 1:24:A:PRO:HD3  | 10                  | 0.15     | 0.0                 | 0.15       |
| (1,372) | 1:7:A:LEU:HB2   | 1:7:A:LEU:HB3   | 10                  | 0.15     | 0.0                 | 0.15       |
| (1,341) | 1:5:A:VAL:HA    | 1:5:A:VAL:HG21  | 10                  | 0.15     | 0.01                | 0.16       |
| (1,341) | 1:5:A:VAL:HA    | 1:5:A:VAL:HG22  | 10                  | 0.15     | 0.01                | 0.16       |
| (1,341) | 1:5:A:VAL:HA    | 1:5:A:VAL:HG23  | 10                  | 0.15     | 0.01                | 0.16       |
| (1,478) | 1:22:A:PRO:HD2  | 1:22:A:PRO:HD3  | 10                  | 0.14     | 0.0                 | 0.14       |
| (1,520) | 1:24:A:PRO:HA   | 1:24:A:PRO:HB3  | 10                  | 0.14     | 0.01                | 0.15       |
| (1,435) | 1:17:A:PRO:HA   | 1:17:A:PRO:HD2  | 10                  | 0.13     | 0.0                 | 0.13       |
| (1,469) | 1:21:A:ARG:HB2  | 1:21:A:ARG:HB3  | 10                  | 0.12     | 0.0                 | 0.12       |
| (1,344) | 1:5:A:VAL:HB    | 1:5:A:VAL:HG11  | 10                  | 0.12     | 0.01                | 0.12       |
| (1,344) | 1:5:A:VAL:HB    | 1:5:A:VAL:HG12  | 10                  | 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) |
|---------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,344) | 1:5:A:VAL:HB   | 1:5:A:VAL:HG13  | 10                  | 0.12     | 0.01                | 0.12       |
| (1,300) | 1:12:A:LEU:H   | 1:12:A:LEU:HD21 | 9                   | 1.06     | 0.02                | 1.06       |
| (1,300) | 1:12:A:LEU:H   | 1:12:A:LEU:HD22 | 9                   | 1.06     | 0.02                | 1.06       |
| (1,300) | 1:12:A:LEU:H   | 1:12:A:LEU:HD23 | 9                   | 1.06     | 0.02                | 1.06       |
| (1,730) | 1:2:A:GLU:HG3  | 1:6:A:ARG:HG3   | 9                   | 0.9      | 0.23                | 0.98       |
| (1,355) | 1:6:A:ARG:HB2  | 1:6:A:ARG:HD2   | 9                   | 0.84     | 0.06                | 0.8        |
| (1,672) | 1:9:A:ILE:HA   | 1:12:A:LEU:HD21 | 9                   | 0.76     | 0.06                | 0.72       |
| (1,672) | 1:9:A:ILE:HA   | 1:12:A:LEU:HD22 | 9                   | 0.76     | 0.06                | 0.72       |
| (1,672) | 1:9:A:ILE:HA   | 1:12:A:LEU:HD23 | 9                   | 0.76     | 0.06                | 0.72       |
| (1,299) | 1:8:A:TYR:H    | 1:9:A:ILE:HB    | 9                   | 0.72     | 0.1                 | 0.68       |
| (1,268) | 1:8:A:TYR:HD1  | 1:9:A:ILE:H     | 9                   | 0.66     | 0.02                | 0.66       |
| (1,268) | 1:8:A:TYR:HD2  | 1:9:A:ILE:H     | 9                   | 0.66     | 0.02                | 0.66       |
| (1,1)   | 1:7:A:LEU:HB2  | 1:8:A:TYR:H     | 9                   | 0.64     | 0.04                | 0.66       |
| (1,30)  | 1:4:A:CYS:H    | 1:4:A:CYS:HB2   | 9                   | 0.62     | 0.03                | 0.63       |
| (1,145) | 1:11:A:TRP:H   | 1:12:A:LEU:HA   | 9                   | 0.62     | 0.07                | 0.63       |
| (1,671) | 1:8:A:TYR:HA   | 1:12:A:LEU:HD21 | 9                   | 0.59     | 0.09                | 0.53       |
| (1,671) | 1:8:A:TYR:HA   | 1:12:A:LEU:HD22 | 9                   | 0.59     | 0.09                | 0.53       |
| (1,671) | 1:8:A:TYR:HA   | 1:12:A:LEU:HD23 | 9                   | 0.59     | 0.09                | 0.53       |
| (1,350) | 1:6:A:ARG:HA   | 1:6:A:ARG:HG3   | 9                   | 0.55     | 0.05                | 0.55       |
| (1,111) | 1:10:A:GLN:HB3 | 1:11:A:TRP:H    | 9                   | 0.52     | 0.12                | 0.57       |
| (1,190) | 1:11:A:TRP:HD1 | 1:24:A:PRO:HD2  | 9                   | 0.52     | 0.02                | 0.52       |
| (1,26)  | 1:2:A:GLU:HB2  | 1:3:A:GLU:H     | 9                   | 0.51     | 0.19                | 0.56       |
| (1,535) | 1:23:A:PRO:HB3 | 1:24:A:PRO:HD2  | 9                   | 0.49     | 0.13                | 0.49       |
| (1,665) | 1:3:A:GLU:HG2  | 1:4:A:CYS:HA    | 9                   | 0.49     | 0.08                | 0.5        |
| (1,665) | 1:3:A:GLU:HG3  | 1:4:A:CYS:HA    | 9                   | 0.49     | 0.08                | 0.5        |
| (1,666) | 1:24:A:PRO:HG2 | 1:25:A:CYS:HB2  | 9                   | 0.45     | 0.18                | 0.47       |
| (1,259) | 1:4:A:CYS:HB3  | 1:5:A:VAL:H     | 9                   | 0.43     | 0.15                | 0.43       |
| (1,682) | 1:4:A:CYS:HB2  | 1:5:A:VAL:HG11  | 9                   | 0.42     | 0.12                | 0.43       |
| (1,682) | 1:4:A:CYS:HB2  | 1:5:A:VAL:HG12  | 9                   | 0.42     | 0.12                | 0.43       |
| (1,682) | 1:4:A:CYS:HB2  | 1:5:A:VAL:HG13  | 9                   | 0.42     | 0.12                | 0.43       |
| (1,118) | 1:12:A:LEU:H   | 1:12:A:LEU:HG   | 9                   | 0.39     | 0.02                | 0.39       |
| (1,450) | 1:18:A:SER:HA  | 1:18:A:SER:HB3  | 9                   | 0.31     | 0.06                | 0.35       |
| (1,614) | 1:19:A:SER:HG  | 1:20:A:GLY:H    | 9                   | 0.3      | 0.16                | 0.22       |
| (1,728) | 1:2:A:GLU:HG2  | 1:6:A:ARG:HG2   | 9                   | 0.29     | 0.1                 | 0.26       |
| (1,177) | 1:8:A:TYR:HD1  | 1:12:A:LEU:HA   | 9                   | 0.28     | 0.09                | 0.25       |
| (1,177) | 1:8:A:TYR:HD2  | 1:12:A:LEU:HA   | 9                   | 0.28     | 0.09                | 0.25       |
| (1,704) | 1:9:A:ILE:HG21 | 1:13:A:LYS:HD3  | 9                   | 0.26     | 0.07                | 0.21       |
| (1,704) | 1:9:A:ILE:HG22 | 1:13:A:LYS:HD3  | 9                   | 0.26     | 0.07                | 0.21       |
| (1,704) | 1:9:A:ILE:HG23 | 1:13:A:LYS:HD3  | 9                   | 0.26     | 0.07                | 0.21       |
| (1,239) | 1:8:A:TYR:HE1  | 1:12:A:LEU:HG   | 9                   | 0.25     | 0.03                | 0.25       |
| (1,239) | 1:8:A:TYR:HE2  | 1:12:A:LEU:HG   | 9                   | 0.25     | 0.03                | 0.25       |
| (1,581) | 1:5:A:VAL:HG11 | 1:6:A:ARG:HA    | 9                   | 0.2      | 0.06                | 0.18       |

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| Key     | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,581) | 1:5:A:VAL:HG12  | 1:6:A:ARG:HA    | 9                   | 0.2      | 0.06                | 0.18       |
| (1,581) | 1:5:A:VAL:HG13  | 1:6:A:ARG:HA    | 9                   | 0.2      | 0.06                | 0.18       |
| (1,394) | 1:10:A:GLN:HA   | 1:10:A:GLN:HB2  | 9                   | 0.2      | 0.08                | 0.22       |
| (1,408) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD11 | 9                   | 0.19     | 0.12                | 0.16       |
| (1,408) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD12 | 9                   | 0.19     | 0.12                | 0.16       |
| (1,408) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD13 | 9                   | 0.19     | 0.12                | 0.16       |
| (1,220) | 1:8:A:TYR:HD1   | 1:9:A:ILE:HG12  | 9                   | 0.17     | 0.03                | 0.17       |
| (1,220) | 1:8:A:TYR:HD2   | 1:9:A:ILE:HG12  | 9                   | 0.17     | 0.03                | 0.17       |
| (1,155) | 1:7:A:LEU:H     | 1:7:A:LEU:HD11  | 9                   | 0.16     | 0.03                | 0.16       |
| (1,155) | 1:7:A:LEU:H     | 1:7:A:LEU:HD12  | 9                   | 0.16     | 0.03                | 0.16       |
| (1,155) | 1:7:A:LEU:H     | 1:7:A:LEU:HD13  | 9                   | 0.16     | 0.03                | 0.16       |
| (1,155) | 1:7:A:LEU:H     | 1:7:A:LEU:HD21  | 9                   | 0.16     | 0.03                | 0.16       |
| (1,155) | 1:7:A:LEU:H     | 1:7:A:LEU:HD22  | 9                   | 0.16     | 0.03                | 0.16       |
| (1,155) | 1:7:A:LEU:H     | 1:7:A:LEU:HD23  | 9                   | 0.16     | 0.03                | 0.16       |
| (1,195) | 1:8:A:TYR:HE1   | 1:24:A:PRO:HD3  | 9                   | 0.16     | 0.02                | 0.16       |
| (1,195) | 1:8:A:TYR:HE2   | 1:24:A:PRO:HD3  | 9                   | 0.16     | 0.02                | 0.16       |
| (1,115) | 1:9:A:ILE:H     | 1:9:A:ILE:HG13  | 9                   | 0.16     | 0.03                | 0.17       |
| (1,335) | 1:3:A:GLU:HA    | 1:3:A:GLU:HB2   | 9                   | 0.15     | 0.01                | 0.16       |
| (1,335) | 1:3:A:GLU:HA    | 1:3:A:GLU:HB3   | 9                   | 0.15     | 0.01                | 0.16       |
| (1,413) | 1:12:A:LEU:HD11 | 1:12:A:LEU:HG   | 9                   | 0.12     | 0.04                | 0.11       |
| (1,413) | 1:12:A:LEU:HD12 | 1:12:A:LEU:HG   | 9                   | 0.12     | 0.04                | 0.11       |
| (1,413) | 1:12:A:LEU:HD13 | 1:12:A:LEU:HG   | 9                   | 0.12     | 0.04                | 0.11       |
| (1,384) | 1:9:A:ILE:HB    | 1:9:A:ILE:HG12  | 9                   | 0.1      | 0.0                 | 0.1        |
| (1,291) | 1:11:A:TRP:HD1  | 1:21:A:ARG:HD2  | 8                   | 1.25     | 0.11                | 1.28       |
| (1,67)  | 1:18:A:SER:H    | 1:18:A:SER:HB2  | 8                   | 0.67     | 0.05                | 0.66       |
| (1,463) | 1:21:A:ARG:HB3  | 1:21:A:ARG:HD3  | 8                   | 0.59     | 0.05                | 0.58       |
| (1,651) | 1:3:A:GLU:HA    | 1:6:A:ARG:HD2   | 8                   | 0.55     | 0.27                | 0.54       |
| (1,723) | 1:12:A:LEU:HB3  | 1:13:A:LYS:HG2  | 8                   | 0.45     | 0.14                | 0.48       |
| (1,723) | 1:12:A:LEU:HB3  | 1:13:A:LYS:HG3  | 8                   | 0.45     | 0.14                | 0.48       |
| (1,391) | 1:10:A:GLN:HA   | 1:10:A:GLN:HG2  | 8                   | 0.42     | 0.15                | 0.43       |
| (1,512) | 1:23:A:PRO:HB3  | 1:23:A:PRO:HD3  | 8                   | 0.4      | 0.09                | 0.46       |
| (1,716) | 1:9:A:ILE:HG12  | 1:12:A:LEU:HD11 | 8                   | 0.37     | 0.21                | 0.4        |
| (1,716) | 1:9:A:ILE:HG12  | 1:12:A:LEU:HD12 | 8                   | 0.37     | 0.21                | 0.4        |
| (1,716) | 1:9:A:ILE:HG12  | 1:12:A:LEU:HD13 | 8                   | 0.37     | 0.21                | 0.4        |
| (1,719) | 1:9:A:ILE:HG12  | 1:12:A:LEU:HG   | 8                   | 0.35     | 0.17                | 0.42       |
| (1,465) | 1:21:A:ARG:HB2  | 1:21:A:ARG:HD2  | 8                   | 0.31     | 0.04                | 0.32       |
| (1,208) | 1:11:A:TRP:HZ3  | 1:12:A:LEU:HD11 | 8                   | 0.3      | 0.14                | 0.31       |
| (1,208) | 1:11:A:TRP:HZ3  | 1:12:A:LEU:HD12 | 8                   | 0.3      | 0.14                | 0.31       |
| (1,208) | 1:11:A:TRP:HZ3  | 1:12:A:LEU:HD13 | 8                   | 0.3      | 0.14                | 0.31       |
| (1,720) | 1:7:A:LEU:HB2   | 1:24:A:PRO:HB2  | 8                   | 0.24     | 0.07                | 0.24       |
| (1,262) | 1:10:A:GLN:HA   | 1:10:A:GLN:HE22 | 8                   | 0.24     | 0.15                | 0.18       |
| (1,497) | 1:23:A:PRO:HA   | 1:23:A:PRO:HB2  | 8                   | 0.16     | 0.02                | 0.16       |

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| Key     | Atom-1          | Atom-2         | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|----------------|---------------------|----------|---------------------|------------|
| (1,152) | 1:8:A:TYR:HB2   | 1:9:A:ILE:H    | 8                   | 0.15     | 0.03                | 0.16       |
| (1,152) | 1:8:A:TYR:HB3   | 1:9:A:ILE:H    | 8                   | 0.15     | 0.03                | 0.16       |
| (1,21)  | 1:12:A:LEU:HB2  | 1:13:A:LYS:H   | 8                   | 0.15     | 0.01                | 0.15       |
| (1,254) | 1:11:A:TRP:HZ2  | 1:17:A:PRO:HB2 | 8                   | 0.14     | 0.02                | 0.15       |
| (1,706) | 1:6:A:ARG:HG3   | 1:7:A:LEU:HD11 | 8                   | 0.14     | 0.02                | 0.14       |
| (1,706) | 1:6:A:ARG:HG3   | 1:7:A:LEU:HD12 | 8                   | 0.14     | 0.02                | 0.14       |
| (1,706) | 1:6:A:ARG:HG3   | 1:7:A:LEU:HD13 | 8                   | 0.14     | 0.02                | 0.14       |
| (1,706) | 1:6:A:ARG:HG3   | 1:7:A:LEU:HD21 | 8                   | 0.14     | 0.02                | 0.14       |
| (1,706) | 1:6:A:ARG:HG3   | 1:7:A:LEU:HD22 | 8                   | 0.14     | 0.02                | 0.14       |
| (1,706) | 1:6:A:ARG:HG3   | 1:7:A:LEU:HD23 | 8                   | 0.14     | 0.02                | 0.14       |
| (1,377) | 1:9:A:ILE:HA    | 1:9:A:ILE:HG13 | 8                   | 0.13     | 0.03                | 0.12       |
| (1,22)  | 1:13:A:LYS:H    | 1:13:A:LYS:HG2 | 7                   | 0.74     | 0.05                | 0.72       |
| (1,22)  | 1:13:A:LYS:H    | 1:13:A:LYS:HG3 | 7                   | 0.74     | 0.05                | 0.72       |
| (1,663) | 1:10:A:GLN:HA   | 1:13:A:LYS:HB2 | 7                   | 0.73     | 0.02                | 0.72       |
| (1,663) | 1:10:A:GLN:HA   | 1:13:A:LYS:HB3 | 7                   | 0.73     | 0.02                | 0.72       |
| (1,315) | 1:10:A:GLN:HE22 | 1:13:A:LYS:HE2 | 7                   | 0.72     | 0.29                | 0.69       |
| (1,315) | 1:10:A:GLN:HE22 | 1:13:A:LYS:HE3 | 7                   | 0.72     | 0.29                | 0.69       |
| (1,222) | 1:8:A:TYR:HD1   | 1:23:A:PRO:HB2 | 7                   | 0.65     | 0.25                | 0.78       |
| (1,222) | 1:8:A:TYR:HD2   | 1:23:A:PRO:HB2 | 7                   | 0.65     | 0.25                | 0.78       |
| (1,24)  | 1:13:A:LYS:H    | 1:13:A:LYS:HD3 | 7                   | 0.6      | 0.05                | 0.58       |
| (1,618) | 1:10:A:GLN:HE21 | 1:13:A:LYS:HD3 | 7                   | 0.51     | 0.2                 | 0.58       |
| (1,425) | 1:13:A:LYS:HB2  | 1:13:A:LYS:HD2 | 7                   | 0.49     | 0.02                | 0.5        |
| (1,425) | 1:13:A:LYS:HB3  | 1:13:A:LYS:HD2 | 7                   | 0.49     | 0.02                | 0.5        |
| (1,47)  | 1:10:A:GLN:HE21 | 1:10:A:GLN:HG2 | 7                   | 0.49     | 0.02                | 0.5        |
| (1,93)  | 1:19:A:SER:HG   | 1:21:A:ARG:H   | 7                   | 0.28     | 0.1                 | 0.3        |
| (1,108) | 1:14:A:ASP:H    | 1:15:A:GLY:H   | 7                   | 0.23     | 0.11                | 0.22       |
| (1,35)  | 1:10:A:GLN:H    | 1:10:A:GLN:HB2 | 7                   | 0.2      | 0.08                | 0.19       |
| (1,75)  | 1:25:A:CYS:H    | 1:25:A:CYS:HB2 | 7                   | 0.18     | 0.05                | 0.21       |
| (1,537) | 1:23:A:PRO:HB2  | 1:24:A:PRO:HD2 | 7                   | 0.17     | 0.05                | 0.15       |
| (1,390) | 1:9:A:ILE:HG12  | 1:9:A:ILE:HG21 | 7                   | 0.12     | 0.01                | 0.12       |
| (1,390) | 1:9:A:ILE:HG12  | 1:9:A:ILE:HG22 | 7                   | 0.12     | 0.01                | 0.12       |
| (1,390) | 1:9:A:ILE:HG12  | 1:9:A:ILE:HG23 | 7                   | 0.12     | 0.01                | 0.12       |
| (1,117) | 1:12:A:LEU:H    | 1:12:A:LEU:HB3 | 7                   | 0.11     | 0.01                | 0.11       |
| (1,668) | 1:19:A:SER:HB2  | 1:21:A:ARG:HG2 | 6                   | 0.9      | 0.22                | 1.02       |
| (1,668) | 1:19:A:SER:HB2  | 1:21:A:ARG:HG3 | 6                   | 0.9      | 0.22                | 1.02       |
| (1,709) | 1:12:A:LEU:HD11 | 1:23:A:PRO:HB2 | 6                   | 0.7      | 0.21                | 0.72       |
| (1,709) | 1:12:A:LEU:HD12 | 1:23:A:PRO:HB2 | 6                   | 0.7      | 0.21                | 0.72       |
| (1,709) | 1:12:A:LEU:HD13 | 1:23:A:PRO:HB2 | 6                   | 0.7      | 0.21                | 0.72       |
| (1,200) | 1:11:A:TRP:HE3  | 1:23:A:PRO:HB3 | 6                   | 0.62     | 0.32                | 0.8        |
| (1,295) | 1:11:A:TRP:HE1  | 1:21:A:ARG:HB2 | 6                   | 0.59     | 0.03                | 0.59       |
| (1,596) | 1:1:A:GLU:HA    | 1:1:A:GLU:HG2  | 6                   | 0.57     | 0.18                | 0.66       |
| (1,596) | 1:1:A:GLU:HA    | 1:1:A:GLU:HG3  | 6                   | 0.57     | 0.18                | 0.66       |

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| Key     | Atom-1          | Atom-2         | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|----------------|---------------------|----------|---------------------|------------|
| (1,227) | 1:11:A:TRP:HZ2  | 1:23:A:PRO:HG2 | 6                   | 0.53     | 0.19                | 0.62       |
| (1,711) | 1:12:A:LEU:HD21 | 1:23:A:PRO:HB2 | 6                   | 0.48     | 0.16                | 0.42       |
| (1,711) | 1:12:A:LEU:HD22 | 1:23:A:PRO:HB2 | 6                   | 0.48     | 0.16                | 0.42       |
| (1,711) | 1:12:A:LEU:HD23 | 1:23:A:PRO:HB2 | 6                   | 0.48     | 0.16                | 0.42       |
| (1,459) | 1:21:A:ARG:HA   | 1:21:A:ARG:HB3 | 6                   | 0.47     | 0.01                | 0.47       |
| (1,230) | 1:11:A:TRP:HD1  | 1:21:A:ARG:HB2 | 6                   | 0.43     | 0.05                | 0.43       |
| (1,196) | 1:11:A:TRP:HH2  | 1:23:A:PRO:HB3 | 6                   | 0.42     | 0.08                | 0.46       |
| (1,277) | 1:20:A:GLY:H    | 1:21:A:ARG:H   | 6                   | 0.36     | 0.07                | 0.36       |
| (1,569) | 1:8:A:TYR:HA    | 1:11:A:TRP:HB3 | 6                   | 0.32     | 0.06                | 0.3        |
| (1,554) | 1:22:A:PRO:HB3  | 1:23:A:PRO:HD2 | 6                   | 0.27     | 0.12                | 0.33       |
| (1,621) | 1:2:A:GLU:HB2   | 1:6:A:ARG:H    | 6                   | 0.23     | 0.07                | 0.22       |
| (1,226) | 1:11:A:TRP:HH2  | 1:23:A:PRO:HG2 | 6                   | 0.2      | 0.08                | 0.18       |
| (1,179) | 1:11:A:TRP:HB2  | 1:11:A:TRP:HD1 | 6                   | 0.19     | 0.01                | 0.19       |
| (1,551) | 1:16:A:GLY:HA3  | 1:17:A:PRO:HD3 | 6                   | 0.18     | 0.06                | 0.16       |
| (1,397) | 1:10:A:GLN:HB2  | 1:10:A:GLN:HG2 | 6                   | 0.16     | 0.03                | 0.17       |
| (1,65)  | 1:20:A:GLY:H    | 1:20:A:GLY:HA2 | 6                   | 0.12     | 0.02                | 0.12       |
| (1,625) | 1:10:A:GLN:HE21 | 1:14:A:ASP:HB3 | 5                   | 0.54     | 0.31                | 0.39       |
| (1,648) | 1:15:A:GLY:HA2  | 1:19:A:SER:HB2 | 5                   | 0.31     | 0.07                | 0.32       |
| (1,563) | 1:7:A:LEU:HA    | 1:10:A:GLN:HB3 | 5                   | 0.28     | 0.14                | 0.23       |
| (1,55)  | 1:21:A:ARG:H    | 1:21:A:ARG:HD2 | 5                   | 0.28     | 0.07                | 0.28       |
| (1,250) | 1:11:A:TRP:HE3  | 1:23:A:PRO:HA  | 5                   | 0.27     | 0.01                | 0.26       |
| (1,565) | 1:4:A:CYS:HA    | 1:7:A:LEU:HG   | 5                   | 0.27     | 0.12                | 0.25       |
| (1,615) | 1:16:A:GLY:H    | 1:19:A:SER:HB3 | 5                   | 0.24     | 0.13                | 0.17       |
| (1,550) | 1:11:A:TRP:HB3  | 1:24:A:PRO:HD3 | 5                   | 0.23     | 0.05                | 0.22       |
| (1,641) | 1:8:A:TYR:HD1   | 1:25:A:CYS:HB3 | 5                   | 0.22     | 0.16                | 0.15       |
| (1,641) | 1:8:A:TYR:HD2   | 1:25:A:CYS:HB3 | 5                   | 0.22     | 0.16                | 0.15       |
| (1,61)  | 1:11:A:TRP:HB2  | 1:12:A:LEU:H   | 5                   | 0.21     | 0.01                | 0.21       |
| (1,545) | 1:13:A:LYS:HB2  | 1:13:A:LYS:HE2 | 5                   | 0.21     | 0.07                | 0.22       |
| (1,545) | 1:13:A:LYS:HB2  | 1:13:A:LYS:HE3 | 5                   | 0.21     | 0.07                | 0.22       |
| (1,545) | 1:13:A:LYS:HB3  | 1:13:A:LYS:HE2 | 5                   | 0.21     | 0.07                | 0.22       |
| (1,545) | 1:13:A:LYS:HB3  | 1:13:A:LYS:HE3 | 5                   | 0.21     | 0.07                | 0.22       |
| (1,552) | 1:11:A:TRP:HB2  | 1:24:A:PRO:HD2 | 5                   | 0.21     | 0.15                | 0.15       |
| (1,98)  | 1:11:A:TRP:HE1  | 1:19:A:SER:HG  | 5                   | 0.19     | 0.02                | 0.2        |
| (1,284) | 1:2:A:GLU:HA    | 1:3:A:GLU:H    | 5                   | 0.18     | 0.03                | 0.19       |
| (1,633) | 1:11:A:TRP:HZ3  | 1:23:A:PRO:HB2 | 5                   | 0.16     | 0.03                | 0.17       |
| (1,112) | 1:7:A:LEU:H     | 1:7:A:LEU:HB3  | 5                   | 0.1      | 0.0                 | 0.1        |
| (1,296) | 1:11:A:TRP:HE1  | 1:21:A:ARG:HB3 | 4                   | 0.7      | 0.06                | 0.68       |
| (1,231) | 1:11:A:TRP:HD1  | 1:21:A:ARG:HB3 | 4                   | 0.66     | 0.04                | 0.65       |
| (1,650) | 1:15:A:GLY:HA3  | 1:19:A:SER:HA  | 4                   | 0.6      | 0.02                | 0.6        |
| (1,223) | 1:8:A:TYR:HE1   | 1:23:A:PRO:HB2 | 4                   | 0.54     | 0.03                | 0.55       |
| (1,223) | 1:8:A:TYR:HE2   | 1:23:A:PRO:HB2 | 4                   | 0.54     | 0.03                | 0.55       |
| (1,238) | 1:8:A:TYR:HE1   | 1:23:A:PRO:HG3 | 4                   | 0.42     | 0.11                | 0.44       |

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| Key     | Atom-1         | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,238) | 1:8:A:TYR:HE2  | 1:23:A:PRO:HG3  | 4                   | 0.42     | 0.11                | 0.44       |
| (1,225) | 1:23:A:PRO:HB2 | 1:25:A:CYS:H    | 4                   | 0.31     | 0.08                | 0.33       |
| (1,623) | 1:2:A:GLU:HB3  | 1:6:A:ARG:H     | 4                   | 0.26     | 0.06                | 0.25       |
| (1,210) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD11 | 4                   | 0.22     | 0.02                | 0.22       |
| (1,210) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD12 | 4                   | 0.22     | 0.02                | 0.22       |
| (1,210) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD13 | 4                   | 0.22     | 0.02                | 0.22       |
| (1,293) | 1:11:A:TRP:HE1 | 1:24:A:PRO:HD2  | 4                   | 0.22     | 0.02                | 0.22       |
| (1,334) | 1:3:A:GLU:HA   | 1:3:A:GLU:HG2   | 4                   | 0.2      | 0.15                | 0.12       |
| (1,334) | 1:3:A:GLU:HA   | 1:3:A:GLU:HG3   | 4                   | 0.2      | 0.15                | 0.12       |
| (1,634) | 1:11:A:TRP:HE3 | 1:23:A:PRO:HB2  | 4                   | 0.19     | 0.03                | 0.2        |
| (1,94)  | 1:20:A:GLY:HA3 | 1:21:A:ARG:H    | 4                   | 0.15     | 0.02                | 0.16       |
| (1,695) | 1:5:A:VAL:HG11 | 1:9:A:ILE:HB    | 4                   | 0.15     | 0.03                | 0.16       |
| (1,695) | 1:5:A:VAL:HG12 | 1:9:A:ILE:HB    | 4                   | 0.15     | 0.03                | 0.16       |
| (1,695) | 1:5:A:VAL:HG13 | 1:9:A:ILE:HB    | 4                   | 0.15     | 0.03                | 0.16       |
| (1,471) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HG2  | 4                   | 0.14     | 0.02                | 0.14       |
| (1,471) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HG3  | 4                   | 0.14     | 0.02                | 0.14       |
| (1,453) | 1:19:A:SER:HA  | 1:19:A:SER:HB2  | 4                   | 0.13     | 0.01                | 0.14       |
| (1,255) | 1:11:A:TRP:HH2 | 1:17:A:PRO:HB2  | 4                   | 0.13     | 0.02                | 0.12       |
| (1,68)  | 1:18:A:SER:H   | 1:18:A:SER:HB3  | 3                   | 0.74     | 0.08                | 0.73       |
| (1,451) | 1:18:A:SER:HA  | 1:18:A:SER:HB2  | 3                   | 0.53     | 0.08                | 0.58       |
| (1,464) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD2  | 3                   | 0.36     | 0.17                | 0.46       |
| (1,664) | 1:21:A:ARG:HB3 | 1:22:A:PRO:HD2  | 3                   | 0.33     | 0.15                | 0.39       |
| (1,352) | 1:6:A:ARG:HB3  | 1:6:A:ARG:HD2   | 3                   | 0.31     | 0.22                | 0.21       |
| (1,424) | 1:13:A:LYS:HB2 | 1:13:A:LYS:HD3  | 3                   | 0.3      | 0.07                | 0.31       |
| (1,424) | 1:13:A:LYS:HB3 | 1:13:A:LYS:HD3  | 3                   | 0.3      | 0.07                | 0.31       |
| (1,76)  | 1:25:A:CYS:H   | 1:25:A:CYS:HB3  | 3                   | 0.27     | 0.06                | 0.28       |
| (1,171) | 1:11:A:TRP:HH2 | 1:23:A:PRO:HD3  | 3                   | 0.27     | 0.01                | 0.26       |
| (1,263) | 1:18:A:SER:HA  | 1:20:A:GLY:H    | 3                   | 0.18     | 0.06                | 0.15       |
| (1,646) | 1:15:A:GLY:HA2 | 1:18:A:SER:HB3  | 3                   | 0.17     | 0.08                | 0.14       |
| (1,123) | 1:24:A:PRO:HG2 | 1:25:A:CYS:H    | 3                   | 0.14     | 0.02                | 0.13       |
| (1,290) | 1:11:A:TRP:HD1 | 1:21:A:ARG:HD3  | 2                   | 1.24     | 0.14                | 1.24       |
| (1,594) | 1:9:A:ILE:HG21 | 1:13:A:LYS:HE2  | 2                   | 0.93     | 0.07                | 0.93       |
| (1,594) | 1:9:A:ILE:HG22 | 1:13:A:LYS:HE2  | 2                   | 0.93     | 0.07                | 0.93       |
| (1,594) | 1:9:A:ILE:HG23 | 1:13:A:LYS:HE2  | 2                   | 0.93     | 0.07                | 0.93       |
| (1,594) | 1:9:A:ILE:HG21 | 1:13:A:LYS:HE3  | 2                   | 0.93     | 0.07                | 0.93       |
| (1,594) | 1:9:A:ILE:HG22 | 1:13:A:LYS:HE3  | 2                   | 0.93     | 0.07                | 0.93       |
| (1,594) | 1:9:A:ILE:HG23 | 1:13:A:LYS:HE3  | 2                   | 0.93     | 0.07                | 0.93       |
| (1,248) | 1:8:A:TYR:HD1  | 1:23:A:PRO:HA   | 2                   | 0.48     | 0.28                | 0.48       |
| (1,248) | 1:8:A:TYR:HD2  | 1:23:A:PRO:HA   | 2                   | 0.48     | 0.28                | 0.48       |
| (1,657) | 1:4:A:CYS:HB2  | 1:25:A:CYS:HB3  | 2                   | 0.34     | 0.11                | 0.34       |
| (1,56)  | 1:21:A:ARG:H   | 1:21:A:ARG:HD3  | 2                   | 0.28     | 0.0                 | 0.28       |
| (1,479) | 1:22:A:PRO:HB3 | 1:22:A:PRO:HD3  | 2                   | 0.23     | 0.04                | 0.23       |

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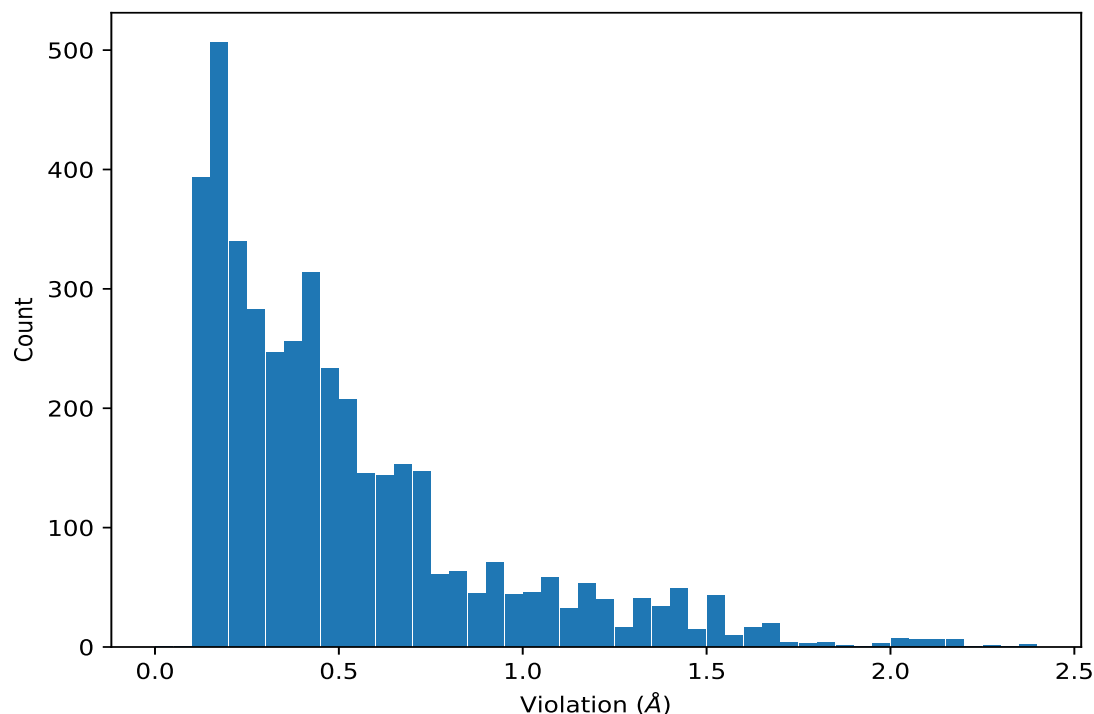
| Key     | Atom-1         | Atom-2         | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|----------------|----------------|---------------------|----------|---------------------|------------|
| (1,647) | 1:15:A:GLY:HA2 | 1:18:A:SER:HB2 | 2                   | 0.2      | 0.02                | 0.2        |
| (1,8)   | 1:5:A:VAL:H    | 1:5:A:VAL:HG21 | 2                   | 0.17     | 0.04                | 0.17       |
| (1,8)   | 1:5:A:VAL:H    | 1:5:A:VAL:HG22 | 2                   | 0.17     | 0.04                | 0.17       |
| (1,8)   | 1:5:A:VAL:H    | 1:5:A:VAL:HG23 | 2                   | 0.17     | 0.04                | 0.17       |
| (1,16)  | 1:5:A:VAL:H    | 1:5:A:VAL:HG21 | 2                   | 0.17     | 0.04                | 0.17       |
| (1,16)  | 1:5:A:VAL:H    | 1:5:A:VAL:HG22 | 2                   | 0.17     | 0.04                | 0.17       |
| (1,16)  | 1:5:A:VAL:H    | 1:5:A:VAL:HG23 | 2                   | 0.17     | 0.04                | 0.17       |
| (1,642) | 1:8:A:TYR:HD1  | 1:25:A:CYS:HB2 | 2                   | 0.16     | 0.02                | 0.16       |
| (1,642) | 1:8:A:TYR:HD2  | 1:25:A:CYS:HB2 | 2                   | 0.16     | 0.02                | 0.16       |
| (1,515) | 1:23:A:PRO:HB2 | 1:23:A:PRO:HG2 | 2                   | 0.14     | 0.0                 | 0.14       |
| (1,694) | 1:9:A:ILE:HG21 | 1:12:A:LEU:HB3 | 2                   | 0.13     | 0.02                | 0.13       |
| (1,694) | 1:9:A:ILE:HG22 | 1:12:A:LEU:HB3 | 2                   | 0.13     | 0.02                | 0.13       |
| (1,694) | 1:9:A:ILE:HG23 | 1:12:A:LEU:HB3 | 2                   | 0.13     | 0.02                | 0.13       |

<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

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

| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,727) | 1:22:A:PRO:HB3 | 1:23:A:PRO:HG3  | 7        | 2.39          |
| (1,727) | 1:22:A:PRO:HB3 | 1:23:A:PRO:HG3  | 4        | 2.35          |
| (1,727) | 1:22:A:PRO:HB3 | 1:23:A:PRO:HG3  | 2        | 2.25          |
| (1,727) | 1:22:A:PRO:HB3 | 1:23:A:PRO:HG3  | 8        | 2.19          |
| (1,727) | 1:22:A:PRO:HB3 | 1:23:A:PRO:HG3  | 3        | 2.16          |
| (1,727) | 1:22:A:PRO:HB3 | 1:23:A:PRO:HG3  | 10       | 2.15          |
| (1,681) | 1:11:A:TRP:HB3 | 1:12:A:LEU:HD21 | 6        | 2.15          |
| (1,681) | 1:11:A:TRP:HB3 | 1:12:A:LEU:HD22 | 6        | 2.15          |
| (1,681) | 1:11:A:TRP:HB3 | 1:12:A:LEU:HD23 | 6        | 2.15          |
| (1,681) | 1:11:A:TRP:HB3 | 1:12:A:LEU:HD21 | 5        | 2.11          |
| (1,681) | 1:11:A:TRP:HB3 | 1:12:A:LEU:HD22 | 5        | 2.11          |
| (1,681) | 1:11:A:TRP:HB3 | 1:12:A:LEU:HD23 | 5        | 2.11          |
| (1,681) | 1:11:A:TRP:HB3 | 1:12:A:LEU:HD21 | 1        | 2.1           |
| (1,681) | 1:11:A:TRP:HB3 | 1:12:A:LEU:HD22 | 1        | 2.1           |
| (1,681) | 1:11:A:TRP:HB3 | 1:12:A:LEU:HD23 | 1        | 2.1           |
| (1,681) | 1:11:A:TRP:HB3 | 1:12:A:LEU:HD21 | 2        | 2.07          |
| (1,681) | 1:11:A:TRP:HB3 | 1:12:A:LEU:HD22 | 2        | 2.07          |
| (1,681) | 1:11:A:TRP:HB3 | 1:12:A:LEU:HD23 | 2        | 2.07          |
| (1,680) | 1:11:A:TRP:HB3 | 1:12:A:LEU:HD21 | 6        | 2.06          |
| (1,680) | 1:11:A:TRP:HB3 | 1:12:A:LEU:HD22 | 6        | 2.06          |
| (1,680) | 1:11:A:TRP:HB3 | 1:12:A:LEU:HD23 | 6        | 2.06          |
| (1,680) | 1:11:A:TRP:HB3 | 1:12:A:LEU:HD21 | 5        | 2.03          |
| (1,680) | 1:11:A:TRP:HB3 | 1:12:A:LEU:HD22 | 5        | 2.03          |
| (1,680) | 1:11:A:TRP:HB3 | 1:12:A:LEU:HD23 | 5        | 2.03          |
| (1,680) | 1:11:A:TRP:HB3 | 1:12:A:LEU:HD21 | 1        | 2.02          |
| (1,680) | 1:11:A:TRP:HB3 | 1:12:A:LEU:HD22 | 1        | 2.02          |
| (1,680) | 1:11:A:TRP:HB3 | 1:12:A:LEU:HD23 | 1        | 2.02          |
| (1,727) | 1:22:A:PRO:HB3 | 1:23:A:PRO:HG3  | 9        | 2.0           |
| (1,680) | 1:11:A:TRP:HB3 | 1:12:A:LEU:HD21 | 2        | 1.98          |
| (1,680) | 1:11:A:TRP:HB3 | 1:12:A:LEU:HD22 | 2        | 1.98          |
| (1,680) | 1:11:A:TRP:HB3 | 1:12:A:LEU:HD23 | 2        | 1.98          |
| (1,729) | 1:2:A:GLU:HG2  | 1:6:A:ARG:HG3   | 10       | 1.85          |
| (1,729) | 1:2:A:GLU:HG2  | 1:6:A:ARG:HG3   | 8        | 1.84          |
| (1,727) | 1:22:A:PRO:HB3 | 1:23:A:PRO:HG3  | 1        | 1.82          |
| (1,727) | 1:22:A:PRO:HB3 | 1:23:A:PRO:HG3  | 6        | 1.82          |
| (1,727) | 1:22:A:PRO:HB3 | 1:23:A:PRO:HG3  | 5        | 1.8           |
| (1,729) | 1:2:A:GLU:HG2  | 1:6:A:ARG:HG3   | 2        | 1.79          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,729) | 1:2:A:GLU:HG2   | 1:6:A:ARG:HG3  | 3        | 1.77          |
| (1,729) | 1:2:A:GLU:HG2   | 1:6:A:ARG:HG3  | 6        | 1.75          |
| (1,729) | 1:2:A:GLU:HG2   | 1:6:A:ARG:HG3  | 4        | 1.74          |
| (1,696) | 1:5:A:VAL:HG21  | 1:9:A:ILE:HB   | 3        | 1.74          |
| (1,696) | 1:5:A:VAL:HG22  | 1:9:A:ILE:HB   | 3        | 1.74          |
| (1,696) | 1:5:A:VAL:HG23  | 1:9:A:ILE:HB   | 3        | 1.74          |
| (1,661) | 1:17:A:PRO:HB3  | 1:18:A:SER:HB3 | 4        | 1.69          |
| (1,661) | 1:17:A:PRO:HB3  | 1:18:A:SER:HB3 | 9        | 1.68          |
| (1,541) | 1:12:A:LEU:HD11 | 1:17:A:PRO:HG2 | 3        | 1.68          |
| (1,541) | 1:12:A:LEU:HD12 | 1:17:A:PRO:HG2 | 3        | 1.68          |
| (1,541) | 1:12:A:LEU:HD13 | 1:17:A:PRO:HG2 | 3        | 1.68          |
| (1,541) | 1:12:A:LEU:HD11 | 1:17:A:PRO:HG3 | 3        | 1.68          |
| (1,541) | 1:12:A:LEU:HD12 | 1:17:A:PRO:HG3 | 3        | 1.68          |
| (1,541) | 1:12:A:LEU:HD13 | 1:17:A:PRO:HG3 | 3        | 1.68          |
| (1,109) | 1:9:A:ILE:HB    | 1:11:A:TRP:H   | 5        | 1.68          |
| (1,109) | 1:9:A:ILE:HB    | 1:11:A:TRP:H   | 6        | 1.67          |
| (1,729) | 1:2:A:GLU:HG2   | 1:6:A:ARG:HG3  | 1        | 1.66          |
| (1,661) | 1:17:A:PRO:HB3  | 1:18:A:SER:HB3 | 7        | 1.66          |
| (1,661) | 1:17:A:PRO:HB3  | 1:18:A:SER:HB3 | 8        | 1.66          |
| (1,661) | 1:17:A:PRO:HB3  | 1:18:A:SER:HB3 | 10       | 1.66          |
| (1,696) | 1:5:A:VAL:HG21  | 1:9:A:ILE:HB   | 1        | 1.65          |
| (1,696) | 1:5:A:VAL:HG22  | 1:9:A:ILE:HB   | 1        | 1.65          |
| (1,696) | 1:5:A:VAL:HG23  | 1:9:A:ILE:HB   | 1        | 1.65          |
| (1,696) | 1:5:A:VAL:HG21  | 1:9:A:ILE:HB   | 9        | 1.65          |
| (1,696) | 1:5:A:VAL:HG22  | 1:9:A:ILE:HB   | 9        | 1.65          |
| (1,696) | 1:5:A:VAL:HG23  | 1:9:A:ILE:HB   | 9        | 1.65          |
| (1,696) | 1:5:A:VAL:HG21  | 1:9:A:ILE:HB   | 4        | 1.64          |
| (1,696) | 1:5:A:VAL:HG22  | 1:9:A:ILE:HB   | 4        | 1.64          |
| (1,696) | 1:5:A:VAL:HG23  | 1:9:A:ILE:HB   | 4        | 1.64          |
| (1,661) | 1:17:A:PRO:HB3  | 1:18:A:SER:HB3 | 3        | 1.64          |
| (1,696) | 1:5:A:VAL:HG21  | 1:9:A:ILE:HB   | 5        | 1.63          |
| (1,696) | 1:5:A:VAL:HG22  | 1:9:A:ILE:HB   | 5        | 1.63          |
| (1,696) | 1:5:A:VAL:HG23  | 1:9:A:ILE:HB   | 5        | 1.63          |
| (1,661) | 1:17:A:PRO:HB3  | 1:18:A:SER:HB3 | 1        | 1.63          |
| (1,696) | 1:5:A:VAL:HG21  | 1:9:A:ILE:HB   | 2        | 1.62          |
| (1,696) | 1:5:A:VAL:HG22  | 1:9:A:ILE:HB   | 2        | 1.62          |
| (1,696) | 1:5:A:VAL:HG23  | 1:9:A:ILE:HB   | 2        | 1.62          |
| (1,661) | 1:17:A:PRO:HB3  | 1:18:A:SER:HB3 | 5        | 1.62          |
| (1,109) | 1:9:A:ILE:HB    | 1:11:A:TRP:H   | 1        | 1.62          |
| (1,109) | 1:9:A:ILE:HB    | 1:11:A:TRP:H   | 9        | 1.61          |
| (1,726) | 1:22:A:PRO:HB2  | 1:23:A:PRO:HG2 | 4        | 1.6           |
| (1,726) | 1:22:A:PRO:HB2  | 1:23:A:PRO:HG2 | 7        | 1.6           |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,696) | 1:5:A:VAL:HG21 | 1:9:A:ILE:HB    | 7        | 1.59          |
| (1,696) | 1:5:A:VAL:HG22 | 1:9:A:ILE:HB    | 7        | 1.59          |
| (1,696) | 1:5:A:VAL:HG23 | 1:9:A:ILE:HB    | 7        | 1.59          |
| (1,696) | 1:5:A:VAL:HG21 | 1:9:A:ILE:HB    | 10       | 1.59          |
| (1,696) | 1:5:A:VAL:HG22 | 1:9:A:ILE:HB    | 10       | 1.59          |
| (1,696) | 1:5:A:VAL:HG23 | 1:9:A:ILE:HB    | 10       | 1.59          |
| (1,696) | 1:5:A:VAL:HG21 | 1:9:A:ILE:HB    | 8        | 1.57          |
| (1,696) | 1:5:A:VAL:HG22 | 1:9:A:ILE:HB    | 8        | 1.57          |
| (1,696) | 1:5:A:VAL:HG23 | 1:9:A:ILE:HB    | 8        | 1.57          |
| (1,109) | 1:9:A:ILE:HB   | 1:11:A:TRP:H    | 2        | 1.55          |
| (1,696) | 1:5:A:VAL:HG21 | 1:9:A:ILE:HB    | 6        | 1.54          |
| (1,696) | 1:5:A:VAL:HG22 | 1:9:A:ILE:HB    | 6        | 1.54          |
| (1,696) | 1:5:A:VAL:HG23 | 1:9:A:ILE:HB    | 6        | 1.54          |
| (1,673) | 1:9:A:ILE:HA   | 1:12:A:LEU:HD11 | 3        | 1.54          |
| (1,673) | 1:9:A:ILE:HA   | 1:12:A:LEU:HD12 | 3        | 1.54          |
| (1,673) | 1:9:A:ILE:HA   | 1:12:A:LEU:HD13 | 3        | 1.54          |
| (1,681) | 1:11:A:TRP:HB3 | 1:12:A:LEU:HD21 | 9        | 1.53          |
| (1,681) | 1:11:A:TRP:HB3 | 1:12:A:LEU:HD22 | 9        | 1.53          |
| (1,681) | 1:11:A:TRP:HB3 | 1:12:A:LEU:HD23 | 9        | 1.53          |
| (1,216) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD21 | 1        | 1.52          |
| (1,216) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD22 | 1        | 1.52          |
| (1,216) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD23 | 1        | 1.52          |
| (1,216) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD21 | 7        | 1.52          |
| (1,216) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD22 | 7        | 1.52          |
| (1,216) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD23 | 7        | 1.52          |
| (1,216) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD21 | 9        | 1.52          |
| (1,216) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD22 | 9        | 1.52          |
| (1,216) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD23 | 9        | 1.52          |
| (1,681) | 1:11:A:TRP:HB3 | 1:12:A:LEU:HD21 | 7        | 1.51          |
| (1,681) | 1:11:A:TRP:HB3 | 1:12:A:LEU:HD22 | 7        | 1.51          |
| (1,681) | 1:11:A:TRP:HB3 | 1:12:A:LEU:HD23 | 7        | 1.51          |
| (1,216) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD21 | 2        | 1.51          |
| (1,216) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD22 | 2        | 1.51          |
| (1,216) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD23 | 2        | 1.51          |
| (1,216) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD21 | 4        | 1.51          |
| (1,216) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD22 | 4        | 1.51          |
| (1,216) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD23 | 4        | 1.51          |
| (1,216) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD21 | 5        | 1.51          |
| (1,216) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD22 | 5        | 1.51          |
| (1,216) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD23 | 5        | 1.51          |
| (1,216) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD21 | 6        | 1.51          |
| (1,216) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD22 | 6        | 1.51          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,216) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD23 | 6        | 1.51          |
| (1,216) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD21 | 8        | 1.51          |
| (1,216) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD22 | 8        | 1.51          |
| (1,216) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD23 | 8        | 1.51          |
| (1,216) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD21 | 10       | 1.51          |
| (1,216) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD22 | 10       | 1.51          |
| (1,216) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD23 | 10       | 1.51          |
| (1,674) | 1:9:A:ILE:HA   | 1:12:A:LEU:HD11 | 3        | 1.5           |
| (1,674) | 1:9:A:ILE:HA   | 1:12:A:LEU:HD12 | 3        | 1.5           |
| (1,674) | 1:9:A:ILE:HA   | 1:12:A:LEU:HD13 | 3        | 1.5           |
| (1,568) | 1:8:A:TYR:HA   | 1:24:A:PRO:HD2  | 6        | 1.5           |
| (1,729) | 1:2:A:GLU:HG2  | 1:6:A:ARG:HG3   | 7        | 1.49          |
| (1,568) | 1:8:A:TYR:HA   | 1:24:A:PRO:HD2  | 5        | 1.47          |
| (1,109) | 1:9:A:ILE:HB   | 1:11:A:TRP:H    | 7        | 1.47          |
| (1,713) | 1:5:A:VAL:HG21 | 1:9:A:ILE:HG12  | 6        | 1.46          |
| (1,713) | 1:5:A:VAL:HG22 | 1:9:A:ILE:HG12  | 6        | 1.46          |
| (1,713) | 1:5:A:VAL:HG23 | 1:9:A:ILE:HG12  | 6        | 1.46          |
| (1,681) | 1:11:A:TRP:HB3 | 1:12:A:LEU:HD21 | 4        | 1.46          |
| (1,681) | 1:11:A:TRP:HB3 | 1:12:A:LEU:HD22 | 4        | 1.46          |
| (1,681) | 1:11:A:TRP:HB3 | 1:12:A:LEU:HD23 | 4        | 1.46          |
| (1,215) | 1:11:A:TRP:HZ3 | 1:12:A:LEU:HD21 | 3        | 1.46          |
| (1,215) | 1:11:A:TRP:HZ3 | 1:12:A:LEU:HD22 | 3        | 1.46          |
| (1,215) | 1:11:A:TRP:HZ3 | 1:12:A:LEU:HD23 | 3        | 1.46          |
| (1,726) | 1:22:A:PRO:HB2 | 1:23:A:PRO:HG2  | 9        | 1.45          |
| (1,568) | 1:8:A:TYR:HA   | 1:24:A:PRO:HD2  | 2        | 1.45          |
| (1,568) | 1:8:A:TYR:HA   | 1:24:A:PRO:HD2  | 3        | 1.45          |
| (1,713) | 1:5:A:VAL:HG21 | 1:9:A:ILE:HG12  | 3        | 1.44          |
| (1,713) | 1:5:A:VAL:HG22 | 1:9:A:ILE:HG12  | 3        | 1.44          |
| (1,713) | 1:5:A:VAL:HG23 | 1:9:A:ILE:HG12  | 3        | 1.44          |
| (1,713) | 1:5:A:VAL:HG21 | 1:9:A:ILE:HG12  | 7        | 1.44          |
| (1,713) | 1:5:A:VAL:HG22 | 1:9:A:ILE:HG12  | 7        | 1.44          |
| (1,713) | 1:5:A:VAL:HG23 | 1:9:A:ILE:HG12  | 7        | 1.44          |
| (1,687) | 1:2:A:GLU:HG3  | 1:5:A:VAL:HG11  | 7        | 1.44          |
| (1,687) | 1:2:A:GLU:HG3  | 1:5:A:VAL:HG12  | 7        | 1.44          |
| (1,687) | 1:2:A:GLU:HG3  | 1:5:A:VAL:HG13  | 7        | 1.44          |
| (1,680) | 1:11:A:TRP:HB3 | 1:12:A:LEU:HD21 | 9        | 1.44          |
| (1,680) | 1:11:A:TRP:HB3 | 1:12:A:LEU:HD22 | 9        | 1.44          |
| (1,680) | 1:11:A:TRP:HB3 | 1:12:A:LEU:HD23 | 9        | 1.44          |
| (1,713) | 1:5:A:VAL:HG21 | 1:9:A:ILE:HG12  | 1        | 1.43          |
| (1,713) | 1:5:A:VAL:HG22 | 1:9:A:ILE:HG12  | 1        | 1.43          |
| (1,713) | 1:5:A:VAL:HG23 | 1:9:A:ILE:HG12  | 1        | 1.43          |
| (1,713) | 1:5:A:VAL:HG21 | 1:9:A:ILE:HG12  | 5        | 1.43          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,713) | 1:5:A:VAL:HG22 | 1:9:A:ILE:HG12  | 5        | 1.43          |
| (1,713) | 1:5:A:VAL:HG23 | 1:9:A:ILE:HG12  | 5        | 1.43          |
| (1,568) | 1:8:A:TYR:HA   | 1:24:A:PRO:HD2  | 1        | 1.43          |
| (1,729) | 1:2:A:GLU:HG2  | 1:6:A:ARG:HG3   | 5        | 1.42          |
| (1,713) | 1:5:A:VAL:HG21 | 1:9:A:ILE:HG12  | 2        | 1.42          |
| (1,713) | 1:5:A:VAL:HG22 | 1:9:A:ILE:HG12  | 2        | 1.42          |
| (1,713) | 1:5:A:VAL:HG23 | 1:9:A:ILE:HG12  | 2        | 1.42          |
| (1,713) | 1:5:A:VAL:HG21 | 1:9:A:ILE:HG12  | 8        | 1.42          |
| (1,713) | 1:5:A:VAL:HG22 | 1:9:A:ILE:HG12  | 8        | 1.42          |
| (1,713) | 1:5:A:VAL:HG23 | 1:9:A:ILE:HG12  | 8        | 1.42          |
| (1,681) | 1:11:A:TRP:HB3 | 1:12:A:LEU:HD21 | 8        | 1.42          |
| (1,681) | 1:11:A:TRP:HB3 | 1:12:A:LEU:HD22 | 8        | 1.42          |
| (1,681) | 1:11:A:TRP:HB3 | 1:12:A:LEU:HD23 | 8        | 1.42          |
| (1,681) | 1:11:A:TRP:HB3 | 1:12:A:LEU:HD21 | 10       | 1.42          |
| (1,681) | 1:11:A:TRP:HB3 | 1:12:A:LEU:HD22 | 10       | 1.42          |
| (1,681) | 1:11:A:TRP:HB3 | 1:12:A:LEU:HD23 | 10       | 1.42          |
| (1,680) | 1:11:A:TRP:HB3 | 1:12:A:LEU:HD21 | 7        | 1.42          |
| (1,680) | 1:11:A:TRP:HB3 | 1:12:A:LEU:HD22 | 7        | 1.42          |
| (1,680) | 1:11:A:TRP:HB3 | 1:12:A:LEU:HD23 | 7        | 1.42          |
| (1,687) | 1:2:A:GLU:HG3  | 1:5:A:VAL:HG11  | 9        | 1.41          |
| (1,687) | 1:2:A:GLU:HG3  | 1:5:A:VAL:HG12  | 9        | 1.41          |
| (1,687) | 1:2:A:GLU:HG3  | 1:5:A:VAL:HG13  | 9        | 1.41          |
| (1,726) | 1:22:A:PRO:HB2 | 1:23:A:PRO:HG2  | 2        | 1.4           |
| (1,713) | 1:5:A:VAL:HG21 | 1:9:A:ILE:HG12  | 9        | 1.4           |
| (1,713) | 1:5:A:VAL:HG22 | 1:9:A:ILE:HG12  | 9        | 1.4           |
| (1,713) | 1:5:A:VAL:HG23 | 1:9:A:ILE:HG12  | 9        | 1.4           |
| (1,687) | 1:2:A:GLU:HG3  | 1:5:A:VAL:HG11  | 8        | 1.4           |
| (1,687) | 1:2:A:GLU:HG3  | 1:5:A:VAL:HG12  | 8        | 1.4           |
| (1,687) | 1:2:A:GLU:HG3  | 1:5:A:VAL:HG13  | 8        | 1.4           |
| (1,687) | 1:2:A:GLU:HG3  | 1:5:A:VAL:HG11  | 10       | 1.4           |
| (1,687) | 1:2:A:GLU:HG3  | 1:5:A:VAL:HG12  | 10       | 1.4           |
| (1,687) | 1:2:A:GLU:HG3  | 1:5:A:VAL:HG13  | 10       | 1.4           |
| (1,504) | 1:11:A:TRP:HD1 | 1:23:A:PRO:HD3  | 7        | 1.4           |
| (1,713) | 1:5:A:VAL:HG21 | 1:9:A:ILE:HG12  | 10       | 1.39          |
| (1,713) | 1:5:A:VAL:HG22 | 1:9:A:ILE:HG12  | 10       | 1.39          |
| (1,713) | 1:5:A:VAL:HG23 | 1:9:A:ILE:HG12  | 10       | 1.39          |
| (1,687) | 1:2:A:GLU:HG3  | 1:5:A:VAL:HG11  | 1        | 1.39          |
| (1,687) | 1:2:A:GLU:HG3  | 1:5:A:VAL:HG12  | 1        | 1.39          |
| (1,687) | 1:2:A:GLU:HG3  | 1:5:A:VAL:HG13  | 1        | 1.39          |
| (1,687) | 1:2:A:GLU:HG3  | 1:5:A:VAL:HG11  | 2        | 1.39          |
| (1,687) | 1:2:A:GLU:HG3  | 1:5:A:VAL:HG12  | 2        | 1.39          |
| (1,687) | 1:2:A:GLU:HG3  | 1:5:A:VAL:HG13  | 2        | 1.39          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,315) | 1:10:A:GLN:HE22 | 1:13:A:LYS:HE2  | 9        | 1.39          |
| (1,315) | 1:10:A:GLN:HE22 | 1:13:A:LYS:HE3  | 9        | 1.39          |
| (1,291) | 1:11:A:TRP:HD1  | 1:21:A:ARG:HD2  | 7        | 1.39          |
| (1,713) | 1:5:A:VAL:HG21  | 1:9:A:ILE:HG12  | 4        | 1.38          |
| (1,713) | 1:5:A:VAL:HG22  | 1:9:A:ILE:HG12  | 4        | 1.38          |
| (1,713) | 1:5:A:VAL:HG23  | 1:9:A:ILE:HG12  | 4        | 1.38          |
| (1,687) | 1:2:A:GLU:HG3   | 1:5:A:VAL:HG11  | 6        | 1.38          |
| (1,687) | 1:2:A:GLU:HG3   | 1:5:A:VAL:HG12  | 6        | 1.38          |
| (1,687) | 1:2:A:GLU:HG3   | 1:5:A:VAL:HG13  | 6        | 1.38          |
| (1,572) | 1:4:A:CYS:HB2   | 1:25:A:CYS:HB2  | 3        | 1.38          |
| (1,291) | 1:11:A:TRP:HD1  | 1:21:A:ARG:HD2  | 2        | 1.38          |
| (1,687) | 1:2:A:GLU:HG3   | 1:5:A:VAL:HG11  | 4        | 1.37          |
| (1,687) | 1:2:A:GLU:HG3   | 1:5:A:VAL:HG12  | 4        | 1.37          |
| (1,687) | 1:2:A:GLU:HG3   | 1:5:A:VAL:HG13  | 4        | 1.37          |
| (1,680) | 1:11:A:TRP:HB3  | 1:12:A:LEU:HD21 | 4        | 1.37          |
| (1,680) | 1:11:A:TRP:HB3  | 1:12:A:LEU:HD22 | 4        | 1.37          |
| (1,680) | 1:11:A:TRP:HB3  | 1:12:A:LEU:HD23 | 4        | 1.37          |
| (1,547) | 1:13:A:LYS:HD2  | 1:13:A:LYS:HE2  | 2        | 1.37          |
| (1,547) | 1:13:A:LYS:HD2  | 1:13:A:LYS:HE3  | 2        | 1.37          |
| (1,504) | 1:11:A:TRP:HD1  | 1:23:A:PRO:HD3  | 4        | 1.37          |
| (1,290) | 1:11:A:TRP:HD1  | 1:21:A:ARG:HD3  | 8        | 1.37          |
| (1,547) | 1:13:A:LYS:HD2  | 1:13:A:LYS:HE2  | 5        | 1.35          |
| (1,547) | 1:13:A:LYS:HD2  | 1:13:A:LYS:HE3  | 5        | 1.35          |
| (1,109) | 1:9:A:ILE:HB    | 1:11:A:TRP:H    | 4        | 1.35          |
| (1,109) | 1:9:A:ILE:HB    | 1:11:A:TRP:H    | 10       | 1.35          |
| (1,680) | 1:11:A:TRP:HB3  | 1:12:A:LEU:HD21 | 10       | 1.34          |
| (1,680) | 1:11:A:TRP:HB3  | 1:12:A:LEU:HD22 | 10       | 1.34          |
| (1,680) | 1:11:A:TRP:HB3  | 1:12:A:LEU:HD23 | 10       | 1.34          |
| (1,547) | 1:13:A:LYS:HD2  | 1:13:A:LYS:HE2  | 3        | 1.34          |
| (1,547) | 1:13:A:LYS:HD2  | 1:13:A:LYS:HE3  | 3        | 1.34          |
| (1,473) | 1:22:A:PRO:HA   | 1:22:A:PRO:HD3  | 7        | 1.34          |
| (1,680) | 1:11:A:TRP:HB3  | 1:12:A:LEU:HD21 | 8        | 1.33          |
| (1,680) | 1:11:A:TRP:HB3  | 1:12:A:LEU:HD22 | 8        | 1.33          |
| (1,680) | 1:11:A:TRP:HB3  | 1:12:A:LEU:HD23 | 8        | 1.33          |
| (1,547) | 1:13:A:LYS:HD2  | 1:13:A:LYS:HE2  | 1        | 1.33          |
| (1,547) | 1:13:A:LYS:HD2  | 1:13:A:LYS:HE3  | 1        | 1.33          |
| (1,547) | 1:13:A:LYS:HD2  | 1:13:A:LYS:HE2  | 6        | 1.33          |
| (1,547) | 1:13:A:LYS:HD2  | 1:13:A:LYS:HE3  | 6        | 1.33          |
| (1,547) | 1:13:A:LYS:HD2  | 1:13:A:LYS:HE2  | 9        | 1.33          |
| (1,547) | 1:13:A:LYS:HD2  | 1:13:A:LYS:HE3  | 9        | 1.33          |
| (1,547) | 1:13:A:LYS:HD2  | 1:13:A:LYS:HE2  | 10       | 1.33          |
| (1,547) | 1:13:A:LYS:HD2  | 1:13:A:LYS:HE3  | 10       | 1.33          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,726) | 1:22:A:PRO:HB2  | 1:23:A:PRO:HG2  | 8        | 1.32          |
| (1,687) | 1:2:A:GLU:HG3   | 1:5:A:VAL:HG11  | 3        | 1.32          |
| (1,687) | 1:2:A:GLU:HG3   | 1:5:A:VAL:HG12  | 3        | 1.32          |
| (1,687) | 1:2:A:GLU:HG3   | 1:5:A:VAL:HG13  | 3        | 1.32          |
| (1,547) | 1:13:A:LYS:HD2  | 1:13:A:LYS:HE2  | 8        | 1.32          |
| (1,547) | 1:13:A:LYS:HD2  | 1:13:A:LYS:HE3  | 8        | 1.32          |
| (1,504) | 1:11:A:TRP:HD1  | 1:23:A:PRO:HD3  | 3        | 1.32          |
| (1,407) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD21 | 3        | 1.32          |
| (1,407) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD22 | 3        | 1.32          |
| (1,407) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD23 | 3        | 1.32          |
| (1,189) | 1:8:A:TYR:HD1   | 1:24:A:PRO:HD2  | 3        | 1.32          |
| (1,189) | 1:8:A:TYR:HD2   | 1:24:A:PRO:HD2  | 3        | 1.32          |
| (1,109) | 1:9:A:ILE:HB    | 1:11:A:TRP:H    | 8        | 1.32          |
| (1,549) | 1:12:A:LEU:HD11 | 1:16:A:GLY:HA3  | 3        | 1.31          |
| (1,549) | 1:12:A:LEU:HD12 | 1:16:A:GLY:HA3  | 3        | 1.31          |
| (1,549) | 1:12:A:LEU:HD13 | 1:16:A:GLY:HA3  | 3        | 1.31          |
| (1,504) | 1:11:A:TRP:HD1  | 1:23:A:PRO:HD3  | 8        | 1.31          |
| (1,726) | 1:22:A:PRO:HB2  | 1:23:A:PRO:HG2  | 10       | 1.3           |
| (1,547) | 1:13:A:LYS:HD2  | 1:13:A:LYS:HE2  | 4        | 1.3           |
| (1,547) | 1:13:A:LYS:HD2  | 1:13:A:LYS:HE3  | 4        | 1.3           |
| (1,547) | 1:13:A:LYS:HD2  | 1:13:A:LYS:HE2  | 7        | 1.3           |
| (1,547) | 1:13:A:LYS:HD2  | 1:13:A:LYS:HE3  | 7        | 1.3           |
| (1,473) | 1:22:A:PRO:HA   | 1:22:A:PRO:HD3  | 4        | 1.3           |
| (1,50)  | 1:2:A:GLU:HG2   | 1:6:A:ARG:H     | 5        | 1.3           |
| (1,504) | 1:11:A:TRP:HD1  | 1:23:A:PRO:HD3  | 10       | 1.29          |
| (1,291) | 1:11:A:TRP:HD1  | 1:21:A:ARG:HD2  | 5        | 1.29          |
| (1,291) | 1:11:A:TRP:HD1  | 1:21:A:ARG:HD2  | 9        | 1.29          |
| (1,236) | 1:11:A:TRP:HH2  | 1:22:A:PRO:HB2  | 9        | 1.29          |
| (1,687) | 1:2:A:GLU:HG3   | 1:5:A:VAL:HG11  | 5        | 1.28          |
| (1,687) | 1:2:A:GLU:HG3   | 1:5:A:VAL:HG12  | 5        | 1.28          |
| (1,687) | 1:2:A:GLU:HG3   | 1:5:A:VAL:HG13  | 5        | 1.28          |
| (1,568) | 1:8:A:TYR:HA    | 1:24:A:PRO:HD2  | 10       | 1.28          |
| (1,49)  | 1:10:A:GLN:HB3  | 1:10:A:GLN:HE21 | 4        | 1.28          |
| (1,291) | 1:11:A:TRP:HD1  | 1:21:A:ARG:HD2  | 6        | 1.27          |
| (1,726) | 1:22:A:PRO:HB2  | 1:23:A:PRO:HG2  | 3        | 1.26          |
| (1,726) | 1:22:A:PRO:HB2  | 1:23:A:PRO:HG2  | 5        | 1.26          |
| (1,504) | 1:11:A:TRP:HD1  | 1:23:A:PRO:HD3  | 9        | 1.26          |
| (1,129) | 1:10:A:GLN:HA   | 1:10:A:GLN:HE21 | 1        | 1.26          |
| (1,645) | 1:19:A:SER:HB2  | 1:19:A:SER:HG   | 3        | 1.25          |
| (1,473) | 1:22:A:PRO:HA   | 1:22:A:PRO:HD3  | 9        | 1.25          |
| (1,645) | 1:19:A:SER:HB2  | 1:19:A:SER:HG   | 2        | 1.24          |
| (1,645) | 1:19:A:SER:HB2  | 1:19:A:SER:HG   | 8        | 1.24          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,553) | 1:11:A:TRP:HB2 | 1:24:A:PRO:HD3 | 5        | 1.24          |
| (1,50)  | 1:2:A:GLU:HG2  | 1:6:A:ARG:H    | 6        | 1.24          |
| (1,645) | 1:19:A:SER:HB2 | 1:19:A:SER:HG  | 4        | 1.23          |
| (1,645) | 1:19:A:SER:HB2 | 1:19:A:SER:HG  | 7        | 1.23          |
| (1,568) | 1:8:A:TYR:HA   | 1:24:A:PRO:HD2 | 4        | 1.23          |
| (1,548) | 1:13:A:LYS:HE2 | 1:13:A:LYS:HG2 | 4        | 1.23          |
| (1,548) | 1:13:A:LYS:HE2 | 1:13:A:LYS:HG3 | 4        | 1.23          |
| (1,548) | 1:13:A:LYS:HE3 | 1:13:A:LYS:HG2 | 4        | 1.23          |
| (1,548) | 1:13:A:LYS:HE3 | 1:13:A:LYS:HG3 | 4        | 1.23          |
| (1,726) | 1:22:A:PRO:HB2 | 1:23:A:PRO:HG2 | 6        | 1.22          |
| (1,645) | 1:19:A:SER:HB2 | 1:19:A:SER:HG  | 1        | 1.22          |
| (1,645) | 1:19:A:SER:HB2 | 1:19:A:SER:HG  | 9        | 1.22          |
| (1,645) | 1:19:A:SER:HB2 | 1:19:A:SER:HG  | 10       | 1.22          |
| (1,568) | 1:8:A:TYR:HA   | 1:24:A:PRO:HD2 | 8        | 1.22          |
| (1,548) | 1:13:A:LYS:HE2 | 1:13:A:LYS:HG2 | 2        | 1.22          |
| (1,548) | 1:13:A:LYS:HE2 | 1:13:A:LYS:HG3 | 2        | 1.22          |
| (1,548) | 1:13:A:LYS:HE3 | 1:13:A:LYS:HG2 | 2        | 1.22          |
| (1,548) | 1:13:A:LYS:HE3 | 1:13:A:LYS:HG3 | 2        | 1.22          |
| (1,473) | 1:22:A:PRO:HA  | 1:22:A:PRO:HD3 | 5        | 1.22          |
| (1,473) | 1:22:A:PRO:HA  | 1:22:A:PRO:HD3 | 10       | 1.22          |
| (1,257) | 1:24:A:PRO:HD2 | 1:25:A:CYS:H   | 7        | 1.22          |
| (1,50)  | 1:2:A:GLU:HG2  | 1:6:A:ARG:H    | 4        | 1.22          |
| (1,726) | 1:22:A:PRO:HB2 | 1:23:A:PRO:HG2 | 1        | 1.21          |
| (1,645) | 1:19:A:SER:HB2 | 1:19:A:SER:HG  | 5        | 1.21          |
| (1,553) | 1:11:A:TRP:HB2 | 1:24:A:PRO:HD3 | 2        | 1.21          |
| (1,473) | 1:22:A:PRO:HA  | 1:22:A:PRO:HD3 | 1        | 1.21          |
| (1,473) | 1:22:A:PRO:HA  | 1:22:A:PRO:HD3 | 3        | 1.21          |
| (1,473) | 1:22:A:PRO:HA  | 1:22:A:PRO:HD3 | 6        | 1.21          |
| (1,473) | 1:22:A:PRO:HA  | 1:22:A:PRO:HD3 | 8        | 1.21          |
| (1,257) | 1:24:A:PRO:HD2 | 1:25:A:CYS:H   | 9        | 1.21          |
| (1,669) | 1:9:A:ILE:HA   | 1:12:A:LEU:HB2 | 6        | 1.2           |
| (1,669) | 1:9:A:ILE:HA   | 1:12:A:LEU:HB2 | 9        | 1.2           |
| (1,645) | 1:19:A:SER:HB2 | 1:19:A:SER:HG  | 6        | 1.2           |
| (1,548) | 1:13:A:LYS:HE2 | 1:13:A:LYS:HG2 | 7        | 1.2           |
| (1,548) | 1:13:A:LYS:HE2 | 1:13:A:LYS:HG3 | 7        | 1.2           |
| (1,548) | 1:13:A:LYS:HE3 | 1:13:A:LYS:HG2 | 7        | 1.2           |
| (1,548) | 1:13:A:LYS:HE3 | 1:13:A:LYS:HG3 | 7        | 1.2           |
| (1,291) | 1:11:A:TRP:HD1 | 1:21:A:ARG:HD2 | 4        | 1.2           |
| (1,669) | 1:9:A:ILE:HA   | 1:12:A:LEU:HB2 | 2        | 1.19          |
| (1,669) | 1:9:A:ILE:HA   | 1:12:A:LEU:HB2 | 4        | 1.19          |
| (1,669) | 1:9:A:ILE:HA   | 1:12:A:LEU:HB2 | 5        | 1.19          |
| (1,669) | 1:9:A:ILE:HA   | 1:12:A:LEU:HB2 | 7        | 1.19          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,473) | 1:22:A:PRO:HA  | 1:22:A:PRO:HD3  | 2        | 1.19          |
| (1,669) | 1:9:A:ILE:HA   | 1:12:A:LEU:HB2  | 1        | 1.18          |
| (1,669) | 1:9:A:ILE:HA   | 1:12:A:LEU:HB2  | 3        | 1.18          |
| (1,669) | 1:9:A:ILE:HA   | 1:12:A:LEU:HB2  | 8        | 1.18          |
| (1,669) | 1:9:A:ILE:HA   | 1:12:A:LEU:HB2  | 10       | 1.18          |
| (1,662) | 1:17:A:PRO:HB3 | 1:18:A:SER:HB2  | 2        | 1.18          |
| (1,568) | 1:8:A:TYR:HA   | 1:24:A:PRO:HD2  | 7        | 1.18          |
| (1,240) | 1:8:A:TYR:HD1  | 1:9:A:ILE:HG13  | 2        | 1.18          |
| (1,240) | 1:8:A:TYR:HD2  | 1:9:A:ILE:HG13  | 2        | 1.18          |
| (1,240) | 1:8:A:TYR:HD1  | 1:9:A:ILE:HG13  | 10       | 1.18          |
| (1,240) | 1:8:A:TYR:HD2  | 1:9:A:ILE:HG13  | 10       | 1.18          |
| (1,50)  | 1:2:A:GLU:HG2  | 1:6:A:ARG:H     | 7        | 1.18          |
| (1,557) | 1:9:A:ILE:HA   | 1:12:A:LEU:HG   | 3        | 1.17          |
| (1,556) | 1:11:A:TRP:HB2 | 1:24:A:PRO:HG2  | 3        | 1.17          |
| (1,240) | 1:8:A:TYR:HD1  | 1:9:A:ILE:HG13  | 1        | 1.17          |
| (1,240) | 1:8:A:TYR:HD2  | 1:9:A:ILE:HG13  | 1        | 1.17          |
| (1,240) | 1:8:A:TYR:HD1  | 1:9:A:ILE:HG13  | 5        | 1.17          |
| (1,240) | 1:8:A:TYR:HD2  | 1:9:A:ILE:HG13  | 5        | 1.17          |
| (1,240) | 1:8:A:TYR:HD1  | 1:9:A:ILE:HG13  | 6        | 1.17          |
| (1,240) | 1:8:A:TYR:HD2  | 1:9:A:ILE:HG13  | 6        | 1.17          |
| (1,240) | 1:8:A:TYR:HD1  | 1:9:A:ILE:HG13  | 8        | 1.17          |
| (1,240) | 1:8:A:TYR:HD2  | 1:9:A:ILE:HG13  | 8        | 1.17          |
| (1,50)  | 1:2:A:GLU:HG2  | 1:6:A:ARG:H     | 9        | 1.17          |
| (1,561) | 1:8:A:TYR:HA   | 1:24:A:PRO:HG2  | 6        | 1.16          |
| (1,557) | 1:9:A:ILE:HA   | 1:12:A:LEU:HG   | 8        | 1.16          |
| (1,557) | 1:9:A:ILE:HA   | 1:12:A:LEU:HG   | 10       | 1.16          |
| (1,553) | 1:11:A:TRP:HB2 | 1:24:A:PRO:HD3  | 1        | 1.16          |
| (1,543) | 1:2:A:GLU:HG2  | 1:9:A:ILE:HD11  | 3        | 1.16          |
| (1,543) | 1:2:A:GLU:HG2  | 1:9:A:ILE:HD12  | 3        | 1.16          |
| (1,543) | 1:2:A:GLU:HG2  | 1:9:A:ILE:HD13  | 3        | 1.16          |
| (1,543) | 1:2:A:GLU:HG2  | 1:9:A:ILE:HD11  | 5        | 1.16          |
| (1,543) | 1:2:A:GLU:HG2  | 1:9:A:ILE:HD12  | 5        | 1.16          |
| (1,543) | 1:2:A:GLU:HG2  | 1:9:A:ILE:HD13  | 5        | 1.16          |
| (1,257) | 1:24:A:PRO:HD2 | 1:25:A:CYS:H    | 8        | 1.16          |
| (1,240) | 1:8:A:TYR:HD1  | 1:9:A:ILE:HG13  | 4        | 1.16          |
| (1,240) | 1:8:A:TYR:HD2  | 1:9:A:ILE:HG13  | 4        | 1.16          |
| (1,240) | 1:8:A:TYR:HD1  | 1:9:A:ILE:HG13  | 7        | 1.16          |
| (1,240) | 1:8:A:TYR:HD2  | 1:9:A:ILE:HG13  | 7        | 1.16          |
| (1,240) | 1:8:A:TYR:HD1  | 1:9:A:ILE:HG13  | 9        | 1.16          |
| (1,240) | 1:8:A:TYR:HD2  | 1:9:A:ILE:HG13  | 9        | 1.16          |
| (1,129) | 1:10:A:GLN:HA  | 1:10:A:GLN:HE21 | 7        | 1.16          |
| (1,568) | 1:8:A:TYR:HA   | 1:24:A:PRO:HD2  | 9        | 1.15          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,561) | 1:8:A:TYR:HA   | 1:24:A:PRO:HG2  | 10       | 1.15          |
| (1,215) | 1:11:A:TRP:HZ3 | 1:12:A:LEU:HD21 | 8        | 1.15          |
| (1,215) | 1:11:A:TRP:HZ3 | 1:12:A:LEU:HD22 | 8        | 1.15          |
| (1,215) | 1:11:A:TRP:HZ3 | 1:12:A:LEU:HD23 | 8        | 1.15          |
| (1,215) | 1:11:A:TRP:HZ3 | 1:12:A:LEU:HD21 | 10       | 1.15          |
| (1,215) | 1:11:A:TRP:HZ3 | 1:12:A:LEU:HD22 | 10       | 1.15          |
| (1,215) | 1:11:A:TRP:HZ3 | 1:12:A:LEU:HD23 | 10       | 1.15          |
| (1,705) | 1:9:A:ILE:HG21 | 1:13:A:LYS:HD2  | 2        | 1.14          |
| (1,705) | 1:9:A:ILE:HG22 | 1:13:A:LYS:HD2  | 2        | 1.14          |
| (1,705) | 1:9:A:ILE:HG23 | 1:13:A:LYS:HD2  | 2        | 1.14          |
| (1,662) | 1:17:A:PRO:HB3 | 1:18:A:SER:HB2  | 6        | 1.14          |
| (1,561) | 1:8:A:TYR:HA   | 1:24:A:PRO:HG2  | 4        | 1.14          |
| (1,257) | 1:24:A:PRO:HD2 | 1:25:A:CYS:H    | 4        | 1.14          |
| (1,561) | 1:8:A:TYR:HA   | 1:24:A:PRO:HG2  | 1        | 1.13          |
| (1,561) | 1:8:A:TYR:HA   | 1:24:A:PRO:HG2  | 3        | 1.13          |
| (1,561) | 1:8:A:TYR:HA   | 1:24:A:PRO:HG2  | 7        | 1.13          |
| (1,561) | 1:8:A:TYR:HA   | 1:24:A:PRO:HG2  | 8        | 1.13          |
| (1,561) | 1:8:A:TYR:HA   | 1:24:A:PRO:HG2  | 9        | 1.13          |
| (1,553) | 1:11:A:TRP:HB2 | 1:24:A:PRO:HD3  | 6        | 1.13          |
| (1,50)  | 1:2:A:GLU:HG2  | 1:6:A:ARG:H     | 1        | 1.13          |
| (1,705) | 1:9:A:ILE:HG21 | 1:13:A:LYS:HD2  | 1        | 1.12          |
| (1,705) | 1:9:A:ILE:HG22 | 1:13:A:LYS:HD2  | 1        | 1.12          |
| (1,705) | 1:9:A:ILE:HG23 | 1:13:A:LYS:HD2  | 1        | 1.12          |
| (1,668) | 1:19:A:SER:HB2 | 1:21:A:ARG:HG2  | 4        | 1.12          |
| (1,668) | 1:19:A:SER:HB2 | 1:21:A:ARG:HG3  | 4        | 1.12          |
| (1,561) | 1:8:A:TYR:HA   | 1:24:A:PRO:HG2  | 2        | 1.12          |
| (1,561) | 1:8:A:TYR:HA   | 1:24:A:PRO:HG2  | 5        | 1.12          |
| (1,504) | 1:11:A:TRP:HD1 | 1:23:A:PRO:HD3  | 1        | 1.12          |
| (1,651) | 1:3:A:GLU:HA   | 1:6:A:ARG:HD2   | 2        | 1.11          |
| (1,504) | 1:11:A:TRP:HD1 | 1:23:A:PRO:HD3  | 6        | 1.11          |
| (1,236) | 1:11:A:TRP:HH2 | 1:22:A:PRO:HB2  | 10       | 1.11          |
| (1,548) | 1:13:A:LYS:HE2 | 1:13:A:LYS:HG2  | 1        | 1.1           |
| (1,548) | 1:13:A:LYS:HE2 | 1:13:A:LYS:HG3  | 1        | 1.1           |
| (1,548) | 1:13:A:LYS:HE3 | 1:13:A:LYS:HG2  | 1        | 1.1           |
| (1,548) | 1:13:A:LYS:HE3 | 1:13:A:LYS:HG3  | 1        | 1.1           |
| (1,291) | 1:11:A:TRP:HD1 | 1:21:A:ARG:HD2  | 3        | 1.1           |
| (1,290) | 1:11:A:TRP:HD1 | 1:21:A:ARG:HD3  | 10       | 1.1           |
| (1,236) | 1:11:A:TRP:HH2 | 1:22:A:PRO:HB2  | 8        | 1.1           |
| (1,50)  | 1:2:A:GLU:HG2  | 1:6:A:ARG:H     | 3        | 1.1           |
| (1,291) | 1:11:A:TRP:HD1 | 1:21:A:ARG:HD2  | 1        | 1.09          |
| (1,215) | 1:11:A:TRP:HZ3 | 1:12:A:LEU:HD21 | 4        | 1.09          |
| (1,215) | 1:11:A:TRP:HZ3 | 1:12:A:LEU:HD22 | 4        | 1.09          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,215) | 1:11:A:TRP:HZ3 | 1:12:A:LEU:HD23 | 4        | 1.09          |
| (1,722) | 1:9:A:ILE:HG12 | 1:12:A:LEU:HB3  | 3        | 1.08          |
| (1,557) | 1:9:A:ILE:HA   | 1:12:A:LEU:HG   | 7        | 1.08          |
| (1,548) | 1:13:A:LYS:HE2 | 1:13:A:LYS:HG2  | 3        | 1.08          |
| (1,548) | 1:13:A:LYS:HE2 | 1:13:A:LYS:HG3  | 3        | 1.08          |
| (1,548) | 1:13:A:LYS:HE3 | 1:13:A:LYS:HG2  | 3        | 1.08          |
| (1,548) | 1:13:A:LYS:HE3 | 1:13:A:LYS:HG3  | 3        | 1.08          |
| (1,504) | 1:11:A:TRP:HD1 | 1:23:A:PRO:HD3  | 5        | 1.08          |
| (1,300) | 1:12:A:LEU:H   | 1:12:A:LEU:HD21 | 7        | 1.08          |
| (1,300) | 1:12:A:LEU:H   | 1:12:A:LEU:HD22 | 7        | 1.08          |
| (1,300) | 1:12:A:LEU:H   | 1:12:A:LEU:HD23 | 7        | 1.08          |
| (1,129) | 1:10:A:GLN:HA  | 1:10:A:GLN:HE21 | 6        | 1.08          |
| (1,557) | 1:9:A:ILE:HA   | 1:12:A:LEU:HG   | 4        | 1.07          |
| (1,543) | 1:2:A:GLU:HG2  | 1:9:A:ILE:HD11  | 4        | 1.07          |
| (1,543) | 1:2:A:GLU:HG2  | 1:9:A:ILE:HD12  | 4        | 1.07          |
| (1,543) | 1:2:A:GLU:HG2  | 1:9:A:ILE:HD13  | 4        | 1.07          |
| (1,300) | 1:12:A:LEU:H   | 1:12:A:LEU:HD21 | 4        | 1.07          |
| (1,300) | 1:12:A:LEU:H   | 1:12:A:LEU:HD22 | 4        | 1.07          |
| (1,300) | 1:12:A:LEU:H   | 1:12:A:LEU:HD23 | 4        | 1.07          |
| (1,300) | 1:12:A:LEU:H   | 1:12:A:LEU:HD21 | 8        | 1.07          |
| (1,300) | 1:12:A:LEU:H   | 1:12:A:LEU:HD22 | 8        | 1.07          |
| (1,300) | 1:12:A:LEU:H   | 1:12:A:LEU:HD23 | 8        | 1.07          |
| (1,300) | 1:12:A:LEU:H   | 1:12:A:LEU:HD21 | 10       | 1.07          |
| (1,300) | 1:12:A:LEU:H   | 1:12:A:LEU:HD22 | 10       | 1.07          |
| (1,300) | 1:12:A:LEU:H   | 1:12:A:LEU:HD23 | 10       | 1.07          |
| (1,257) | 1:24:A:PRO:HD2 | 1:25:A:CYS:H    | 10       | 1.07          |
| (1,557) | 1:9:A:ILE:HA   | 1:12:A:LEU:HG   | 9        | 1.06          |
| (1,543) | 1:2:A:GLU:HG2  | 1:9:A:ILE:HD11  | 2        | 1.06          |
| (1,543) | 1:2:A:GLU:HG2  | 1:9:A:ILE:HD12  | 2        | 1.06          |
| (1,543) | 1:2:A:GLU:HG2  | 1:9:A:ILE:HD13  | 2        | 1.06          |
| (1,543) | 1:2:A:GLU:HG2  | 1:9:A:ILE:HD11  | 10       | 1.06          |
| (1,543) | 1:2:A:GLU:HG2  | 1:9:A:ILE:HD12  | 10       | 1.06          |
| (1,543) | 1:2:A:GLU:HG2  | 1:9:A:ILE:HD13  | 10       | 1.06          |
| (1,300) | 1:12:A:LEU:H   | 1:12:A:LEU:HD21 | 9        | 1.06          |
| (1,300) | 1:12:A:LEU:H   | 1:12:A:LEU:HD22 | 9        | 1.06          |
| (1,300) | 1:12:A:LEU:H   | 1:12:A:LEU:HD23 | 9        | 1.06          |
| (1,129) | 1:10:A:GLN:HA  | 1:10:A:GLN:HE21 | 2        | 1.06          |
| (1,50)  | 1:2:A:GLU:HG2  | 1:6:A:ARG:H     | 8        | 1.06          |
| (1,668) | 1:19:A:SER:HB2 | 1:21:A:ARG:HG2  | 1        | 1.05          |
| (1,668) | 1:19:A:SER:HB2 | 1:21:A:ARG:HG3  | 1        | 1.05          |
| (1,543) | 1:2:A:GLU:HG2  | 1:9:A:ILE:HD11  | 1        | 1.05          |
| (1,543) | 1:2:A:GLU:HG2  | 1:9:A:ILE:HD12  | 1        | 1.05          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,543) | 1:2:A:GLU:HG2  | 1:9:A:ILE:HD13  | 1        | 1.05          |
| (1,504) | 1:11:A:TRP:HD1 | 1:23:A:PRO:HD3  | 2        | 1.05          |
| (1,300) | 1:12:A:LEU:H   | 1:12:A:LEU:HD21 | 2        | 1.05          |
| (1,300) | 1:12:A:LEU:H   | 1:12:A:LEU:HD22 | 2        | 1.05          |
| (1,300) | 1:12:A:LEU:H   | 1:12:A:LEU:HD23 | 2        | 1.05          |
| (1,216) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD21 | 3        | 1.05          |
| (1,216) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD22 | 3        | 1.05          |
| (1,216) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD23 | 3        | 1.05          |
| (1,215) | 1:11:A:TRP:HZ3 | 1:12:A:LEU:HD21 | 7        | 1.05          |
| (1,215) | 1:11:A:TRP:HZ3 | 1:12:A:LEU:HD22 | 7        | 1.05          |
| (1,215) | 1:11:A:TRP:HZ3 | 1:12:A:LEU:HD23 | 7        | 1.05          |
| (1,129) | 1:10:A:GLN:HA  | 1:10:A:GLN:HE21 | 5        | 1.05          |
| (1,50)  | 1:2:A:GLU:HG2  | 1:6:A:ARG:H     | 10       | 1.05          |
| (1,668) | 1:19:A:SER:HB2 | 1:21:A:ARG:HG2  | 7        | 1.04          |
| (1,668) | 1:19:A:SER:HB2 | 1:21:A:ARG:HG3  | 7        | 1.04          |
| (1,407) | 1:12:A:LEU:HA  | 1:12:A:LEU:HD21 | 8        | 1.04          |
| (1,407) | 1:12:A:LEU:HA  | 1:12:A:LEU:HD22 | 8        | 1.04          |
| (1,407) | 1:12:A:LEU:HA  | 1:12:A:LEU:HD23 | 8        | 1.04          |
| (1,300) | 1:12:A:LEU:H   | 1:12:A:LEU:HD21 | 1        | 1.04          |
| (1,300) | 1:12:A:LEU:H   | 1:12:A:LEU:HD22 | 1        | 1.04          |
| (1,300) | 1:12:A:LEU:H   | 1:12:A:LEU:HD23 | 1        | 1.04          |
| (1,300) | 1:12:A:LEU:H   | 1:12:A:LEU:HD21 | 6        | 1.04          |
| (1,300) | 1:12:A:LEU:H   | 1:12:A:LEU:HD22 | 6        | 1.04          |
| (1,300) | 1:12:A:LEU:H   | 1:12:A:LEU:HD23 | 6        | 1.04          |
| (1,236) | 1:11:A:TRP:HH2 | 1:22:A:PRO:HB2  | 3        | 1.04          |
| (1,50)  | 1:2:A:GLU:HG2  | 1:6:A:ARG:H     | 2        | 1.04          |
| (1,543) | 1:2:A:GLU:HG2  | 1:9:A:ILE:HD11  | 6        | 1.03          |
| (1,543) | 1:2:A:GLU:HG2  | 1:9:A:ILE:HD12  | 6        | 1.03          |
| (1,543) | 1:2:A:GLU:HG2  | 1:9:A:ILE:HD13  | 6        | 1.03          |
| (1,407) | 1:12:A:LEU:HA  | 1:12:A:LEU:HD21 | 10       | 1.03          |
| (1,407) | 1:12:A:LEU:HA  | 1:12:A:LEU:HD22 | 10       | 1.03          |
| (1,407) | 1:12:A:LEU:HA  | 1:12:A:LEU:HD23 | 10       | 1.03          |
| (1,300) | 1:12:A:LEU:H   | 1:12:A:LEU:HD21 | 5        | 1.03          |
| (1,300) | 1:12:A:LEU:H   | 1:12:A:LEU:HD22 | 5        | 1.03          |
| (1,300) | 1:12:A:LEU:H   | 1:12:A:LEU:HD23 | 5        | 1.03          |
| (1,236) | 1:11:A:TRP:HH2 | 1:22:A:PRO:HB2  | 2        | 1.03          |
| (1,730) | 1:2:A:GLU:HG3  | 1:6:A:ARG:HG3   | 1        | 1.02          |
| (1,407) | 1:12:A:LEU:HA  | 1:12:A:LEU:HD21 | 4        | 1.02          |
| (1,407) | 1:12:A:LEU:HA  | 1:12:A:LEU:HD22 | 4        | 1.02          |
| (1,407) | 1:12:A:LEU:HA  | 1:12:A:LEU:HD23 | 4        | 1.02          |
| (1,257) | 1:24:A:PRO:HD2 | 1:25:A:CYS:H    | 2        | 1.02          |
| (1,257) | 1:24:A:PRO:HD2 | 1:25:A:CYS:H    | 5        | 1.02          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,215) | 1:11:A:TRP:HZ3 | 1:12:A:LEU:HD21 | 9        | 1.01          |
| (1,215) | 1:11:A:TRP:HZ3 | 1:12:A:LEU:HD22 | 9        | 1.01          |
| (1,215) | 1:11:A:TRP:HZ3 | 1:12:A:LEU:HD23 | 9        | 1.01          |
| (1,730) | 1:2:A:GLU:HG3  | 1:6:A:ARG:HG3   | 8        | 1.0           |
| (1,668) | 1:19:A:SER:HB2 | 1:21:A:ARG:HG2  | 5        | 1.0           |
| (1,668) | 1:19:A:SER:HB2 | 1:21:A:ARG:HG3  | 5        | 1.0           |
| (1,594) | 1:9:A:ILE:HG21 | 1:13:A:LYS:HE2  | 3        | 1.0           |
| (1,594) | 1:9:A:ILE:HG22 | 1:13:A:LYS:HE2  | 3        | 1.0           |
| (1,594) | 1:9:A:ILE:HG23 | 1:13:A:LYS:HE2  | 3        | 1.0           |
| (1,594) | 1:9:A:ILE:HG21 | 1:13:A:LYS:HE3  | 3        | 1.0           |
| (1,594) | 1:9:A:ILE:HG22 | 1:13:A:LYS:HE3  | 3        | 1.0           |
| (1,594) | 1:9:A:ILE:HG23 | 1:13:A:LYS:HE3  | 3        | 1.0           |
| (1,543) | 1:2:A:GLU:HG2  | 1:9:A:ILE:HD11  | 8        | 1.0           |
| (1,543) | 1:2:A:GLU:HG2  | 1:9:A:ILE:HD12  | 8        | 1.0           |
| (1,543) | 1:2:A:GLU:HG2  | 1:9:A:ILE:HD13  | 8        | 1.0           |
| (1,189) | 1:8:A:TYR:HD1  | 1:24:A:PRO:HD2  | 4        | 1.0           |
| (1,189) | 1:8:A:TYR:HD2  | 1:24:A:PRO:HD2  | 4        | 1.0           |
| (1,730) | 1:2:A:GLU:HG3  | 1:6:A:ARG:HG3   | 2        | 0.99          |
| (1,649) | 1:15:A:GLY:HA2 | 1:19:A:SER:HB3  | 3        | 0.99          |
| (1,189) | 1:8:A:TYR:HD1  | 1:24:A:PRO:HD2  | 10       | 0.99          |
| (1,189) | 1:8:A:TYR:HD2  | 1:24:A:PRO:HD2  | 10       | 0.99          |
| (1,730) | 1:2:A:GLU:HG3  | 1:6:A:ARG:HG3   | 3        | 0.98          |
| (1,730) | 1:2:A:GLU:HG3  | 1:6:A:ARG:HG3   | 5        | 0.98          |
| (1,730) | 1:2:A:GLU:HG3  | 1:6:A:ARG:HG3   | 10       | 0.98          |
| (1,407) | 1:12:A:LEU:HA  | 1:12:A:LEU:HD21 | 9        | 0.98          |
| (1,407) | 1:12:A:LEU:HA  | 1:12:A:LEU:HD22 | 9        | 0.98          |
| (1,407) | 1:12:A:LEU:HA  | 1:12:A:LEU:HD23 | 9        | 0.98          |
| (1,189) | 1:8:A:TYR:HD1  | 1:24:A:PRO:HD2  | 6        | 0.98          |
| (1,189) | 1:8:A:TYR:HD2  | 1:24:A:PRO:HD2  | 6        | 0.98          |
| (1,730) | 1:2:A:GLU:HG3  | 1:6:A:ARG:HG3   | 6        | 0.97          |
| (1,461) | 1:21:A:ARG:HA  | 1:21:A:ARG:HG2  | 10       | 0.97          |
| (1,461) | 1:21:A:ARG:HA  | 1:21:A:ARG:HG3  | 10       | 0.97          |
| (1,189) | 1:8:A:TYR:HD1  | 1:24:A:PRO:HD2  | 2        | 0.97          |
| (1,189) | 1:8:A:TYR:HD2  | 1:24:A:PRO:HD2  | 2        | 0.97          |
| (1,189) | 1:8:A:TYR:HD1  | 1:24:A:PRO:HD2  | 7        | 0.97          |
| (1,189) | 1:8:A:TYR:HD2  | 1:24:A:PRO:HD2  | 7        | 0.97          |
| (1,189) | 1:8:A:TYR:HD1  | 1:24:A:PRO:HD2  | 9        | 0.97          |
| (1,189) | 1:8:A:TYR:HD2  | 1:24:A:PRO:HD2  | 9        | 0.97          |
| (1,548) | 1:13:A:LYS:HE2 | 1:13:A:LYS:HG2  | 8        | 0.96          |
| (1,548) | 1:13:A:LYS:HE2 | 1:13:A:LYS:HG3  | 8        | 0.96          |
| (1,548) | 1:13:A:LYS:HE3 | 1:13:A:LYS:HG2  | 8        | 0.96          |
| (1,548) | 1:13:A:LYS:HE3 | 1:13:A:LYS:HG3  | 8        | 0.96          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,407) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD21 | 7        | 0.96          |
| (1,407) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD22 | 7        | 0.96          |
| (1,407) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD23 | 7        | 0.96          |
| (1,257) | 1:24:A:PRO:HD2  | 1:25:A:CYS:H    | 6        | 0.96          |
| (1,189) | 1:8:A:TYR:HD1   | 1:24:A:PRO:HD2  | 1        | 0.96          |
| (1,189) | 1:8:A:TYR:HD2   | 1:24:A:PRO:HD2  | 1        | 0.96          |
| (1,121) | 1:2:A:GLU:HB2   | 1:5:A:VAL:H     | 9        | 0.96          |
| (1,730) | 1:2:A:GLU:HG3   | 1:6:A:ARG:HG3   | 4        | 0.95          |
| (1,700) | 1:9:A:ILE:HG13  | 1:12:A:LEU:HD11 | 3        | 0.95          |
| (1,700) | 1:9:A:ILE:HG13  | 1:12:A:LEU:HD12 | 3        | 0.95          |
| (1,700) | 1:9:A:ILE:HG13  | 1:12:A:LEU:HD13 | 3        | 0.95          |
| (1,548) | 1:13:A:LYS:HE2  | 1:13:A:LYS:HG2  | 9        | 0.95          |
| (1,548) | 1:13:A:LYS:HE2  | 1:13:A:LYS:HG3  | 9        | 0.95          |
| (1,548) | 1:13:A:LYS:HE3  | 1:13:A:LYS:HG2  | 9        | 0.95          |
| (1,548) | 1:13:A:LYS:HE3  | 1:13:A:LYS:HG3  | 9        | 0.95          |
| (1,257) | 1:24:A:PRO:HD2  | 1:25:A:CYS:H    | 1        | 0.95          |
| (1,222) | 1:8:A:TYR:HD1   | 1:23:A:PRO:HB2  | 5        | 0.95          |
| (1,222) | 1:8:A:TYR:HD2   | 1:23:A:PRO:HB2  | 5        | 0.95          |
| (1,121) | 1:2:A:GLU:HB2   | 1:5:A:VAL:H     | 10       | 0.95          |
| (1,649) | 1:15:A:GLY:HA2  | 1:19:A:SER:HB3  | 2        | 0.94          |
| (1,625) | 1:10:A:GLN:HE21 | 1:14:A:ASP:HB3  | 1        | 0.94          |
| (1,593) | 1:11:A:TRP:HA   | 1:14:A:ASP:HB3  | 4        | 0.94          |
| (1,548) | 1:13:A:LYS:HE2  | 1:13:A:LYS:HG2  | 6        | 0.94          |
| (1,548) | 1:13:A:LYS:HE2  | 1:13:A:LYS:HG3  | 6        | 0.94          |
| (1,548) | 1:13:A:LYS:HE3  | 1:13:A:LYS:HG2  | 6        | 0.94          |
| (1,548) | 1:13:A:LYS:HE3  | 1:13:A:LYS:HG3  | 6        | 0.94          |
| (1,548) | 1:13:A:LYS:HE2  | 1:13:A:LYS:HG2  | 10       | 0.94          |
| (1,548) | 1:13:A:LYS:HE2  | 1:13:A:LYS:HG3  | 10       | 0.94          |
| (1,548) | 1:13:A:LYS:HE3  | 1:13:A:LYS:HG2  | 10       | 0.94          |
| (1,548) | 1:13:A:LYS:HE3  | 1:13:A:LYS:HG3  | 10       | 0.94          |
| (1,476) | 1:22:A:PRO:HA   | 1:22:A:PRO:HG3  | 9        | 0.94          |
| (1,461) | 1:21:A:ARG:HA   | 1:21:A:ARG:HG2  | 2        | 0.94          |
| (1,461) | 1:21:A:ARG:HA   | 1:21:A:ARG:HG3  | 2        | 0.94          |
| (1,461) | 1:21:A:ARG:HA   | 1:21:A:ARG:HG2  | 3        | 0.94          |
| (1,461) | 1:21:A:ARG:HA   | 1:21:A:ARG:HG3  | 3        | 0.94          |
| (1,355) | 1:6:A:ARG:HB2   | 1:6:A:ARG:HD2   | 8        | 0.94          |
| (1,207) | 1:11:A:TRP:HH2  | 1:12:A:LEU:HD11 | 3        | 0.94          |
| (1,207) | 1:11:A:TRP:HH2  | 1:12:A:LEU:HD12 | 3        | 0.94          |
| (1,207) | 1:11:A:TRP:HH2  | 1:12:A:LEU:HD13 | 3        | 0.94          |
| (1,166) | 1:5:A:VAL:HA    | 1:8:A:TYR:HD1   | 3        | 0.94          |
| (1,166) | 1:5:A:VAL:HA    | 1:8:A:TYR:HD2   | 3        | 0.94          |
| (1,121) | 1:2:A:GLU:HB2   | 1:5:A:VAL:H     | 3        | 0.94          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,675) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD21 | 3        | 0.93          |
| (1,675) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD22 | 3        | 0.93          |
| (1,675) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD23 | 3        | 0.93          |
| (1,587) | 1:8:A:TYR:HB2   | 1:12:A:LEU:HD21 | 3        | 0.93          |
| (1,587) | 1:8:A:TYR:HB2   | 1:12:A:LEU:HD22 | 3        | 0.93          |
| (1,587) | 1:8:A:TYR:HB2   | 1:12:A:LEU:HD23 | 3        | 0.93          |
| (1,587) | 1:8:A:TYR:HB3   | 1:12:A:LEU:HD21 | 3        | 0.93          |
| (1,587) | 1:8:A:TYR:HB3   | 1:12:A:LEU:HD22 | 3        | 0.93          |
| (1,587) | 1:8:A:TYR:HB3   | 1:12:A:LEU:HD23 | 3        | 0.93          |
| (1,189) | 1:8:A:TYR:HD1   | 1:24:A:PRO:HD2  | 8        | 0.93          |
| (1,189) | 1:8:A:TYR:HD2   | 1:24:A:PRO:HD2  | 8        | 0.93          |
| (1,176) | 1:11:A:TRP:HB2  | 1:11:A:TRP:HZ3  | 4        | 0.93          |
| (1,176) | 1:11:A:TRP:HB2  | 1:11:A:TRP:HZ3  | 8        | 0.93          |
| (1,176) | 1:11:A:TRP:HB2  | 1:11:A:TRP:HZ3  | 10       | 0.93          |
| (1,709) | 1:12:A:LEU:HD11 | 1:23:A:PRO:HB2  | 7        | 0.92          |
| (1,709) | 1:12:A:LEU:HD12 | 1:23:A:PRO:HB2  | 7        | 0.92          |
| (1,709) | 1:12:A:LEU:HD13 | 1:23:A:PRO:HB2  | 7        | 0.92          |
| (1,476) | 1:22:A:PRO:HA   | 1:22:A:PRO:HG3  | 5        | 0.92          |
| (1,461) | 1:21:A:ARG:HA   | 1:21:A:ARG:HG2  | 8        | 0.92          |
| (1,461) | 1:21:A:ARG:HA   | 1:21:A:ARG:HG3  | 8        | 0.92          |
| (1,355) | 1:6:A:ARG:HB2   | 1:6:A:ARG:HD2   | 2        | 0.92          |
| (1,212) | 1:8:A:TYR:HD1   | 1:9:A:ILE:HG21  | 3        | 0.92          |
| (1,212) | 1:8:A:TYR:HD1   | 1:9:A:ILE:HG22  | 3        | 0.92          |
| (1,212) | 1:8:A:TYR:HD1   | 1:9:A:ILE:HG23  | 3        | 0.92          |
| (1,212) | 1:8:A:TYR:HD2   | 1:9:A:ILE:HG21  | 3        | 0.92          |
| (1,212) | 1:8:A:TYR:HD2   | 1:9:A:ILE:HG22  | 3        | 0.92          |
| (1,212) | 1:8:A:TYR:HD2   | 1:9:A:ILE:HG23  | 3        | 0.92          |
| (1,176) | 1:11:A:TRP:HB2  | 1:11:A:TRP:HZ3  | 7        | 0.92          |
| (1,200) | 1:11:A:TRP:HE3  | 1:23:A:PRO:HB3  | 5        | 0.91          |
| (1,176) | 1:11:A:TRP:HB2  | 1:11:A:TRP:HZ3  | 3        | 0.91          |
| (1,176) | 1:11:A:TRP:HB2  | 1:11:A:TRP:HZ3  | 9        | 0.91          |
| (1,732) | 1:2:A:GLU:HG3   | 1:6:A:ARG:HB3   | 9        | 0.9           |
| (1,709) | 1:12:A:LEU:HD11 | 1:23:A:PRO:HB2  | 4        | 0.9           |
| (1,709) | 1:12:A:LEU:HD12 | 1:23:A:PRO:HB2  | 4        | 0.9           |
| (1,709) | 1:12:A:LEU:HD13 | 1:23:A:PRO:HB2  | 4        | 0.9           |
| (1,649) | 1:15:A:GLY:HA2  | 1:19:A:SER:HB3  | 6        | 0.9           |
| (1,571) | 1:14:A:ASP:HB3  | 1:19:A:SER:HB2  | 6        | 0.9           |
| (1,557) | 1:9:A:ILE:HA    | 1:12:A:LEU:HG   | 5        | 0.9           |
| (1,557) | 1:9:A:ILE:HA    | 1:12:A:LEU:HG   | 6        | 0.9           |
| (1,548) | 1:13:A:LYS:HE2  | 1:13:A:LYS:HG2  | 5        | 0.9           |
| (1,548) | 1:13:A:LYS:HE2  | 1:13:A:LYS:HG3  | 5        | 0.9           |
| (1,548) | 1:13:A:LYS:HE3  | 1:13:A:LYS:HG2  | 5        | 0.9           |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,548) | 1:13:A:LYS:HE3  | 1:13:A:LYS:HG3  | 5        | 0.9           |
| (1,476) | 1:22:A:PRO:HA   | 1:22:A:PRO:HG3  | 6        | 0.9           |
| (1,355) | 1:6:A:ARG:HB2   | 1:6:A:ARG:HD2   | 1        | 0.9           |
| (1,236) | 1:11:A:TRP:HH2  | 1:22:A:PRO:HB2  | 4        | 0.9           |
| (1,189) | 1:8:A:TYR:HD1   | 1:24:A:PRO:HD2  | 5        | 0.9           |
| (1,189) | 1:8:A:TYR:HD2   | 1:24:A:PRO:HD2  | 5        | 0.9           |
| (1,543) | 1:2:A:GLU:HG2   | 1:9:A:ILE:HD11  | 9        | 0.89          |
| (1,543) | 1:2:A:GLU:HG2   | 1:9:A:ILE:HD12  | 9        | 0.89          |
| (1,543) | 1:2:A:GLU:HG2   | 1:9:A:ILE:HD13  | 9        | 0.89          |
| (1,476) | 1:22:A:PRO:HA   | 1:22:A:PRO:HG3  | 1        | 0.89          |
| (1,732) | 1:2:A:GLU:HG3   | 1:6:A:ARG:HB3   | 7        | 0.88          |
| (1,721) | 1:9:A:ILE:HG13  | 1:12:A:LEU:HB2  | 3        | 0.88          |
| (1,702) | 1:9:A:ILE:HG13  | 1:12:A:LEU:HD21 | 3        | 0.88          |
| (1,702) | 1:9:A:ILE:HG13  | 1:12:A:LEU:HD22 | 3        | 0.88          |
| (1,702) | 1:9:A:ILE:HG13  | 1:12:A:LEU:HD23 | 3        | 0.88          |
| (1,649) | 1:15:A:GLY:HA2  | 1:19:A:SER:HB3  | 5        | 0.88          |
| (1,602) | 1:8:A:TYR:H     | 1:10:A:GLN:H    | 3        | 0.88          |
| (1,557) | 1:9:A:ILE:HA    | 1:12:A:LEU:HG   | 1        | 0.88          |
| (1,441) | 1:17:A:PRO:HB2  | 1:17:A:PRO:HD2  | 1        | 0.88          |
| (1,441) | 1:17:A:PRO:HB2  | 1:17:A:PRO:HD2  | 10       | 0.88          |
| (1,222) | 1:8:A:TYR:HD1   | 1:23:A:PRO:HB2  | 1        | 0.88          |
| (1,222) | 1:8:A:TYR:HD2   | 1:23:A:PRO:HB2  | 1        | 0.88          |
| (1,198) | 1:11:A:TRP:HZ3  | 1:23:A:PRO:HB3  | 1        | 0.88          |
| (1,198) | 1:11:A:TRP:HZ3  | 1:23:A:PRO:HB3  | 6        | 0.88          |
| (1,625) | 1:10:A:GLN:HE21 | 1:14:A:ASP:HB3  | 2        | 0.87          |
| (1,571) | 1:14:A:ASP:HB3  | 1:19:A:SER:HB2  | 1        | 0.87          |
| (1,517) | 1:23:A:PRO:HB3  | 1:23:A:PRO:HG3  | 4        | 0.87          |
| (1,517) | 1:23:A:PRO:HB3  | 1:23:A:PRO:HG3  | 7        | 0.87          |
| (1,441) | 1:17:A:PRO:HB2  | 1:17:A:PRO:HD2  | 3        | 0.87          |
| (1,200) | 1:11:A:TRP:HE3  | 1:23:A:PRO:HB3  | 1        | 0.87          |
| (1,594) | 1:9:A:ILE:HG21  | 1:13:A:LYS:HE2  | 1        | 0.86          |
| (1,594) | 1:9:A:ILE:HG22  | 1:13:A:LYS:HE2  | 1        | 0.86          |
| (1,594) | 1:9:A:ILE:HG23  | 1:13:A:LYS:HE2  | 1        | 0.86          |
| (1,594) | 1:9:A:ILE:HG21  | 1:13:A:LYS:HE3  | 1        | 0.86          |
| (1,594) | 1:9:A:ILE:HG22  | 1:13:A:LYS:HE3  | 1        | 0.86          |
| (1,594) | 1:9:A:ILE:HG23  | 1:13:A:LYS:HE3  | 1        | 0.86          |
| (1,557) | 1:9:A:ILE:HA    | 1:12:A:LEU:HG   | 2        | 0.86          |
| (1,441) | 1:17:A:PRO:HB2  | 1:17:A:PRO:HD2  | 6        | 0.86          |
| (1,441) | 1:17:A:PRO:HB2  | 1:17:A:PRO:HD2  | 8        | 0.86          |
| (1,355) | 1:6:A:ARG:HB2   | 1:6:A:ARG:HD2   | 10       | 0.86          |
| (1,346) | 1:6:A:ARG:HA    | 1:6:A:ARG:HD3   | 9        | 0.86          |
| (1,649) | 1:15:A:GLY:HA2  | 1:19:A:SER:HB3  | 1        | 0.85          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,639) | 1:10:A:GLN:HE22 | 1:14:A:ASP:HB3  | 3        | 0.85          |
| (1,553) | 1:11:A:TRP:HB2  | 1:24:A:PRO:HD3  | 10       | 0.85          |
| (1,441) | 1:17:A:PRO:HB2  | 1:17:A:PRO:HD2  | 2        | 0.85          |
| (1,299) | 1:8:A:TYR:H     | 1:9:A:ILE:HB    | 5        | 0.85          |
| (1,222) | 1:8:A:TYR:HD1   | 1:23:A:PRO:HB2  | 6        | 0.85          |
| (1,222) | 1:8:A:TYR:HD2   | 1:23:A:PRO:HB2  | 6        | 0.85          |
| (1,176) | 1:11:A:TRP:HB2  | 1:11:A:TRP:HZ3  | 5        | 0.85          |
| (1,129) | 1:10:A:GLN:HA   | 1:10:A:GLN:HE21 | 3        | 0.85          |
| (1,68)  | 1:18:A:SER:H    | 1:18:A:SER:HB3  | 2        | 0.85          |
| (1,716) | 1:9:A:ILE:HG12  | 1:12:A:LEU:HD11 | 3        | 0.84          |
| (1,716) | 1:9:A:ILE:HG12  | 1:12:A:LEU:HD12 | 3        | 0.84          |
| (1,716) | 1:9:A:ILE:HG12  | 1:12:A:LEU:HD13 | 3        | 0.84          |
| (1,672) | 1:9:A:ILE:HA    | 1:12:A:LEU:HD21 | 1        | 0.84          |
| (1,672) | 1:9:A:ILE:HA    | 1:12:A:LEU:HD22 | 1        | 0.84          |
| (1,672) | 1:9:A:ILE:HA    | 1:12:A:LEU:HD23 | 1        | 0.84          |
| (1,605) | 1:8:A:TYR:HE1   | 1:11:A:TRP:HZ3  | 3        | 0.84          |
| (1,605) | 1:8:A:TYR:HE2   | 1:11:A:TRP:HZ3  | 3        | 0.84          |
| (1,441) | 1:17:A:PRO:HB2  | 1:17:A:PRO:HD2  | 4        | 0.84          |
| (1,441) | 1:17:A:PRO:HB2  | 1:17:A:PRO:HD2  | 7        | 0.84          |
| (1,317) | 1:12:A:LEU:HD11 | 1:16:A:GLY:H    | 3        | 0.84          |
| (1,317) | 1:12:A:LEU:HD12 | 1:16:A:GLY:H    | 3        | 0.84          |
| (1,317) | 1:12:A:LEU:HD13 | 1:16:A:GLY:H    | 3        | 0.84          |
| (1,236) | 1:11:A:TRP:HH2  | 1:22:A:PRO:HB2  | 7        | 0.84          |
| (1,200) | 1:11:A:TRP:HE3  | 1:23:A:PRO:HB3  | 6        | 0.84          |
| (1,176) | 1:11:A:TRP:HB2  | 1:11:A:TRP:HZ3  | 1        | 0.84          |
| (1,176) | 1:11:A:TRP:HB2  | 1:11:A:TRP:HZ3  | 2        | 0.84          |
| (1,176) | 1:11:A:TRP:HB2  | 1:11:A:TRP:HZ3  | 6        | 0.84          |
| (1,672) | 1:9:A:ILE:HA    | 1:12:A:LEU:HD21 | 2        | 0.83          |
| (1,672) | 1:9:A:ILE:HA    | 1:12:A:LEU:HD22 | 2        | 0.83          |
| (1,672) | 1:9:A:ILE:HA    | 1:12:A:LEU:HD23 | 2        | 0.83          |
| (1,672) | 1:9:A:ILE:HA    | 1:12:A:LEU:HD21 | 5        | 0.83          |
| (1,672) | 1:9:A:ILE:HA    | 1:12:A:LEU:HD22 | 5        | 0.83          |
| (1,672) | 1:9:A:ILE:HA    | 1:12:A:LEU:HD23 | 5        | 0.83          |
| (1,672) | 1:9:A:ILE:HA    | 1:12:A:LEU:HD21 | 6        | 0.83          |
| (1,672) | 1:9:A:ILE:HA    | 1:12:A:LEU:HD22 | 6        | 0.83          |
| (1,672) | 1:9:A:ILE:HA    | 1:12:A:LEU:HD23 | 6        | 0.83          |
| (1,649) | 1:15:A:GLY:HA2  | 1:19:A:SER:HB3  | 9        | 0.83          |
| (1,649) | 1:15:A:GLY:HA2  | 1:19:A:SER:HB3  | 10       | 0.83          |
| (1,644) | 1:22:A:PRO:HA   | 1:23:A:PRO:HD2  | 8        | 0.83          |
| (1,644) | 1:22:A:PRO:HA   | 1:23:A:PRO:HD2  | 9        | 0.83          |
| (1,644) | 1:22:A:PRO:HA   | 1:23:A:PRO:HD2  | 10       | 0.83          |
| (1,441) | 1:17:A:PRO:HB2  | 1:17:A:PRO:HD2  | 5        | 0.83          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,299) | 1:8:A:TYR:H    | 1:9:A:ILE:HB    | 1        | 0.83          |
| (1,198) | 1:11:A:TRP:HZ3 | 1:23:A:PRO:HB3  | 5        | 0.83          |
| (1,160) | 1:11:A:TRP:HZ2 | 1:22:A:PRO:HA   | 5        | 0.83          |
| (1,121) | 1:2:A:GLU:HB2  | 1:5:A:VAL:H     | 5        | 0.83          |
| (1,22)  | 1:13:A:LYS:H   | 1:13:A:LYS:HG2  | 9        | 0.83          |
| (1,22)  | 1:13:A:LYS:H   | 1:13:A:LYS:HG3  | 9        | 0.83          |
| (1,649) | 1:15:A:GLY:HA2 | 1:19:A:SER:HB3  | 8        | 0.82          |
| (1,299) | 1:8:A:TYR:H    | 1:9:A:ILE:HB    | 2        | 0.82          |
| (1,160) | 1:11:A:TRP:HZ2 | 1:22:A:PRO:HA   | 1        | 0.82          |
| (1,129) | 1:10:A:GLN:HA  | 1:10:A:GLN:HE21 | 8        | 0.82          |
| (1,121) | 1:2:A:GLU:HB2  | 1:5:A:VAL:H     | 7        | 0.82          |
| (1,553) | 1:11:A:TRP:HB2 | 1:24:A:PRO:HD3  | 8        | 0.81          |
| (1,468) | 1:21:A:ARG:HD3 | 1:21:A:ARG:HG2  | 2        | 0.81          |
| (1,468) | 1:21:A:ARG:HD3 | 1:21:A:ARG:HG3  | 2        | 0.81          |
| (1,468) | 1:21:A:ARG:HD3 | 1:21:A:ARG:HG2  | 3        | 0.81          |
| (1,468) | 1:21:A:ARG:HD3 | 1:21:A:ARG:HG3  | 3        | 0.81          |
| (1,441) | 1:17:A:PRO:HB2 | 1:17:A:PRO:HD2  | 9        | 0.81          |
| (1,299) | 1:8:A:TYR:H    | 1:9:A:ILE:HB    | 6        | 0.81          |
| (1,160) | 1:11:A:TRP:HZ2 | 1:22:A:PRO:HA   | 6        | 0.81          |
| (1,109) | 1:9:A:ILE:HB   | 1:11:A:TRP:H    | 3        | 0.81          |
| (1,701) | 1:5:A:VAL:HG11 | 1:9:A:ILE:HG13  | 10       | 0.8           |
| (1,701) | 1:5:A:VAL:HG12 | 1:9:A:ILE:HG13  | 10       | 0.8           |
| (1,701) | 1:5:A:VAL:HG13 | 1:9:A:ILE:HG13  | 10       | 0.8           |
| (1,644) | 1:22:A:PRO:HA  | 1:23:A:PRO:HD2  | 2        | 0.8           |
| (1,644) | 1:22:A:PRO:HA  | 1:23:A:PRO:HD2  | 3        | 0.8           |
| (1,593) | 1:11:A:TRP:HA  | 1:14:A:ASP:HB3  | 7        | 0.8           |
| (1,593) | 1:11:A:TRP:HA  | 1:14:A:ASP:HB3  | 10       | 0.8           |
| (1,355) | 1:6:A:ARG:HB2  | 1:6:A:ARG:HD2   | 4        | 0.8           |
| (1,355) | 1:6:A:ARG:HB2  | 1:6:A:ARG:HD2   | 5        | 0.8           |
| (1,296) | 1:11:A:TRP:HE1 | 1:21:A:ARG:HB3  | 2        | 0.8           |
| (1,597) | 1:1:A:GLU:HA   | 1:1:A:GLU:HB2   | 2        | 0.79          |
| (1,597) | 1:1:A:GLU:HA   | 1:1:A:GLU:HB2   | 9        | 0.79          |
| (1,571) | 1:14:A:ASP:HB3 | 1:19:A:SER:HB2  | 2        | 0.79          |
| (1,553) | 1:11:A:TRP:HB2 | 1:24:A:PRO:HD3  | 9        | 0.79          |
| (1,517) | 1:23:A:PRO:HB3 | 1:23:A:PRO:HG3  | 5        | 0.79          |
| (1,355) | 1:6:A:ARG:HB2  | 1:6:A:ARG:HD2   | 7        | 0.79          |
| (1,198) | 1:11:A:TRP:HZ3 | 1:23:A:PRO:HB3  | 2        | 0.79          |
| (1,517) | 1:23:A:PRO:HB3 | 1:23:A:PRO:HG3  | 1        | 0.78          |
| (1,517) | 1:23:A:PRO:HB3 | 1:23:A:PRO:HG3  | 6        | 0.78          |
| (1,517) | 1:23:A:PRO:HB3 | 1:23:A:PRO:HG3  | 8        | 0.78          |
| (1,517) | 1:23:A:PRO:HB3 | 1:23:A:PRO:HG3  | 9        | 0.78          |
| (1,355) | 1:6:A:ARG:HB2  | 1:6:A:ARG:HD2   | 3        | 0.78          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,222) | 1:8:A:TYR:HD1  | 1:23:A:PRO:HB2  | 2        | 0.78          |
| (1,222) | 1:8:A:TYR:HD2  | 1:23:A:PRO:HB2  | 2        | 0.78          |
| (1,517) | 1:23:A:PRO:HB3 | 1:23:A:PRO:HG3  | 2        | 0.77          |
| (1,517) | 1:23:A:PRO:HB3 | 1:23:A:PRO:HG3  | 3        | 0.77          |
| (1,517) | 1:23:A:PRO:HB3 | 1:23:A:PRO:HG3  | 10       | 0.77          |
| (1,200) | 1:11:A:TRP:HE3 | 1:23:A:PRO:HB3  | 2        | 0.77          |
| (1,198) | 1:11:A:TRP:HZ3 | 1:23:A:PRO:HB3  | 3        | 0.77          |
| (1,67)  | 1:18:A:SER:H   | 1:18:A:SER:HB2  | 4        | 0.77          |
| (1,22)  | 1:13:A:LYS:H   | 1:13:A:LYS:HG2  | 4        | 0.77          |
| (1,22)  | 1:13:A:LYS:H   | 1:13:A:LYS:HG3  | 4        | 0.77          |
| (1,722) | 1:9:A:ILE:HG12 | 1:12:A:LEU:HB3  | 2        | 0.76          |
| (1,722) | 1:9:A:ILE:HG12 | 1:12:A:LEU:HB3  | 4        | 0.76          |
| (1,722) | 1:9:A:ILE:HG12 | 1:12:A:LEU:HB3  | 9        | 0.76          |
| (1,701) | 1:5:A:VAL:HG11 | 1:9:A:ILE:HG13  | 8        | 0.76          |
| (1,701) | 1:5:A:VAL:HG12 | 1:9:A:ILE:HG13  | 8        | 0.76          |
| (1,701) | 1:5:A:VAL:HG13 | 1:9:A:ILE:HG13  | 8        | 0.76          |
| (1,663) | 1:10:A:GLN:HA  | 1:13:A:LYS:HB2  | 6        | 0.76          |
| (1,663) | 1:10:A:GLN:HA  | 1:13:A:LYS:HB3  | 6        | 0.76          |
| (1,649) | 1:15:A:GLY:HA2 | 1:19:A:SER:HB3  | 4        | 0.76          |
| (1,649) | 1:15:A:GLY:HA2 | 1:19:A:SER:HB3  | 7        | 0.76          |
| (1,553) | 1:11:A:TRP:HB2 | 1:24:A:PRO:HD3  | 7        | 0.76          |
| (1,543) | 1:2:A:GLU:HG2  | 1:9:A:ILE:HD11  | 7        | 0.76          |
| (1,543) | 1:2:A:GLU:HG2  | 1:9:A:ILE:HD12  | 7        | 0.76          |
| (1,543) | 1:2:A:GLU:HG2  | 1:9:A:ILE:HD13  | 7        | 0.76          |
| (1,355) | 1:6:A:ARG:HB2  | 1:6:A:ARG:HD2   | 6        | 0.76          |
| (1,248) | 1:8:A:TYR:HD1  | 1:23:A:PRO:HA   | 3        | 0.76          |
| (1,248) | 1:8:A:TYR:HD2  | 1:23:A:PRO:HA   | 3        | 0.76          |
| (1,705) | 1:9:A:ILE:HG21 | 1:13:A:LYS:HD2  | 3        | 0.75          |
| (1,705) | 1:9:A:ILE:HG22 | 1:13:A:LYS:HD2  | 3        | 0.75          |
| (1,705) | 1:9:A:ILE:HG23 | 1:13:A:LYS:HD2  | 3        | 0.75          |
| (1,701) | 1:5:A:VAL:HG11 | 1:9:A:ILE:HG13  | 4        | 0.75          |
| (1,701) | 1:5:A:VAL:HG12 | 1:9:A:ILE:HG13  | 4        | 0.75          |
| (1,701) | 1:5:A:VAL:HG13 | 1:9:A:ILE:HG13  | 4        | 0.75          |
| (1,663) | 1:10:A:GLN:HA  | 1:13:A:LYS:HB2  | 4        | 0.75          |
| (1,663) | 1:10:A:GLN:HA  | 1:13:A:LYS:HB3  | 4        | 0.75          |
| (1,663) | 1:10:A:GLN:HA  | 1:13:A:LYS:HB2  | 8        | 0.75          |
| (1,663) | 1:10:A:GLN:HA  | 1:13:A:LYS:HB3  | 8        | 0.75          |
| (1,626) | 1:14:A:ASP:HB3 | 1:15:A:GLY:H    | 3        | 0.75          |
| (1,597) | 1:1:A:GLU:HA   | 1:1:A:GLU:HB2   | 10       | 0.75          |
| (1,593) | 1:11:A:TRP:HA  | 1:14:A:ASP:HB3  | 8        | 0.75          |
| (1,476) | 1:22:A:PRO:HA  | 1:22:A:PRO:HG3  | 10       | 0.75          |
| (1,407) | 1:12:A:LEU:HA  | 1:12:A:LEU:HD21 | 5        | 0.75          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,407) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD22 | 5        | 0.75          |
| (1,407) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD23 | 5        | 0.75          |
| (1,407) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD21 | 6        | 0.75          |
| (1,407) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD22 | 6        | 0.75          |
| (1,407) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD23 | 6        | 0.75          |
| (1,129) | 1:10:A:GLN:HA   | 1:10:A:GLN:HE21 | 10       | 0.75          |
| (1,26)  | 1:2:A:GLU:HB2   | 1:3:A:GLU:H     | 2        | 0.75          |
| (1,722) | 1:9:A:ILE:HG12  | 1:12:A:LEU:HB3  | 1        | 0.74          |
| (1,722) | 1:9:A:ILE:HG12  | 1:12:A:LEU:HB3  | 8        | 0.74          |
| (1,722) | 1:9:A:ILE:HG12  | 1:12:A:LEU:HB3  | 10       | 0.74          |
| (1,709) | 1:12:A:LEU:HD11 | 1:23:A:PRO:HB2  | 8        | 0.74          |
| (1,709) | 1:12:A:LEU:HD12 | 1:23:A:PRO:HB2  | 8        | 0.74          |
| (1,709) | 1:12:A:LEU:HD13 | 1:23:A:PRO:HB2  | 8        | 0.74          |
| (1,701) | 1:5:A:VAL:HG11  | 1:9:A:ILE:HG13  | 6        | 0.74          |
| (1,701) | 1:5:A:VAL:HG12  | 1:9:A:ILE:HG13  | 6        | 0.74          |
| (1,701) | 1:5:A:VAL:HG13  | 1:9:A:ILE:HG13  | 6        | 0.74          |
| (1,618) | 1:10:A:GLN:HE21 | 1:13:A:LYS:HD3  | 1        | 0.74          |
| (1,598) | 1:1:A:GLU:HA    | 1:1:A:GLU:HB3   | 1        | 0.74          |
| (1,574) | 1:5:A:VAL:HA    | 1:8:A:TYR:HB2   | 3        | 0.74          |
| (1,574) | 1:5:A:VAL:HA    | 1:8:A:TYR:HB3   | 3        | 0.74          |
| (1,315) | 1:10:A:GLN:HE22 | 1:13:A:LYS:HE2  | 4        | 0.74          |
| (1,315) | 1:10:A:GLN:HE22 | 1:13:A:LYS:HE3  | 4        | 0.74          |
| (1,172) | 1:11:A:TRP:HZ2  | 1:23:A:PRO:HD3  | 9        | 0.74          |
| (1,121) | 1:2:A:GLU:HB2   | 1:5:A:VAL:H     | 4        | 0.74          |
| (1,598) | 1:1:A:GLU:HA    | 1:1:A:GLU:HB3   | 10       | 0.73          |
| (1,597) | 1:1:A:GLU:HA    | 1:1:A:GLU:HB2   | 7        | 0.73          |
| (1,527) | 1:24:A:PRO:HB2  | 1:24:A:PRO:HD2  | 3        | 0.73          |
| (1,427) | 1:13:A:LYS:HB2  | 1:13:A:LYS:HG2  | 2        | 0.73          |
| (1,427) | 1:13:A:LYS:HB2  | 1:13:A:LYS:HG3  | 2        | 0.73          |
| (1,427) | 1:13:A:LYS:HB3  | 1:13:A:LYS:HG2  | 2        | 0.73          |
| (1,427) | 1:13:A:LYS:HB3  | 1:13:A:LYS:HG3  | 2        | 0.73          |
| (1,427) | 1:13:A:LYS:HB2  | 1:13:A:LYS:HG2  | 3        | 0.73          |
| (1,427) | 1:13:A:LYS:HB2  | 1:13:A:LYS:HG3  | 3        | 0.73          |
| (1,427) | 1:13:A:LYS:HB3  | 1:13:A:LYS:HG2  | 3        | 0.73          |
| (1,427) | 1:13:A:LYS:HB3  | 1:13:A:LYS:HG3  | 3        | 0.73          |
| (1,427) | 1:13:A:LYS:HB2  | 1:13:A:LYS:HG2  | 4        | 0.73          |
| (1,427) | 1:13:A:LYS:HB2  | 1:13:A:LYS:HG3  | 4        | 0.73          |
| (1,427) | 1:13:A:LYS:HB3  | 1:13:A:LYS:HG2  | 4        | 0.73          |
| (1,427) | 1:13:A:LYS:HB3  | 1:13:A:LYS:HG3  | 4        | 0.73          |
| (1,427) | 1:13:A:LYS:HB2  | 1:13:A:LYS:HG2  | 6        | 0.73          |
| (1,427) | 1:13:A:LYS:HB2  | 1:13:A:LYS:HG3  | 6        | 0.73          |
| (1,427) | 1:13:A:LYS:HB3  | 1:13:A:LYS:HG2  | 6        | 0.73          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,427) | 1:13:A:LYS:HB3  | 1:13:A:LYS:HG3  | 6        | 0.73          |
| (1,427) | 1:13:A:LYS:HB2  | 1:13:A:LYS:HG2  | 8        | 0.73          |
| (1,427) | 1:13:A:LYS:HB2  | 1:13:A:LYS:HG3  | 8        | 0.73          |
| (1,427) | 1:13:A:LYS:HB3  | 1:13:A:LYS:HG2  | 8        | 0.73          |
| (1,427) | 1:13:A:LYS:HB3  | 1:13:A:LYS:HG3  | 8        | 0.73          |
| (1,427) | 1:13:A:LYS:HB2  | 1:13:A:LYS:HG2  | 9        | 0.73          |
| (1,427) | 1:13:A:LYS:HB2  | 1:13:A:LYS:HG3  | 9        | 0.73          |
| (1,427) | 1:13:A:LYS:HB3  | 1:13:A:LYS:HG2  | 9        | 0.73          |
| (1,427) | 1:13:A:LYS:HB3  | 1:13:A:LYS:HG3  | 9        | 0.73          |
| (1,427) | 1:13:A:LYS:HB2  | 1:13:A:LYS:HG2  | 10       | 0.73          |
| (1,427) | 1:13:A:LYS:HB2  | 1:13:A:LYS:HG3  | 10       | 0.73          |
| (1,427) | 1:13:A:LYS:HB3  | 1:13:A:LYS:HG2  | 10       | 0.73          |
| (1,427) | 1:13:A:LYS:HB3  | 1:13:A:LYS:HG3  | 10       | 0.73          |
| (1,407) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD21 | 1        | 0.73          |
| (1,407) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD22 | 1        | 0.73          |
| (1,407) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD23 | 1        | 0.73          |
| (1,322) | 1:11:A:TRP:HB3  | 1:11:A:TRP:HE3  | 2        | 0.73          |
| (1,322) | 1:11:A:TRP:HB3  | 1:11:A:TRP:HE3  | 5        | 0.73          |
| (1,322) | 1:11:A:TRP:HB3  | 1:11:A:TRP:HE3  | 6        | 0.73          |
| (1,315) | 1:10:A:GLN:HE22 | 1:13:A:LYS:HE2  | 10       | 0.73          |
| (1,315) | 1:10:A:GLN:HE22 | 1:13:A:LYS:HE3  | 10       | 0.73          |
| (1,68)  | 1:18:A:SER:H    | 1:18:A:SER:HB3  | 6        | 0.73          |
| (1,22)  | 1:13:A:LYS:H    | 1:13:A:LYS:HG2  | 7        | 0.73          |
| (1,22)  | 1:13:A:LYS:H    | 1:13:A:LYS:HG3  | 7        | 0.73          |
| (1,711) | 1:12:A:LEU:HD21 | 1:23:A:PRO:HB2  | 7        | 0.72          |
| (1,711) | 1:12:A:LEU:HD22 | 1:23:A:PRO:HB2  | 7        | 0.72          |
| (1,711) | 1:12:A:LEU:HD23 | 1:23:A:PRO:HB2  | 7        | 0.72          |
| (1,701) | 1:5:A:VAL:HG11  | 1:9:A:ILE:HG13  | 7        | 0.72          |
| (1,701) | 1:5:A:VAL:HG12  | 1:9:A:ILE:HG13  | 7        | 0.72          |
| (1,701) | 1:5:A:VAL:HG13  | 1:9:A:ILE:HG13  | 7        | 0.72          |
| (1,672) | 1:9:A:ILE:HA    | 1:12:A:LEU:HD21 | 7        | 0.72          |
| (1,672) | 1:9:A:ILE:HA    | 1:12:A:LEU:HD22 | 7        | 0.72          |
| (1,672) | 1:9:A:ILE:HA    | 1:12:A:LEU:HD23 | 7        | 0.72          |
| (1,666) | 1:24:A:PRO:HG2  | 1:25:A:CYS:HB2  | 7        | 0.72          |
| (1,663) | 1:10:A:GLN:HA   | 1:13:A:LYS:HB2  | 10       | 0.72          |
| (1,663) | 1:10:A:GLN:HA   | 1:13:A:LYS:HB3  | 10       | 0.72          |
| (1,644) | 1:22:A:PRO:HA   | 1:23:A:PRO:HD2  | 5        | 0.72          |
| (1,618) | 1:10:A:GLN:HE21 | 1:13:A:LYS:HD3  | 7        | 0.72          |
| (1,553) | 1:11:A:TRP:HB2  | 1:24:A:PRO:HD3  | 4        | 0.72          |
| (1,535) | 1:23:A:PRO:HB3  | 1:24:A:PRO:HD2  | 7        | 0.72          |
| (1,476) | 1:22:A:PRO:HA   | 1:22:A:PRO:HG3  | 8        | 0.72          |
| (1,427) | 1:13:A:LYS:HB2  | 1:13:A:LYS:HG2  | 1        | 0.72          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,427) | 1:13:A:LYS:HB2  | 1:13:A:LYS:HG3  | 1        | 0.72          |
| (1,427) | 1:13:A:LYS:HB3  | 1:13:A:LYS:HG2  | 1        | 0.72          |
| (1,427) | 1:13:A:LYS:HB3  | 1:13:A:LYS:HG3  | 1        | 0.72          |
| (1,427) | 1:13:A:LYS:HB2  | 1:13:A:LYS:HG2  | 5        | 0.72          |
| (1,427) | 1:13:A:LYS:HB2  | 1:13:A:LYS:HG3  | 5        | 0.72          |
| (1,427) | 1:13:A:LYS:HB3  | 1:13:A:LYS:HG2  | 5        | 0.72          |
| (1,427) | 1:13:A:LYS:HB3  | 1:13:A:LYS:HG3  | 5        | 0.72          |
| (1,427) | 1:13:A:LYS:HB2  | 1:13:A:LYS:HG2  | 7        | 0.72          |
| (1,427) | 1:13:A:LYS:HB2  | 1:13:A:LYS:HG3  | 7        | 0.72          |
| (1,427) | 1:13:A:LYS:HB3  | 1:13:A:LYS:HG2  | 7        | 0.72          |
| (1,427) | 1:13:A:LYS:HB3  | 1:13:A:LYS:HG3  | 7        | 0.72          |
| (1,407) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD21 | 2        | 0.72          |
| (1,407) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD22 | 2        | 0.72          |
| (1,407) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD23 | 2        | 0.72          |
| (1,322) | 1:11:A:TRP:HB3  | 1:11:A:TRP:HE3  | 1        | 0.72          |
| (1,322) | 1:11:A:TRP:HB3  | 1:11:A:TRP:HE3  | 7        | 0.72          |
| (1,322) | 1:11:A:TRP:HB3  | 1:11:A:TRP:HE3  | 9        | 0.72          |
| (1,322) | 1:11:A:TRP:HB3  | 1:11:A:TRP:HE3  | 10       | 0.72          |
| (1,231) | 1:11:A:TRP:HD1  | 1:21:A:ARG:HB3  | 3        | 0.72          |
| (1,121) | 1:2:A:GLU:HB2   | 1:5:A:VAL:H     | 6        | 0.72          |
| (1,22)  | 1:13:A:LYS:H    | 1:13:A:LYS:HG2  | 5        | 0.72          |
| (1,22)  | 1:13:A:LYS:H    | 1:13:A:LYS:HG3  | 5        | 0.72          |
| (1,722) | 1:9:A:ILE:HG12  | 1:12:A:LEU:HB3  | 7        | 0.71          |
| (1,709) | 1:12:A:LEU:HD11 | 1:23:A:PRO:HB2  | 10       | 0.71          |
| (1,709) | 1:12:A:LEU:HD12 | 1:23:A:PRO:HB2  | 10       | 0.71          |
| (1,709) | 1:12:A:LEU:HD13 | 1:23:A:PRO:HB2  | 10       | 0.71          |
| (1,672) | 1:9:A:ILE:HA    | 1:12:A:LEU:HD21 | 8        | 0.71          |
| (1,672) | 1:9:A:ILE:HA    | 1:12:A:LEU:HD22 | 8        | 0.71          |
| (1,672) | 1:9:A:ILE:HA    | 1:12:A:LEU:HD23 | 8        | 0.71          |
| (1,672) | 1:9:A:ILE:HA    | 1:12:A:LEU:HD21 | 9        | 0.71          |
| (1,672) | 1:9:A:ILE:HA    | 1:12:A:LEU:HD22 | 9        | 0.71          |
| (1,672) | 1:9:A:ILE:HA    | 1:12:A:LEU:HD23 | 9        | 0.71          |
| (1,671) | 1:8:A:TYR:HA    | 1:12:A:LEU:HD21 | 6        | 0.71          |
| (1,671) | 1:8:A:TYR:HA    | 1:12:A:LEU:HD22 | 6        | 0.71          |
| (1,671) | 1:8:A:TYR:HA    | 1:12:A:LEU:HD23 | 6        | 0.71          |
| (1,663) | 1:10:A:GLN:HA   | 1:13:A:LYS:HB2  | 7        | 0.71          |
| (1,663) | 1:10:A:GLN:HA   | 1:13:A:LYS:HB3  | 7        | 0.71          |
| (1,663) | 1:10:A:GLN:HA   | 1:13:A:LYS:HB2  | 9        | 0.71          |
| (1,663) | 1:10:A:GLN:HA   | 1:13:A:LYS:HB3  | 9        | 0.71          |
| (1,608) | 1:8:A:TYR:HE1   | 1:11:A:TRP:HE3  | 3        | 0.71          |
| (1,608) | 1:8:A:TYR:HE2   | 1:11:A:TRP:HE3  | 3        | 0.71          |
| (1,476) | 1:22:A:PRO:HA   | 1:22:A:PRO:HG3  | 3        | 0.71          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,349) | 1:6:A:ARG:HA    | 1:6:A:ARG:HG2   | 9        | 0.71          |
| (1,322) | 1:11:A:TRP:HB3  | 1:11:A:TRP:HE3  | 3        | 0.71          |
| (1,322) | 1:11:A:TRP:HB3  | 1:11:A:TRP:HE3  | 8        | 0.71          |
| (1,282) | 1:15:A:GLY:H    | 1:16:A:GLY:H    | 3        | 0.71          |
| (1,259) | 1:4:A:CYS:HB3   | 1:5:A:VAL:H     | 4        | 0.71          |
| (1,201) | 1:8:A:TYR:HE1   | 1:23:A:PRO:HB3  | 1        | 0.71          |
| (1,201) | 1:8:A:TYR:HE2   | 1:23:A:PRO:HB3  | 1        | 0.71          |
| (1,22)  | 1:13:A:LYS:H    | 1:13:A:LYS:HG2  | 8        | 0.71          |
| (1,22)  | 1:13:A:LYS:H    | 1:13:A:LYS:HG3  | 8        | 0.71          |
| (1,672) | 1:9:A:ILE:HA    | 1:12:A:LEU:HD21 | 10       | 0.7           |
| (1,672) | 1:9:A:ILE:HA    | 1:12:A:LEU:HD22 | 10       | 0.7           |
| (1,672) | 1:9:A:ILE:HA    | 1:12:A:LEU:HD23 | 10       | 0.7           |
| (1,671) | 1:8:A:TYR:HA    | 1:12:A:LEU:HD21 | 5        | 0.7           |
| (1,671) | 1:8:A:TYR:HA    | 1:12:A:LEU:HD22 | 5        | 0.7           |
| (1,671) | 1:8:A:TYR:HA    | 1:12:A:LEU:HD23 | 5        | 0.7           |
| (1,616) | 1:14:A:ASP:HB3  | 1:16:A:GLY:H    | 6        | 0.7           |
| (1,463) | 1:21:A:ARG:HB3  | 1:21:A:ARG:HD3  | 8        | 0.7           |
| (1,401) | 1:11:A:TRP:HA   | 1:11:A:TRP:HB2  | 8        | 0.7           |
| (1,401) | 1:11:A:TRP:HA   | 1:11:A:TRP:HB2  | 10       | 0.7           |
| (1,322) | 1:11:A:TRP:HB3  | 1:11:A:TRP:HE3  | 4        | 0.7           |
| (1,285) | 1:10:A:GLN:HG3  | 1:11:A:TRP:H    | 9        | 0.7           |
| (1,201) | 1:8:A:TYR:HE1   | 1:23:A:PRO:HB3  | 6        | 0.7           |
| (1,201) | 1:8:A:TYR:HE2   | 1:23:A:PRO:HB3  | 6        | 0.7           |
| (1,145) | 1:11:A:TRP:H    | 1:12:A:LEU:HA   | 6        | 0.7           |
| (1,111) | 1:10:A:GLN:HB3  | 1:11:A:TRP:H    | 6        | 0.7           |
| (1,22)  | 1:13:A:LYS:H    | 1:13:A:LYS:HG2  | 10       | 0.7           |
| (1,22)  | 1:13:A:LYS:H    | 1:13:A:LYS:HG3  | 10       | 0.7           |
| (1,1)   | 1:7:A:LEU:HB2   | 1:8:A:TYR:H     | 6        | 0.7           |
| (1,722) | 1:9:A:ILE:HG12  | 1:12:A:LEU:HB3  | 5        | 0.69          |
| (1,711) | 1:12:A:LEU:HD21 | 1:23:A:PRO:HB2  | 4        | 0.69          |
| (1,711) | 1:12:A:LEU:HD22 | 1:23:A:PRO:HB2  | 4        | 0.69          |
| (1,711) | 1:12:A:LEU:HD23 | 1:23:A:PRO:HB2  | 4        | 0.69          |
| (1,701) | 1:5:A:VAL:HG11  | 1:9:A:ILE:HG13  | 9        | 0.69          |
| (1,701) | 1:5:A:VAL:HG12  | 1:9:A:ILE:HG13  | 9        | 0.69          |
| (1,701) | 1:5:A:VAL:HG13  | 1:9:A:ILE:HG13  | 9        | 0.69          |
| (1,672) | 1:9:A:ILE:HA    | 1:12:A:LEU:HD21 | 4        | 0.69          |
| (1,672) | 1:9:A:ILE:HA    | 1:12:A:LEU:HD22 | 4        | 0.69          |
| (1,672) | 1:9:A:ILE:HA    | 1:12:A:LEU:HD23 | 4        | 0.69          |
| (1,663) | 1:10:A:GLN:HA   | 1:13:A:LYS:HB2  | 5        | 0.69          |
| (1,663) | 1:10:A:GLN:HA   | 1:13:A:LYS:HB3  | 5        | 0.69          |
| (1,662) | 1:17:A:PRO:HB3  | 1:18:A:SER:HB2  | 3        | 0.69          |
| (1,644) | 1:22:A:PRO:HA   | 1:23:A:PRO:HD2  | 1        | 0.69          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,598) | 1:1:A:GLU:HA    | 1:1:A:GLU:HB3   | 8        | 0.69          |
| (1,468) | 1:21:A:ARG:HD3  | 1:21:A:ARG:HG2  | 7        | 0.69          |
| (1,468) | 1:21:A:ARG:HD3  | 1:21:A:ARG:HG3  | 7        | 0.69          |
| (1,401) | 1:11:A:TRP:HA   | 1:11:A:TRP:HB2  | 4        | 0.69          |
| (1,315) | 1:10:A:GLN:HE22 | 1:13:A:LYS:HE2  | 8        | 0.69          |
| (1,315) | 1:10:A:GLN:HE22 | 1:13:A:LYS:HE3  | 8        | 0.69          |
| (1,296) | 1:11:A:TRP:HE1  | 1:21:A:ARG:HB3  | 8        | 0.69          |
| (1,282) | 1:15:A:GLY:H    | 1:16:A:GLY:H    | 1        | 0.69          |
| (1,201) | 1:8:A:TYR:HE1   | 1:23:A:PRO:HB3  | 5        | 0.69          |
| (1,201) | 1:8:A:TYR:HE2   | 1:23:A:PRO:HB3  | 5        | 0.69          |
| (1,145) | 1:11:A:TRP:H    | 1:12:A:LEU:HA   | 1        | 0.69          |
| (1,145) | 1:11:A:TRP:H    | 1:12:A:LEU:HA   | 5        | 0.69          |
| (1,145) | 1:11:A:TRP:H    | 1:12:A:LEU:HA   | 9        | 0.69          |
| (1,26)  | 1:2:A:GLU:HB2   | 1:3:A:GLU:H     | 8        | 0.69          |
| (1,22)  | 1:13:A:LYS:H    | 1:13:A:LYS:HG2  | 6        | 0.69          |
| (1,22)  | 1:13:A:LYS:H    | 1:13:A:LYS:HG3  | 6        | 0.69          |
| (1,722) | 1:9:A:ILE:HG12  | 1:12:A:LEU:HB3  | 6        | 0.68          |
| (1,712) | 1:9:A:ILE:HG12  | 1:12:A:LEU:HD21 | 3        | 0.68          |
| (1,712) | 1:9:A:ILE:HG12  | 1:12:A:LEU:HD22 | 3        | 0.68          |
| (1,712) | 1:9:A:ILE:HG12  | 1:12:A:LEU:HD23 | 3        | 0.68          |
| (1,701) | 1:5:A:VAL:HG11  | 1:9:A:ILE:HG13  | 2        | 0.68          |
| (1,701) | 1:5:A:VAL:HG12  | 1:9:A:ILE:HG13  | 2        | 0.68          |
| (1,701) | 1:5:A:VAL:HG13  | 1:9:A:ILE:HG13  | 2        | 0.68          |
| (1,671) | 1:8:A:TYR:HA    | 1:12:A:LEU:HD21 | 1        | 0.68          |
| (1,671) | 1:8:A:TYR:HA    | 1:12:A:LEU:HD22 | 1        | 0.68          |
| (1,671) | 1:8:A:TYR:HA    | 1:12:A:LEU:HD23 | 1        | 0.68          |
| (1,662) | 1:17:A:PRO:HB3  | 1:18:A:SER:HB2  | 9        | 0.68          |
| (1,662) | 1:17:A:PRO:HB3  | 1:18:A:SER:HB2  | 10       | 0.68          |
| (1,651) | 1:3:A:GLU:HA    | 1:6:A:ARG:HD2   | 4        | 0.68          |
| (1,598) | 1:1:A:GLU:HA    | 1:1:A:GLU:HB3   | 2        | 0.68          |
| (1,596) | 1:1:A:GLU:HA    | 1:1:A:GLU:HG2   | 5        | 0.68          |
| (1,596) | 1:1:A:GLU:HA    | 1:1:A:GLU:HG3   | 5        | 0.68          |
| (1,596) | 1:1:A:GLU:HA    | 1:1:A:GLU:HG2   | 6        | 0.68          |
| (1,596) | 1:1:A:GLU:HA    | 1:1:A:GLU:HG3   | 6        | 0.68          |
| (1,476) | 1:22:A:PRO:HA   | 1:22:A:PRO:HG3  | 2        | 0.68          |
| (1,401) | 1:11:A:TRP:HA   | 1:11:A:TRP:HB2  | 7        | 0.68          |
| (1,299) | 1:8:A:TYR:H     | 1:9:A:ILE:HB    | 4        | 0.68          |
| (1,299) | 1:8:A:TYR:H     | 1:9:A:ILE:HB    | 7        | 0.68          |
| (1,282) | 1:15:A:GLY:H    | 1:16:A:GLY:H    | 8        | 0.68          |
| (1,282) | 1:15:A:GLY:H    | 1:16:A:GLY:H    | 10       | 0.68          |
| (1,270) | 1:8:A:TYR:HD1   | 1:25:A:CYS:H    | 6        | 0.68          |
| (1,270) | 1:8:A:TYR:HD2   | 1:25:A:CYS:H    | 6        | 0.68          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,268) | 1:8:A:TYR:HD1   | 1:9:A:ILE:H    | 10       | 0.68          |
| (1,268) | 1:8:A:TYR:HD2   | 1:9:A:ILE:H    | 10       | 0.68          |
| (1,172) | 1:11:A:TRP:HZ2  | 1:23:A:PRO:HD3 | 8        | 0.68          |
| (1,111) | 1:10:A:GLN:HB3  | 1:11:A:TRP:H   | 5        | 0.68          |
| (1,67)  | 1:18:A:SER:H    | 1:18:A:SER:HB2 | 3        | 0.68          |
| (1,1)   | 1:7:A:LEU:HB2   | 1:8:A:TYR:H    | 7        | 0.68          |
| (1,729) | 1:2:A:GLU:HG2   | 1:6:A:ARG:HG3  | 9        | 0.67          |
| (1,709) | 1:12:A:LEU:HD11 | 1:23:A:PRO:HB2 | 9        | 0.67          |
| (1,709) | 1:12:A:LEU:HD12 | 1:23:A:PRO:HB2 | 9        | 0.67          |
| (1,709) | 1:12:A:LEU:HD13 | 1:23:A:PRO:HB2 | 9        | 0.67          |
| (1,701) | 1:5:A:VAL:HG11  | 1:9:A:ILE:HG13 | 5        | 0.67          |
| (1,701) | 1:5:A:VAL:HG12  | 1:9:A:ILE:HG13 | 5        | 0.67          |
| (1,701) | 1:5:A:VAL:HG13  | 1:9:A:ILE:HG13 | 5        | 0.67          |
| (1,668) | 1:19:A:SER:HB2  | 1:21:A:ARG:HG2 | 9        | 0.67          |
| (1,668) | 1:19:A:SER:HB2  | 1:21:A:ARG:HG3 | 9        | 0.67          |
| (1,662) | 1:17:A:PRO:HB3  | 1:18:A:SER:HB2 | 1        | 0.67          |
| (1,651) | 1:3:A:GLU:HA    | 1:6:A:ARG:HD2  | 8        | 0.67          |
| (1,644) | 1:22:A:PRO:HA   | 1:23:A:PRO:HD2 | 6        | 0.67          |
| (1,598) | 1:1:A:GLU:HA    | 1:1:A:GLU:HB3  | 5        | 0.67          |
| (1,593) | 1:11:A:TRP:HA   | 1:14:A:ASP:HB3 | 5        | 0.67          |
| (1,468) | 1:21:A:ARG:HD3  | 1:21:A:ARG:HG2 | 4        | 0.67          |
| (1,468) | 1:21:A:ARG:HD3  | 1:21:A:ARG:HG3 | 4        | 0.67          |
| (1,401) | 1:11:A:TRP:HA   | 1:11:A:TRP:HB2 | 9        | 0.67          |
| (1,296) | 1:11:A:TRP:HE1  | 1:21:A:ARG:HB3 | 3        | 0.67          |
| (1,268) | 1:8:A:TYR:HD1   | 1:9:A:ILE:H    | 5        | 0.67          |
| (1,268) | 1:8:A:TYR:HD2   | 1:9:A:ILE:H    | 5        | 0.67          |
| (1,268) | 1:8:A:TYR:HD1   | 1:9:A:ILE:H    | 8        | 0.67          |
| (1,268) | 1:8:A:TYR:HD2   | 1:9:A:ILE:H    | 8        | 0.67          |
| (1,257) | 1:24:A:PRO:HD2  | 1:25:A:CYS:H   | 3        | 0.67          |
| (1,172) | 1:11:A:TRP:HZ2  | 1:23:A:PRO:HD3 | 10       | 0.67          |
| (1,67)  | 1:18:A:SER:H    | 1:18:A:SER:HB2 | 9        | 0.67          |
| (1,24)  | 1:13:A:LYS:H    | 1:13:A:LYS:HD3 | 8        | 0.67          |
| (1,1)   | 1:7:A:LEU:HB2   | 1:8:A:TYR:H    | 2        | 0.67          |
| (1,1)   | 1:7:A:LEU:HB2   | 1:8:A:TYR:H    | 5        | 0.67          |
| (1,732) | 1:2:A:GLU:HG3   | 1:6:A:ARG:HB3  | 5        | 0.66          |
| (1,701) | 1:5:A:VAL:HG11  | 1:9:A:ILE:HG13 | 1        | 0.66          |
| (1,701) | 1:5:A:VAL:HG12  | 1:9:A:ILE:HG13 | 1        | 0.66          |
| (1,701) | 1:5:A:VAL:HG13  | 1:9:A:ILE:HG13 | 1        | 0.66          |
| (1,662) | 1:17:A:PRO:HB3  | 1:18:A:SER:HB2 | 8        | 0.66          |
| (1,626) | 1:14:A:ASP:HB3  | 1:15:A:GLY:H   | 1        | 0.66          |
| (1,598) | 1:1:A:GLU:HA    | 1:1:A:GLU:HB3  | 3        | 0.66          |
| (1,596) | 1:1:A:GLU:HA    | 1:1:A:GLU:HG2  | 3        | 0.66          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,596) | 1:1:A:GLU:HA   | 1:1:A:GLU:HG3   | 3        | 0.66          |
| (1,596) | 1:1:A:GLU:HA   | 1:1:A:GLU:HG2   | 7        | 0.66          |
| (1,596) | 1:1:A:GLU:HA   | 1:1:A:GLU:HG3   | 7        | 0.66          |
| (1,468) | 1:21:A:ARG:HD3 | 1:21:A:ARG:HG2  | 1        | 0.66          |
| (1,468) | 1:21:A:ARG:HD3 | 1:21:A:ARG:HG3  | 1        | 0.66          |
| (1,468) | 1:21:A:ARG:HD3 | 1:21:A:ARG:HG2  | 5        | 0.66          |
| (1,468) | 1:21:A:ARG:HD3 | 1:21:A:ARG:HG3  | 5        | 0.66          |
| (1,353) | 1:6:A:ARG:HB3  | 1:6:A:ARG:HD3   | 3        | 0.66          |
| (1,296) | 1:11:A:TRP:HE1 | 1:21:A:ARG:HB3  | 10       | 0.66          |
| (1,268) | 1:8:A:TYR:HD1  | 1:9:A:ILE:H     | 6        | 0.66          |
| (1,268) | 1:8:A:TYR:HD2  | 1:9:A:ILE:H     | 6        | 0.66          |
| (1,268) | 1:8:A:TYR:HD1  | 1:9:A:ILE:H     | 7        | 0.66          |
| (1,268) | 1:8:A:TYR:HD2  | 1:9:A:ILE:H     | 7        | 0.66          |
| (1,268) | 1:8:A:TYR:HD1  | 1:9:A:ILE:H     | 9        | 0.66          |
| (1,268) | 1:8:A:TYR:HD2  | 1:9:A:ILE:H     | 9        | 0.66          |
| (1,227) | 1:11:A:TRP:HZ2 | 1:23:A:PRO:HG2  | 2        | 0.66          |
| (1,121) | 1:2:A:GLU:HB2  | 1:5:A:VAL:H     | 1        | 0.66          |
| (1,121) | 1:2:A:GLU:HB2  | 1:5:A:VAL:H     | 2        | 0.66          |
| (1,67)  | 1:18:A:SER:H   | 1:18:A:SER:HB2  | 1        | 0.66          |
| (1,67)  | 1:18:A:SER:H   | 1:18:A:SER:HB2  | 7        | 0.66          |
| (1,67)  | 1:18:A:SER:H   | 1:18:A:SER:HB2  | 8        | 0.66          |
| (1,67)  | 1:18:A:SER:H   | 1:18:A:SER:HB2  | 10       | 0.66          |
| (1,30)  | 1:4:A:CYS:H    | 1:4:A:CYS:HB2   | 4        | 0.66          |
| (1,26)  | 1:2:A:GLU:HB2  | 1:3:A:GLU:H     | 4        | 0.66          |
| (1,24)  | 1:13:A:LYS:H   | 1:13:A:LYS:HD3  | 10       | 0.66          |
| (1,1)   | 1:7:A:LEU:HB2  | 1:8:A:TYR:H     | 1        | 0.66          |
| (1,732) | 1:2:A:GLU:HG3  | 1:6:A:ARG:HB3   | 2        | 0.65          |
| (1,721) | 1:9:A:ILE:HG13 | 1:12:A:LEU:HB2  | 8        | 0.65          |
| (1,721) | 1:9:A:ILE:HG13 | 1:12:A:LEU:HB2  | 10       | 0.65          |
| (1,701) | 1:5:A:VAL:HG11 | 1:9:A:ILE:HG13  | 3        | 0.65          |
| (1,701) | 1:5:A:VAL:HG12 | 1:9:A:ILE:HG13  | 3        | 0.65          |
| (1,701) | 1:5:A:VAL:HG13 | 1:9:A:ILE:HG13  | 3        | 0.65          |
| (1,675) | 1:12:A:LEU:HA  | 1:12:A:LEU:HD21 | 8        | 0.65          |
| (1,675) | 1:12:A:LEU:HA  | 1:12:A:LEU:HD22 | 8        | 0.65          |
| (1,675) | 1:12:A:LEU:HA  | 1:12:A:LEU:HD23 | 8        | 0.65          |
| (1,671) | 1:8:A:TYR:HA   | 1:12:A:LEU:HD21 | 2        | 0.65          |
| (1,671) | 1:8:A:TYR:HA   | 1:12:A:LEU:HD22 | 2        | 0.65          |
| (1,671) | 1:8:A:TYR:HA   | 1:12:A:LEU:HD23 | 2        | 0.65          |
| (1,654) | 1:14:A:ASP:HB3 | 1:19:A:SER:HB3  | 1        | 0.65          |
| (1,651) | 1:3:A:GLU:HA   | 1:6:A:ARG:HD2   | 1        | 0.65          |
| (1,598) | 1:1:A:GLU:HA   | 1:1:A:GLU:HB3   | 6        | 0.65          |
| (1,553) | 1:11:A:TRP:HB2 | 1:24:A:PRO:HD3  | 3        | 0.65          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,535) | 1:23:A:PRO:HB3  | 1:24:A:PRO:HD2  | 4        | 0.65          |
| (1,468) | 1:21:A:ARG:HD3  | 1:21:A:ARG:HG2  | 9        | 0.65          |
| (1,468) | 1:21:A:ARG:HD3  | 1:21:A:ARG:HG3  | 9        | 0.65          |
| (1,401) | 1:11:A:TRP:HA   | 1:11:A:TRP:HB2  | 3        | 0.65          |
| (1,353) | 1:6:A:ARG:HB3   | 1:6:A:ARG:HD3   | 4        | 0.65          |
| (1,350) | 1:6:A:ARG:HA    | 1:6:A:ARG:HG3   | 1        | 0.65          |
| (1,323) | 1:10:A:GLN:HE22 | 1:11:A:TRP:H    | 3        | 0.65          |
| (1,231) | 1:11:A:TRP:HD1  | 1:21:A:ARG:HB3  | 2        | 0.65          |
| (1,231) | 1:11:A:TRP:HD1  | 1:21:A:ARG:HB3  | 10       | 0.65          |
| (1,227) | 1:11:A:TRP:HZ2  | 1:23:A:PRO:HG2  | 5        | 0.65          |
| (1,68)  | 1:18:A:SER:H    | 1:18:A:SER:HB3  | 5        | 0.65          |
| (1,30)  | 1:4:A:CYS:H     | 1:4:A:CYS:HB2   | 5        | 0.65          |
| (1,26)  | 1:2:A:GLU:HB2   | 1:3:A:GLU:H     | 1        | 0.65          |
| (1,662) | 1:17:A:PRO:HB3  | 1:18:A:SER:HB2  | 7        | 0.64          |
| (1,654) | 1:14:A:ASP:HB3  | 1:19:A:SER:HB3  | 6        | 0.64          |
| (1,598) | 1:1:A:GLU:HA    | 1:1:A:GLU:HB3   | 4        | 0.64          |
| (1,593) | 1:11:A:TRP:HA   | 1:14:A:ASP:HB3  | 3        | 0.64          |
| (1,564) | 1:4:A:CYS:HA    | 1:7:A:LEU:HB3   | 4        | 0.64          |
| (1,472) | 1:22:A:PRO:HA   | 1:22:A:PRO:HD2  | 2        | 0.64          |
| (1,468) | 1:21:A:ARG:HD3  | 1:21:A:ARG:HG2  | 6        | 0.64          |
| (1,468) | 1:21:A:ARG:HD3  | 1:21:A:ARG:HG3  | 6        | 0.64          |
| (1,349) | 1:6:A:ARG:HA    | 1:6:A:ARG:HG2   | 5        | 0.64          |
| (1,295) | 1:11:A:TRP:HE1  | 1:21:A:ARG:HB2  | 5        | 0.64          |
| (1,270) | 1:8:A:TYR:HD1   | 1:25:A:CYS:H    | 2        | 0.64          |
| (1,270) | 1:8:A:TYR:HD2   | 1:25:A:CYS:H    | 2        | 0.64          |
| (1,268) | 1:8:A:TYR:HD1   | 1:9:A:ILE:H     | 1        | 0.64          |
| (1,268) | 1:8:A:TYR:HD2   | 1:9:A:ILE:H     | 1        | 0.64          |
| (1,268) | 1:8:A:TYR:HD1   | 1:9:A:ILE:H     | 2        | 0.64          |
| (1,268) | 1:8:A:TYR:HD2   | 1:9:A:ILE:H     | 2        | 0.64          |
| (1,121) | 1:2:A:GLU:HB2   | 1:5:A:VAL:H     | 8        | 0.64          |
| (1,30)  | 1:4:A:CYS:H     | 1:4:A:CYS:HB2   | 9        | 0.64          |
| (1,1)   | 1:7:A:LEU:HB2   | 1:8:A:TYR:H     | 10       | 0.64          |
| (1,732) | 1:2:A:GLU:HG3   | 1:6:A:ARG:HB3   | 10       | 0.63          |
| (1,721) | 1:9:A:ILE:HG13  | 1:12:A:LEU:HB2  | 7        | 0.63          |
| (1,675) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD21 | 10       | 0.63          |
| (1,675) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD22 | 10       | 0.63          |
| (1,675) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD23 | 10       | 0.63          |
| (1,654) | 1:14:A:ASP:HB3  | 1:19:A:SER:HB3  | 2        | 0.63          |
| (1,654) | 1:14:A:ASP:HB3  | 1:19:A:SER:HB3  | 3        | 0.63          |
| (1,650) | 1:15:A:GLY:HA3  | 1:19:A:SER:HA   | 4        | 0.63          |
| (1,574) | 1:5:A:VAL:HA    | 1:8:A:TYR:HB2   | 4        | 0.63          |
| (1,574) | 1:5:A:VAL:HA    | 1:8:A:TYR:HB3   | 4        | 0.63          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,574) | 1:5:A:VAL:HA   | 1:8:A:TYR:HB2   | 10       | 0.63          |
| (1,574) | 1:5:A:VAL:HA   | 1:8:A:TYR:HB3   | 10       | 0.63          |
| (1,472) | 1:22:A:PRO:HA  | 1:22:A:PRO:HD2  | 6        | 0.63          |
| (1,439) | 1:17:A:PRO:HA  | 1:17:A:PRO:HB3  | 2        | 0.63          |
| (1,439) | 1:17:A:PRO:HA  | 1:17:A:PRO:HB3  | 5        | 0.63          |
| (1,353) | 1:6:A:ARG:HB3  | 1:6:A:ARG:HD3   | 6        | 0.63          |
| (1,299) | 1:8:A:TYR:H    | 1:9:A:ILE:HB    | 9        | 0.63          |
| (1,282) | 1:15:A:GLY:H   | 1:16:A:GLY:H    | 2        | 0.63          |
| (1,268) | 1:8:A:TYR:HD1  | 1:9:A:ILE:H     | 4        | 0.63          |
| (1,268) | 1:8:A:TYR:HD2  | 1:9:A:ILE:H     | 4        | 0.63          |
| (1,227) | 1:11:A:TRP:HZ2 | 1:23:A:PRO:HG2  | 6        | 0.63          |
| (1,145) | 1:11:A:TRP:H   | 1:12:A:LEU:HA   | 2        | 0.63          |
| (1,30)  | 1:4:A:CYS:H    | 1:4:A:CYS:HB2   | 2        | 0.63          |
| (1,30)  | 1:4:A:CYS:H    | 1:4:A:CYS:HB2   | 6        | 0.63          |
| (1,30)  | 1:4:A:CYS:H    | 1:4:A:CYS:HB2   | 7        | 0.63          |
| (1,24)  | 1:13:A:LYS:H   | 1:13:A:LYS:HD3  | 6        | 0.63          |
| (1,732) | 1:2:A:GLU:HG3  | 1:6:A:ARG:HB3   | 1        | 0.62          |
| (1,732) | 1:2:A:GLU:HG3  | 1:6:A:ARG:HB3   | 4        | 0.62          |
| (1,732) | 1:2:A:GLU:HG3  | 1:6:A:ARG:HB3   | 6        | 0.62          |
| (1,721) | 1:9:A:ILE:HG13 | 1:12:A:LEU:HB2  | 4        | 0.62          |
| (1,721) | 1:9:A:ILE:HG13 | 1:12:A:LEU:HB2  | 9        | 0.62          |
| (1,675) | 1:12:A:LEU:HA  | 1:12:A:LEU:HD21 | 4        | 0.62          |
| (1,675) | 1:12:A:LEU:HA  | 1:12:A:LEU:HD22 | 4        | 0.62          |
| (1,675) | 1:12:A:LEU:HA  | 1:12:A:LEU:HD23 | 4        | 0.62          |
| (1,665) | 1:3:A:GLU:HG2  | 1:4:A:CYS:HA    | 7        | 0.62          |
| (1,665) | 1:3:A:GLU:HG3  | 1:4:A:CYS:HA    | 7        | 0.62          |
| (1,650) | 1:15:A:GLY:HA3 | 1:19:A:SER:HA   | 7        | 0.62          |
| (1,574) | 1:5:A:VAL:HA   | 1:8:A:TYR:HB2   | 8        | 0.62          |
| (1,574) | 1:5:A:VAL:HA   | 1:8:A:TYR:HB3   | 8        | 0.62          |
| (1,570) | 1:16:A:GLY:HA3 | 1:17:A:PRO:HD2  | 4        | 0.62          |
| (1,472) | 1:22:A:PRO:HA  | 1:22:A:PRO:HD2  | 1        | 0.62          |
| (1,472) | 1:22:A:PRO:HA  | 1:22:A:PRO:HD2  | 3        | 0.62          |
| (1,472) | 1:22:A:PRO:HA  | 1:22:A:PRO:HD2  | 5        | 0.62          |
| (1,472) | 1:22:A:PRO:HA  | 1:22:A:PRO:HD2  | 8        | 0.62          |
| (1,472) | 1:22:A:PRO:HA  | 1:22:A:PRO:HD2  | 10       | 0.62          |
| (1,468) | 1:21:A:ARG:HD3 | 1:21:A:ARG:HG2  | 10       | 0.62          |
| (1,468) | 1:21:A:ARG:HD3 | 1:21:A:ARG:HG3  | 10       | 0.62          |
| (1,463) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD3  | 1        | 0.62          |
| (1,439) | 1:17:A:PRO:HA  | 1:17:A:PRO:HB3  | 6        | 0.62          |
| (1,439) | 1:17:A:PRO:HA  | 1:17:A:PRO:HB3  | 8        | 0.62          |
| (1,439) | 1:17:A:PRO:HA  | 1:17:A:PRO:HB3  | 9        | 0.62          |
| (1,352) | 1:6:A:ARG:HB3  | 1:6:A:ARG:HD2   | 9        | 0.62          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,295) | 1:11:A:TRP:HE1  | 1:21:A:ARG:HB2 | 1        | 0.62          |
| (1,231) | 1:11:A:TRP:HD1  | 1:21:A:ARG:HB3 | 8        | 0.62          |
| (1,227) | 1:11:A:TRP:HZ2  | 1:23:A:PRO:HG2 | 1        | 0.62          |
| (1,201) | 1:8:A:TYR:HE1   | 1:23:A:PRO:HB3 | 3        | 0.62          |
| (1,201) | 1:8:A:TYR:HE2   | 1:23:A:PRO:HB3 | 3        | 0.62          |
| (1,1)   | 1:7:A:LEU:HB2   | 1:8:A:TYR:H    | 8        | 0.62          |
| (1,732) | 1:2:A:GLU:HG3   | 1:6:A:ARG:HB3  | 8        | 0.61          |
| (1,721) | 1:9:A:ILE:HG13  | 1:12:A:LEU:HB2 | 1        | 0.61          |
| (1,666) | 1:24:A:PRO:HG2  | 1:25:A:CYS:HB2 | 2        | 0.61          |
| (1,618) | 1:10:A:GLN:HE21 | 1:13:A:LYS:HD3 | 5        | 0.61          |
| (1,571) | 1:14:A:ASP:HB3  | 1:19:A:SER:HB2 | 4        | 0.61          |
| (1,570) | 1:16:A:GLY:HA3  | 1:17:A:PRO:HD2 | 3        | 0.61          |
| (1,570) | 1:16:A:GLY:HA3  | 1:17:A:PRO:HD2 | 10       | 0.61          |
| (1,564) | 1:4:A:CYS:HA    | 1:7:A:LEU:HB3  | 3        | 0.61          |
| (1,564) | 1:4:A:CYS:HA    | 1:7:A:LEU:HB3  | 6        | 0.61          |
| (1,494) | 1:21:A:ARG:HA   | 1:22:A:PRO:HD3 | 2        | 0.61          |
| (1,439) | 1:17:A:PRO:HA   | 1:17:A:PRO:HB3 | 1        | 0.61          |
| (1,439) | 1:17:A:PRO:HA   | 1:17:A:PRO:HB3 | 3        | 0.61          |
| (1,439) | 1:17:A:PRO:HA   | 1:17:A:PRO:HB3 | 4        | 0.61          |
| (1,439) | 1:17:A:PRO:HA   | 1:17:A:PRO:HB3 | 7        | 0.61          |
| (1,439) | 1:17:A:PRO:HA   | 1:17:A:PRO:HB3 | 10       | 0.61          |
| (1,401) | 1:11:A:TRP:HA   | 1:11:A:TRP:HB2 | 2        | 0.61          |
| (1,401) | 1:11:A:TRP:HA   | 1:11:A:TRP:HB2 | 5        | 0.61          |
| (1,391) | 1:10:A:GLN:HA   | 1:10:A:GLN:HG2 | 5        | 0.61          |
| (1,391) | 1:10:A:GLN:HA   | 1:10:A:GLN:HG2 | 7        | 0.61          |
| (1,349) | 1:6:A:ARG:HA    | 1:6:A:ARG:HG2  | 4        | 0.61          |
| (1,282) | 1:15:A:GLY:H    | 1:16:A:GLY:H   | 4        | 0.61          |
| (1,282) | 1:15:A:GLY:H    | 1:16:A:GLY:H   | 5        | 0.61          |
| (1,282) | 1:15:A:GLY:H    | 1:16:A:GLY:H   | 6        | 0.61          |
| (1,236) | 1:11:A:TRP:HH2  | 1:22:A:PRO:HB2 | 5        | 0.61          |
| (1,201) | 1:8:A:TYR:HE1   | 1:23:A:PRO:HB3 | 4        | 0.61          |
| (1,201) | 1:8:A:TYR:HE2   | 1:23:A:PRO:HB3 | 4        | 0.61          |
| (1,198) | 1:11:A:TRP:HZ3  | 1:23:A:PRO:HB3 | 8        | 0.61          |
| (1,198) | 1:11:A:TRP:HZ3  | 1:23:A:PRO:HB3 | 10       | 0.61          |
| (1,145) | 1:11:A:TRP:H    | 1:12:A:LEU:HA  | 7        | 0.61          |
| (1,721) | 1:9:A:ILE:HG13  | 1:12:A:LEU:HB2 | 2        | 0.6           |
| (1,721) | 1:9:A:ILE:HG13  | 1:12:A:LEU:HB2 | 6        | 0.6           |
| (1,654) | 1:14:A:ASP:HB3  | 1:19:A:SER:HB3 | 8        | 0.6           |
| (1,654) | 1:14:A:ASP:HB3  | 1:19:A:SER:HB3 | 10       | 0.6           |
| (1,640) | 1:11:A:TRP:HE3  | 1:24:A:PRO:HD2 | 3        | 0.6           |
| (1,631) | 1:5:A:VAL:HG11  | 1:8:A:TYR:HD1  | 3        | 0.6           |
| (1,631) | 1:5:A:VAL:HG11  | 1:8:A:TYR:HD2  | 3        | 0.6           |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,631) | 1:5:A:VAL:HG12 | 1:8:A:TYR:HD1  | 3        | 0.6           |
| (1,631) | 1:5:A:VAL:HG12 | 1:8:A:TYR:HD2  | 3        | 0.6           |
| (1,631) | 1:5:A:VAL:HG13 | 1:8:A:TYR:HD1  | 3        | 0.6           |
| (1,631) | 1:5:A:VAL:HG13 | 1:8:A:TYR:HD2  | 3        | 0.6           |
| (1,616) | 1:14:A:ASP:HB3 | 1:16:A:GLY:H   | 3        | 0.6           |
| (1,574) | 1:5:A:VAL:HA   | 1:8:A:TYR:HB2  | 1        | 0.6           |
| (1,574) | 1:5:A:VAL:HA   | 1:8:A:TYR:HB3  | 1        | 0.6           |
| (1,574) | 1:5:A:VAL:HA   | 1:8:A:TYR:HB2  | 2        | 0.6           |
| (1,574) | 1:5:A:VAL:HA   | 1:8:A:TYR:HB3  | 2        | 0.6           |
| (1,574) | 1:5:A:VAL:HA   | 1:8:A:TYR:HB2  | 9        | 0.6           |
| (1,574) | 1:5:A:VAL:HA   | 1:8:A:TYR:HB3  | 9        | 0.6           |
| (1,570) | 1:16:A:GLY:HA3 | 1:17:A:PRO:HD2 | 8        | 0.6           |
| (1,507) | 1:23:A:PRO:HD2 | 1:23:A:PRO:HG2 | 4        | 0.6           |
| (1,507) | 1:23:A:PRO:HD2 | 1:23:A:PRO:HG2 | 7        | 0.6           |
| (1,494) | 1:21:A:ARG:HA  | 1:22:A:PRO:HD3 | 8        | 0.6           |
| (1,463) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD3 | 6        | 0.6           |
| (1,433) | 1:15:A:GLY:HA2 | 1:15:A:GLY:HA3 | 4        | 0.6           |
| (1,433) | 1:15:A:GLY:HA2 | 1:15:A:GLY:HA3 | 7        | 0.6           |
| (1,433) | 1:15:A:GLY:HA2 | 1:15:A:GLY:HA3 | 8        | 0.6           |
| (1,433) | 1:15:A:GLY:HA2 | 1:15:A:GLY:HA3 | 10       | 0.6           |
| (1,431) | 1:14:A:ASP:HA  | 1:14:A:ASP:HB2 | 7        | 0.6           |
| (1,401) | 1:11:A:TRP:HA  | 1:11:A:TRP:HB2 | 1        | 0.6           |
| (1,401) | 1:11:A:TRP:HA  | 1:11:A:TRP:HB2 | 6        | 0.6           |
| (1,353) | 1:6:A:ARG:HB3  | 1:6:A:ARG:HD3  | 5        | 0.6           |
| (1,350) | 1:6:A:ARG:HA   | 1:6:A:ARG:HG3  | 8        | 0.6           |
| (1,349) | 1:6:A:ARG:HA   | 1:6:A:ARG:HG2  | 6        | 0.6           |
| (1,299) | 1:8:A:TYR:H    | 1:9:A:ILE:HB   | 10       | 0.6           |
| (1,295) | 1:11:A:TRP:HE1 | 1:21:A:ARG:HB2 | 9        | 0.6           |
| (1,282) | 1:15:A:GLY:H   | 1:16:A:GLY:H   | 9        | 0.6           |
| (1,30)  | 1:4:A:CYS:H    | 1:4:A:CYS:HB2  | 1        | 0.6           |
| (1,30)  | 1:4:A:CYS:H    | 1:4:A:CYS:HB2  | 10       | 0.6           |
| (1,732) | 1:2:A:GLU:HG3  | 1:6:A:ARG:HB3  | 3        | 0.59          |
| (1,666) | 1:24:A:PRO:HG2 | 1:25:A:CYS:HB2 | 5        | 0.59          |
| (1,665) | 1:3:A:GLU:HG2  | 1:4:A:CYS:HA   | 1        | 0.59          |
| (1,665) | 1:3:A:GLU:HG3  | 1:4:A:CYS:HA   | 1        | 0.59          |
| (1,650) | 1:15:A:GLY:HA3 | 1:19:A:SER:HA  | 8        | 0.59          |
| (1,574) | 1:5:A:VAL:HA   | 1:8:A:TYR:HB2  | 7        | 0.59          |
| (1,574) | 1:5:A:VAL:HA   | 1:8:A:TYR:HB3  | 7        | 0.59          |
| (1,571) | 1:14:A:ASP:HB3 | 1:19:A:SER:HB2 | 7        | 0.59          |
| (1,571) | 1:14:A:ASP:HB3 | 1:19:A:SER:HB2 | 8        | 0.59          |
| (1,570) | 1:16:A:GLY:HA3 | 1:17:A:PRO:HD2 | 7        | 0.59          |
| (1,494) | 1:21:A:ARG:HA  | 1:22:A:PRO:HD3 | 10       | 0.59          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,472) | 1:22:A:PRO:HA   | 1:22:A:PRO:HD2  | 9        | 0.59          |
| (1,463) | 1:21:A:ARG:HB3  | 1:21:A:ARG:HD3  | 5        | 0.59          |
| (1,451) | 1:18:A:SER:HA   | 1:18:A:SER:HB2  | 6        | 0.59          |
| (1,378) | 1:9:A:ILE:HA    | 1:9:A:ILE:HG12  | 6        | 0.59          |
| (1,353) | 1:6:A:ARG:HB3   | 1:6:A:ARG:HD3   | 7        | 0.59          |
| (1,350) | 1:6:A:ARG:HA    | 1:6:A:ARG:HG3   | 2        | 0.59          |
| (1,349) | 1:6:A:ARG:HA    | 1:6:A:ARG:HG2   | 3        | 0.59          |
| (1,270) | 1:8:A:TYR:HD1   | 1:25:A:CYS:H    | 5        | 0.59          |
| (1,270) | 1:8:A:TYR:HD2   | 1:25:A:CYS:H    | 5        | 0.59          |
| (1,262) | 1:10:A:GLN:HA   | 1:10:A:GLN:HE22 | 3        | 0.59          |
| (1,240) | 1:8:A:TYR:HD1   | 1:9:A:ILE:HG13  | 3        | 0.59          |
| (1,240) | 1:8:A:TYR:HD2   | 1:9:A:ILE:HG13  | 3        | 0.59          |
| (1,201) | 1:8:A:TYR:HE1   | 1:23:A:PRO:HB3  | 7        | 0.59          |
| (1,201) | 1:8:A:TYR:HE2   | 1:23:A:PRO:HB3  | 7        | 0.59          |
| (1,201) | 1:8:A:TYR:HE1   | 1:23:A:PRO:HB3  | 10       | 0.59          |
| (1,201) | 1:8:A:TYR:HE2   | 1:23:A:PRO:HB3  | 10       | 0.59          |
| (1,111) | 1:10:A:GLN:HB3  | 1:11:A:TRP:H    | 1        | 0.59          |
| (1,67)  | 1:18:A:SER:H    | 1:18:A:SER:HB2  | 5        | 0.59          |
| (1,1)   | 1:7:A:LEU:HB2   | 1:8:A:TYR:H     | 9        | 0.59          |
| (1,723) | 1:12:A:LEU:HB3  | 1:13:A:LYS:HG2  | 5        | 0.58          |
| (1,723) | 1:12:A:LEU:HB3  | 1:13:A:LYS:HG3  | 5        | 0.58          |
| (1,721) | 1:9:A:ILE:HG13  | 1:12:A:LEU:HB2  | 5        | 0.58          |
| (1,675) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD21 | 9        | 0.58          |
| (1,675) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD22 | 9        | 0.58          |
| (1,675) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD23 | 9        | 0.58          |
| (1,650) | 1:15:A:GLY:HA3  | 1:19:A:SER:HA   | 10       | 0.58          |
| (1,618) | 1:10:A:GLN:HE21 | 1:13:A:LYS:HD3  | 2        | 0.58          |
| (1,614) | 1:19:A:SER:HG   | 1:20:A:GLY:H    | 9        | 0.58          |
| (1,605) | 1:8:A:TYR:HE1   | 1:11:A:TRP:HZ3  | 9        | 0.58          |
| (1,605) | 1:8:A:TYR:HE2   | 1:11:A:TRP:HZ3  | 9        | 0.58          |
| (1,574) | 1:5:A:VAL:HA    | 1:8:A:TYR:HB2   | 5        | 0.58          |
| (1,574) | 1:5:A:VAL:HA    | 1:8:A:TYR:HB3   | 5        | 0.58          |
| (1,574) | 1:5:A:VAL:HA    | 1:8:A:TYR:HB2   | 6        | 0.58          |
| (1,574) | 1:5:A:VAL:HA    | 1:8:A:TYR:HB3   | 6        | 0.58          |
| (1,570) | 1:16:A:GLY:HA3  | 1:17:A:PRO:HD2  | 9        | 0.58          |
| (1,468) | 1:21:A:ARG:HD3  | 1:21:A:ARG:HG2  | 8        | 0.58          |
| (1,468) | 1:21:A:ARG:HD3  | 1:21:A:ARG:HG3  | 8        | 0.58          |
| (1,463) | 1:21:A:ARG:HB3  | 1:21:A:ARG:HD3  | 9        | 0.58          |
| (1,451) | 1:18:A:SER:HA   | 1:18:A:SER:HB2  | 2        | 0.58          |
| (1,353) | 1:6:A:ARG:HB3   | 1:6:A:ARG:HD3   | 10       | 0.58          |
| (1,295) | 1:11:A:TRP:HE1  | 1:21:A:ARG:HB2  | 6        | 0.58          |
| (1,295) | 1:11:A:TRP:HE1  | 1:21:A:ARG:HB2  | 7        | 0.58          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,276) | 1:19:A:SER:H   | 1:20:A:GLY:H    | 1        | 0.58          |
| (1,270) | 1:8:A:TYR:HD1  | 1:25:A:CYS:H    | 1        | 0.58          |
| (1,270) | 1:8:A:TYR:HD2  | 1:25:A:CYS:H    | 1        | 0.58          |
| (1,236) | 1:11:A:TRP:HH2 | 1:22:A:PRO:HB2  | 6        | 0.58          |
| (1,24)  | 1:13:A:LYS:H   | 1:13:A:LYS:HD3  | 5        | 0.58          |
| (1,24)  | 1:13:A:LYS:H   | 1:13:A:LYS:HD3  | 9        | 0.58          |
| (1,10)  | 1:9:A:ILE:H    | 1:12:A:LEU:HD21 | 3        | 0.58          |
| (1,10)  | 1:9:A:ILE:H    | 1:12:A:LEU:HD22 | 3        | 0.58          |
| (1,10)  | 1:9:A:ILE:H    | 1:12:A:LEU:HD23 | 3        | 0.58          |
| (1,723) | 1:12:A:LEU:HB3 | 1:13:A:LYS:HG2  | 6        | 0.57          |
| (1,723) | 1:12:A:LEU:HB3 | 1:13:A:LYS:HG3  | 6        | 0.57          |
| (1,622) | 1:2:A:GLU:HB3  | 1:5:A:VAL:H     | 1        | 0.57          |
| (1,605) | 1:8:A:TYR:HE1  | 1:11:A:TRP:HZ3  | 8        | 0.57          |
| (1,605) | 1:8:A:TYR:HE2  | 1:11:A:TRP:HZ3  | 8        | 0.57          |
| (1,596) | 1:1:A:GLU:HA   | 1:1:A:GLU:HG2   | 9        | 0.57          |
| (1,596) | 1:1:A:GLU:HA   | 1:1:A:GLU:HG3   | 9        | 0.57          |
| (1,570) | 1:16:A:GLY:HA3 | 1:17:A:PRO:HD2  | 1        | 0.57          |
| (1,530) | 1:24:A:PRO:HD2 | 1:24:A:PRO:HG2  | 3        | 0.57          |
| (1,494) | 1:21:A:ARG:HA  | 1:22:A:PRO:HD3  | 3        | 0.57          |
| (1,463) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD3  | 10       | 0.57          |
| (1,433) | 1:15:A:GLY:HA2 | 1:15:A:GLY:HA3  | 1        | 0.57          |
| (1,433) | 1:15:A:GLY:HA2 | 1:15:A:GLY:HA3  | 2        | 0.57          |
| (1,433) | 1:15:A:GLY:HA2 | 1:15:A:GLY:HA3  | 3        | 0.57          |
| (1,433) | 1:15:A:GLY:HA2 | 1:15:A:GLY:HA3  | 5        | 0.57          |
| (1,433) | 1:15:A:GLY:HA2 | 1:15:A:GLY:HA3  | 6        | 0.57          |
| (1,433) | 1:15:A:GLY:HA2 | 1:15:A:GLY:HA3  | 9        | 0.57          |
| (1,378) | 1:9:A:ILE:HA   | 1:9:A:ILE:HG12  | 5        | 0.57          |
| (1,350) | 1:6:A:ARG:HA   | 1:6:A:ARG:HG3   | 10       | 0.57          |
| (1,299) | 1:8:A:TYR:H    | 1:9:A:ILE:HB    | 8        | 0.57          |
| (1,282) | 1:15:A:GLY:H   | 1:16:A:GLY:H    | 7        | 0.57          |
| (1,259) | 1:4:A:CYS:HB3  | 1:5:A:VAL:H     | 6        | 0.57          |
| (1,111) | 1:10:A:GLN:HB3 | 1:11:A:TRP:H    | 7        | 0.57          |
| (1,111) | 1:10:A:GLN:HB3 | 1:11:A:TRP:H    | 9        | 0.57          |
| (1,30)  | 1:4:A:CYS:H    | 1:4:A:CYS:HB2   | 8        | 0.57          |
| (1,1)   | 1:7:A:LEU:HB2  | 1:8:A:TYR:H     | 4        | 0.57          |
| (1,705) | 1:9:A:ILE:HG21 | 1:13:A:LYS:HD2  | 6        | 0.56          |
| (1,705) | 1:9:A:ILE:HG22 | 1:13:A:LYS:HD2  | 6        | 0.56          |
| (1,705) | 1:9:A:ILE:HG23 | 1:13:A:LYS:HD2  | 6        | 0.56          |
| (1,675) | 1:12:A:LEU:HA  | 1:12:A:LEU:HD21 | 7        | 0.56          |
| (1,675) | 1:12:A:LEU:HA  | 1:12:A:LEU:HD22 | 7        | 0.56          |
| (1,675) | 1:12:A:LEU:HA  | 1:12:A:LEU:HD23 | 7        | 0.56          |
| (1,571) | 1:14:A:ASP:HB3 | 1:19:A:SER:HB2  | 9        | 0.56          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,564) | 1:4:A:CYS:HA   | 1:7:A:LEU:HB3  | 10       | 0.56          |
| (1,530) | 1:24:A:PRO:HD2 | 1:24:A:PRO:HG2 | 5        | 0.56          |
| (1,530) | 1:24:A:PRO:HD2 | 1:24:A:PRO:HG2 | 7        | 0.56          |
| (1,530) | 1:24:A:PRO:HD2 | 1:24:A:PRO:HG2 | 9        | 0.56          |
| (1,463) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD3 | 4        | 0.56          |
| (1,378) | 1:9:A:ILE:HA   | 1:9:A:ILE:HG12 | 7        | 0.56          |
| (1,368) | 1:7:A:LEU:HA   | 1:7:A:LEU:HD11 | 4        | 0.56          |
| (1,368) | 1:7:A:LEU:HA   | 1:7:A:LEU:HD12 | 4        | 0.56          |
| (1,368) | 1:7:A:LEU:HA   | 1:7:A:LEU:HD13 | 4        | 0.56          |
| (1,368) | 1:7:A:LEU:HA   | 1:7:A:LEU:HD21 | 4        | 0.56          |
| (1,368) | 1:7:A:LEU:HA   | 1:7:A:LEU:HD22 | 4        | 0.56          |
| (1,368) | 1:7:A:LEU:HA   | 1:7:A:LEU:HD23 | 4        | 0.56          |
| (1,349) | 1:6:A:ARG:HA   | 1:6:A:ARG:HG2  | 10       | 0.56          |
| (1,236) | 1:11:A:TRP:HH2 | 1:22:A:PRO:HB2 | 1        | 0.56          |
| (1,223) | 1:8:A:TYR:HE1  | 1:23:A:PRO:HB2 | 1        | 0.56          |
| (1,223) | 1:8:A:TYR:HE2  | 1:23:A:PRO:HB2 | 1        | 0.56          |
| (1,199) | 1:8:A:TYR:HD1  | 1:23:A:PRO:HB3 | 7        | 0.56          |
| (1,199) | 1:8:A:TYR:HD2  | 1:23:A:PRO:HB3 | 7        | 0.56          |
| (1,26)  | 1:2:A:GLU:HB2  | 1:3:A:GLU:H    | 6        | 0.56          |
| (1,24)  | 1:13:A:LYS:H   | 1:13:A:LYS:HD3 | 7        | 0.56          |
| (1,666) | 1:24:A:PRO:HG2 | 1:25:A:CYS:HB2 | 9        | 0.55          |
| (1,622) | 1:2:A:GLU:HB3  | 1:5:A:VAL:H    | 8        | 0.55          |
| (1,616) | 1:14:A:ASP:HB3 | 1:16:A:GLY:H   | 10       | 0.55          |
| (1,564) | 1:4:A:CYS:HA   | 1:7:A:LEU:HB3  | 2        | 0.55          |
| (1,563) | 1:7:A:LEU:HA   | 1:10:A:GLN:HB3 | 3        | 0.55          |
| (1,530) | 1:24:A:PRO:HD2 | 1:24:A:PRO:HG2 | 1        | 0.55          |
| (1,530) | 1:24:A:PRO:HD2 | 1:24:A:PRO:HG2 | 2        | 0.55          |
| (1,530) | 1:24:A:PRO:HD2 | 1:24:A:PRO:HG2 | 4        | 0.55          |
| (1,530) | 1:24:A:PRO:HD2 | 1:24:A:PRO:HG2 | 6        | 0.55          |
| (1,530) | 1:24:A:PRO:HD2 | 1:24:A:PRO:HG2 | 8        | 0.55          |
| (1,530) | 1:24:A:PRO:HD2 | 1:24:A:PRO:HG2 | 10       | 0.55          |
| (1,507) | 1:23:A:PRO:HD2 | 1:23:A:PRO:HG2 | 8        | 0.55          |
| (1,507) | 1:23:A:PRO:HD2 | 1:23:A:PRO:HG2 | 9        | 0.55          |
| (1,431) | 1:14:A:ASP:HA  | 1:14:A:ASP:HB2 | 5        | 0.55          |
| (1,391) | 1:10:A:GLN:HA  | 1:10:A:GLN:HG2 | 1        | 0.55          |
| (1,378) | 1:9:A:ILE:HA   | 1:9:A:ILE:HG12 | 10       | 0.55          |
| (1,368) | 1:7:A:LEU:HA   | 1:7:A:LEU:HD11 | 7        | 0.55          |
| (1,368) | 1:7:A:LEU:HA   | 1:7:A:LEU:HD12 | 7        | 0.55          |
| (1,368) | 1:7:A:LEU:HA   | 1:7:A:LEU:HD13 | 7        | 0.55          |
| (1,368) | 1:7:A:LEU:HA   | 1:7:A:LEU:HD21 | 7        | 0.55          |
| (1,368) | 1:7:A:LEU:HA   | 1:7:A:LEU:HD22 | 7        | 0.55          |
| (1,368) | 1:7:A:LEU:HA   | 1:7:A:LEU:HD23 | 7        | 0.55          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,353) | 1:6:A:ARG:HB3  | 1:6:A:ARG:HD3   | 2        | 0.55          |
| (1,350) | 1:6:A:ARG:HA   | 1:6:A:ARG:HG3   | 6        | 0.55          |
| (1,223) | 1:8:A:TYR:HE1  | 1:23:A:PRO:HB2  | 2        | 0.55          |
| (1,223) | 1:8:A:TYR:HE2  | 1:23:A:PRO:HB2  | 2        | 0.55          |
| (1,223) | 1:8:A:TYR:HE1  | 1:23:A:PRO:HB2  | 6        | 0.55          |
| (1,223) | 1:8:A:TYR:HE2  | 1:23:A:PRO:HB2  | 6        | 0.55          |
| (1,190) | 1:11:A:TRP:HD1 | 1:24:A:PRO:HD2  | 1        | 0.55          |
| (1,99)  | 1:11:A:TRP:HE1 | 1:22:A:PRO:HA   | 4        | 0.55          |
| (1,728) | 1:2:A:GLU:HG2  | 1:6:A:ARG:HG2   | 5        | 0.54          |
| (1,719) | 1:9:A:ILE:HG12 | 1:12:A:LEU:HG   | 8        | 0.54          |
| (1,640) | 1:11:A:TRP:HE3 | 1:24:A:PRO:HD2  | 8        | 0.54          |
| (1,616) | 1:14:A:ASP:HB3 | 1:16:A:GLY:H    | 1        | 0.54          |
| (1,579) | 1:4:A:CYS:HA   | 1:7:A:LEU:HB2   | 7        | 0.54          |
| (1,579) | 1:4:A:CYS:HA   | 1:7:A:LEU:HB2   | 9        | 0.54          |
| (1,525) | 1:24:A:PRO:HB3 | 1:24:A:PRO:HD3  | 3        | 0.54          |
| (1,507) | 1:23:A:PRO:HD2 | 1:23:A:PRO:HG2  | 10       | 0.54          |
| (1,431) | 1:14:A:ASP:HA  | 1:14:A:ASP:HB2  | 4        | 0.54          |
| (1,431) | 1:14:A:ASP:HA  | 1:14:A:ASP:HB2  | 9        | 0.54          |
| (1,378) | 1:9:A:ILE:HA   | 1:9:A:ILE:HG12  | 1        | 0.54          |
| (1,378) | 1:9:A:ILE:HA   | 1:9:A:ILE:HG12  | 8        | 0.54          |
| (1,378) | 1:9:A:ILE:HA   | 1:9:A:ILE:HG12  | 9        | 0.54          |
| (1,368) | 1:7:A:LEU:HA   | 1:7:A:LEU:HD11  | 1        | 0.54          |
| (1,368) | 1:7:A:LEU:HA   | 1:7:A:LEU:HD12  | 1        | 0.54          |
| (1,368) | 1:7:A:LEU:HA   | 1:7:A:LEU:HD13  | 1        | 0.54          |
| (1,368) | 1:7:A:LEU:HA   | 1:7:A:LEU:HD21  | 1        | 0.54          |
| (1,368) | 1:7:A:LEU:HA   | 1:7:A:LEU:HD22  | 1        | 0.54          |
| (1,368) | 1:7:A:LEU:HA   | 1:7:A:LEU:HD23  | 1        | 0.54          |
| (1,349) | 1:6:A:ARG:HA   | 1:6:A:ARG:HG2   | 7        | 0.54          |
| (1,190) | 1:11:A:TRP:HD1 | 1:24:A:PRO:HD2  | 2        | 0.54          |
| (1,145) | 1:11:A:TRP:H   | 1:12:A:LEU:HA   | 10       | 0.54          |
| (1,99)  | 1:11:A:TRP:HE1 | 1:22:A:PRO:HA   | 6        | 0.54          |
| (1,92)  | 1:19:A:SER:H   | 1:19:A:SER:HG   | 10       | 0.54          |
| (1,24)  | 1:13:A:LYS:H   | 1:13:A:LYS:HD3  | 4        | 0.54          |
| (1,719) | 1:9:A:ILE:HG12 | 1:12:A:LEU:HG   | 10       | 0.53          |
| (1,682) | 1:4:A:CYS:HB2  | 1:5:A:VAL:HG11  | 8        | 0.53          |
| (1,682) | 1:4:A:CYS:HB2  | 1:5:A:VAL:HG12  | 8        | 0.53          |
| (1,682) | 1:4:A:CYS:HB2  | 1:5:A:VAL:HG13  | 8        | 0.53          |
| (1,671) | 1:8:A:TYR:HA   | 1:12:A:LEU:HD21 | 7        | 0.53          |
| (1,671) | 1:8:A:TYR:HA   | 1:12:A:LEU:HD22 | 7        | 0.53          |
| (1,671) | 1:8:A:TYR:HA   | 1:12:A:LEU:HD23 | 7        | 0.53          |
| (1,671) | 1:8:A:TYR:HA   | 1:12:A:LEU:HD21 | 9        | 0.53          |
| (1,671) | 1:8:A:TYR:HA   | 1:12:A:LEU:HD22 | 9        | 0.53          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,671) | 1:8:A:TYR:HA   | 1:12:A:LEU:HD23 | 9        | 0.53          |
| (1,668) | 1:19:A:SER:HB2 | 1:21:A:ARG:HG2  | 6        | 0.53          |
| (1,668) | 1:19:A:SER:HB2 | 1:21:A:ARG:HG3  | 6        | 0.53          |
| (1,665) | 1:3:A:GLU:HG2  | 1:4:A:CYS:HA    | 2        | 0.53          |
| (1,665) | 1:3:A:GLU:HG3  | 1:4:A:CYS:HA    | 2        | 0.53          |
| (1,665) | 1:3:A:GLU:HG2  | 1:4:A:CYS:HA    | 6        | 0.53          |
| (1,665) | 1:3:A:GLU:HG3  | 1:4:A:CYS:HA    | 6        | 0.53          |
| (1,641) | 1:8:A:TYR:HD1  | 1:25:A:CYS:HB3  | 3        | 0.53          |
| (1,641) | 1:8:A:TYR:HD2  | 1:25:A:CYS:HB3  | 3        | 0.53          |
| (1,622) | 1:2:A:GLU:HB3  | 1:5:A:VAL:H     | 2        | 0.53          |
| (1,616) | 1:14:A:ASP:HB3 | 1:16:A:GLY:H    | 5        | 0.53          |
| (1,616) | 1:14:A:ASP:HB3 | 1:16:A:GLY:H    | 8        | 0.53          |
| (1,576) | 1:22:A:PRO:HA  | 1:23:A:PRO:HD3  | 4        | 0.53          |
| (1,570) | 1:16:A:GLY:HA3 | 1:17:A:PRO:HD2  | 2        | 0.53          |
| (1,535) | 1:23:A:PRO:HB3 | 1:24:A:PRO:HD2  | 9        | 0.53          |
| (1,463) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD3  | 7        | 0.53          |
| (1,378) | 1:9:A:ILE:HA   | 1:9:A:ILE:HG12  | 4        | 0.53          |
| (1,368) | 1:7:A:LEU:HA   | 1:7:A:LEU:HD11  | 5        | 0.53          |
| (1,368) | 1:7:A:LEU:HA   | 1:7:A:LEU:HD12  | 5        | 0.53          |
| (1,368) | 1:7:A:LEU:HA   | 1:7:A:LEU:HD13  | 5        | 0.53          |
| (1,368) | 1:7:A:LEU:HA   | 1:7:A:LEU:HD21  | 5        | 0.53          |
| (1,368) | 1:7:A:LEU:HA   | 1:7:A:LEU:HD22  | 5        | 0.53          |
| (1,368) | 1:7:A:LEU:HA   | 1:7:A:LEU:HD23  | 5        | 0.53          |
| (1,350) | 1:6:A:ARG:HA   | 1:6:A:ARG:HG3   | 3        | 0.53          |
| (1,350) | 1:6:A:ARG:HA   | 1:6:A:ARG:HG3   | 5        | 0.53          |
| (1,349) | 1:6:A:ARG:HA   | 1:6:A:ARG:HG2   | 1        | 0.53          |
| (1,349) | 1:6:A:ARG:HA   | 1:6:A:ARG:HG2   | 8        | 0.53          |
| (1,295) | 1:11:A:TRP:HE1 | 1:21:A:ARG:HB2  | 4        | 0.53          |
| (1,238) | 1:8:A:TYR:HE1  | 1:23:A:PRO:HG3  | 5        | 0.53          |
| (1,238) | 1:8:A:TYR:HE2  | 1:23:A:PRO:HG3  | 5        | 0.53          |
| (1,201) | 1:8:A:TYR:HE1  | 1:23:A:PRO:HB3  | 2        | 0.53          |
| (1,201) | 1:8:A:TYR:HE2  | 1:23:A:PRO:HB3  | 2        | 0.53          |
| (1,198) | 1:11:A:TRP:HZ3 | 1:23:A:PRO:HB3  | 4        | 0.53          |
| (1,190) | 1:11:A:TRP:HD1 | 1:24:A:PRO:HD2  | 8        | 0.53          |
| (1,682) | 1:4:A:CYS:HB2  | 1:5:A:VAL:HG11  | 1        | 0.52          |
| (1,682) | 1:4:A:CYS:HB2  | 1:5:A:VAL:HG12  | 1        | 0.52          |
| (1,682) | 1:4:A:CYS:HB2  | 1:5:A:VAL:HG13  | 1        | 0.52          |
| (1,671) | 1:8:A:TYR:HA   | 1:12:A:LEU:HD21 | 4        | 0.52          |
| (1,671) | 1:8:A:TYR:HA   | 1:12:A:LEU:HD22 | 4        | 0.52          |
| (1,671) | 1:8:A:TYR:HA   | 1:12:A:LEU:HD23 | 4        | 0.52          |
| (1,640) | 1:11:A:TRP:HE3 | 1:24:A:PRO:HD2  | 10       | 0.52          |
| (1,614) | 1:19:A:SER:HG  | 1:20:A:GLY:H    | 4        | 0.52          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,576) | 1:22:A:PRO:HA   | 1:23:A:PRO:HD3 | 7        | 0.52          |
| (1,570) | 1:16:A:GLY:HA3  | 1:17:A:PRO:HD2 | 5        | 0.52          |
| (1,507) | 1:23:A:PRO:HD2  | 1:23:A:PRO:HG2 | 1        | 0.52          |
| (1,507) | 1:23:A:PRO:HD2  | 1:23:A:PRO:HG2 | 2        | 0.52          |
| (1,507) | 1:23:A:PRO:HD2  | 1:23:A:PRO:HG2 | 5        | 0.52          |
| (1,507) | 1:23:A:PRO:HD2  | 1:23:A:PRO:HG2 | 6        | 0.52          |
| (1,425) | 1:13:A:LYS:HB2  | 1:13:A:LYS:HD2 | 4        | 0.52          |
| (1,425) | 1:13:A:LYS:HB3  | 1:13:A:LYS:HD2 | 4        | 0.52          |
| (1,425) | 1:13:A:LYS:HB2  | 1:13:A:LYS:HD2 | 7        | 0.52          |
| (1,425) | 1:13:A:LYS:HB3  | 1:13:A:LYS:HD2 | 7        | 0.52          |
| (1,368) | 1:7:A:LEU:HA    | 1:7:A:LEU:HD11 | 6        | 0.52          |
| (1,368) | 1:7:A:LEU:HA    | 1:7:A:LEU:HD12 | 6        | 0.52          |
| (1,368) | 1:7:A:LEU:HA    | 1:7:A:LEU:HD13 | 6        | 0.52          |
| (1,368) | 1:7:A:LEU:HA    | 1:7:A:LEU:HD21 | 6        | 0.52          |
| (1,368) | 1:7:A:LEU:HA    | 1:7:A:LEU:HD22 | 6        | 0.52          |
| (1,368) | 1:7:A:LEU:HA    | 1:7:A:LEU:HD23 | 6        | 0.52          |
| (1,325) | 1:2:A:GLU:HA    | 1:2:A:GLU:HB2  | 1        | 0.52          |
| (1,325) | 1:2:A:GLU:HA    | 1:2:A:GLU:HB2  | 2        | 0.52          |
| (1,315) | 1:10:A:GLN:HE22 | 1:13:A:LYS:HE2 | 6        | 0.52          |
| (1,315) | 1:10:A:GLN:HE22 | 1:13:A:LYS:HE3 | 6        | 0.52          |
| (1,270) | 1:8:A:TYR:HD1   | 1:25:A:CYS:H   | 3        | 0.52          |
| (1,270) | 1:8:A:TYR:HD2   | 1:25:A:CYS:H   | 3        | 0.52          |
| (1,270) | 1:8:A:TYR:HD1   | 1:25:A:CYS:H   | 4        | 0.52          |
| (1,270) | 1:8:A:TYR:HD2   | 1:25:A:CYS:H   | 4        | 0.52          |
| (1,270) | 1:8:A:TYR:HD1   | 1:25:A:CYS:H   | 10       | 0.52          |
| (1,270) | 1:8:A:TYR:HD2   | 1:25:A:CYS:H   | 10       | 0.52          |
| (1,212) | 1:8:A:TYR:HD1   | 1:9:A:ILE:HG21 | 5        | 0.52          |
| (1,212) | 1:8:A:TYR:HD1   | 1:9:A:ILE:HG22 | 5        | 0.52          |
| (1,212) | 1:8:A:TYR:HD1   | 1:9:A:ILE:HG23 | 5        | 0.52          |
| (1,212) | 1:8:A:TYR:HD2   | 1:9:A:ILE:HG21 | 5        | 0.52          |
| (1,212) | 1:8:A:TYR:HD2   | 1:9:A:ILE:HG22 | 5        | 0.52          |
| (1,212) | 1:8:A:TYR:HD2   | 1:9:A:ILE:HG23 | 5        | 0.52          |
| (1,198) | 1:11:A:TRP:HZ3  | 1:23:A:PRO:HB3 | 9        | 0.52          |
| (1,190) | 1:11:A:TRP:HD1  | 1:24:A:PRO:HD2 | 5        | 0.52          |
| (1,190) | 1:11:A:TRP:HD1  | 1:24:A:PRO:HD2 | 10       | 0.52          |
| (1,145) | 1:11:A:TRP:H    | 1:12:A:LEU:HA  | 4        | 0.52          |
| (1,145) | 1:11:A:TRP:H    | 1:12:A:LEU:HA  | 8        | 0.52          |
| (1,626) | 1:14:A:ASP:HB3  | 1:15:A:GLY:H   | 10       | 0.51          |
| (1,605) | 1:8:A:TYR:HE1   | 1:11:A:TRP:HZ3 | 7        | 0.51          |
| (1,605) | 1:8:A:TYR:HE2   | 1:11:A:TRP:HZ3 | 7        | 0.51          |
| (1,579) | 1:4:A:CYS:HA    | 1:7:A:LEU:HB2  | 5        | 0.51          |
| (1,552) | 1:11:A:TRP:HB2  | 1:24:A:PRO:HD2 | 3        | 0.51          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,542) | 1:7:A:LEU:HB2   | 1:24:A:PRO:HB3  | 7        | 0.51          |
| (1,535) | 1:23:A:PRO:HB3  | 1:24:A:PRO:HD2  | 8        | 0.51          |
| (1,507) | 1:23:A:PRO:HD2  | 1:23:A:PRO:HG2  | 3        | 0.51          |
| (1,431) | 1:14:A:ASP:HA   | 1:14:A:ASP:HB2  | 8        | 0.51          |
| (1,431) | 1:14:A:ASP:HA   | 1:14:A:ASP:HB2  | 10       | 0.51          |
| (1,425) | 1:13:A:LYS:HB2  | 1:13:A:LYS:HD2  | 5        | 0.51          |
| (1,425) | 1:13:A:LYS:HB3  | 1:13:A:LYS:HD2  | 5        | 0.51          |
| (1,408) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD11 | 3        | 0.51          |
| (1,408) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD12 | 3        | 0.51          |
| (1,408) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD13 | 3        | 0.51          |
| (1,391) | 1:10:A:GLN:HA   | 1:10:A:GLN:HG2  | 6        | 0.51          |
| (1,350) | 1:6:A:ARG:HA    | 1:6:A:ARG:HG3   | 4        | 0.51          |
| (1,325) | 1:2:A:GLU:HA    | 1:2:A:GLU:HB2   | 4        | 0.51          |
| (1,324) | 1:11:A:TRP:H    | 1:12:A:LEU:H    | 3        | 0.51          |
| (1,321) | 1:11:A:TRP:HB3  | 1:12:A:LEU:H    | 6        | 0.51          |
| (1,276) | 1:19:A:SER:H    | 1:20:A:GLY:H    | 9        | 0.51          |
| (1,232) | 1:11:A:TRP:HE3  | 1:12:A:LEU:HG   | 8        | 0.51          |
| (1,232) | 1:11:A:TRP:HE3  | 1:12:A:LEU:HG   | 10       | 0.51          |
| (1,230) | 1:11:A:TRP:HD1  | 1:21:A:ARG:HB2  | 4        | 0.51          |
| (1,212) | 1:8:A:TYR:HD1   | 1:9:A:ILE:HG21  | 6        | 0.51          |
| (1,212) | 1:8:A:TYR:HD1   | 1:9:A:ILE:HG22  | 6        | 0.51          |
| (1,212) | 1:8:A:TYR:HD1   | 1:9:A:ILE:HG23  | 6        | 0.51          |
| (1,212) | 1:8:A:TYR:HD2   | 1:9:A:ILE:HG21  | 6        | 0.51          |
| (1,212) | 1:8:A:TYR:HD2   | 1:9:A:ILE:HG22  | 6        | 0.51          |
| (1,212) | 1:8:A:TYR:HD2   | 1:9:A:ILE:HG23  | 6        | 0.51          |
| (1,201) | 1:8:A:TYR:HE1   | 1:23:A:PRO:HB3  | 8        | 0.51          |
| (1,201) | 1:8:A:TYR:HE2   | 1:23:A:PRO:HB3  | 8        | 0.51          |
| (1,199) | 1:8:A:TYR:HD1   | 1:23:A:PRO:HB3  | 4        | 0.51          |
| (1,199) | 1:8:A:TYR:HD2   | 1:23:A:PRO:HB3  | 4        | 0.51          |
| (1,198) | 1:11:A:TRP:HZ3  | 1:23:A:PRO:HB3  | 7        | 0.51          |
| (1,190) | 1:11:A:TRP:HD1  | 1:24:A:PRO:HD2  | 4        | 0.51          |
| (1,190) | 1:11:A:TRP:HD1  | 1:24:A:PRO:HD2  | 7        | 0.51          |
| (1,185) | 1:11:A:TRP:HB3  | 1:11:A:TRP:HE3  | 2        | 0.51          |
| (1,185) | 1:11:A:TRP:HB3  | 1:11:A:TRP:HE3  | 6        | 0.51          |
| (1,122) | 1:24:A:PRO:HB2  | 1:25:A:CYS:H    | 3        | 0.51          |
| (1,82)  | 1:3:A:GLU:H     | 1:3:A:GLU:HA    | 5        | 0.51          |
| (1,47)  | 1:10:A:GLN:HE21 | 1:10:A:GLN:HG2  | 10       | 0.51          |
| (1,723) | 1:12:A:LEU:HB3  | 1:13:A:LYS:HG2  | 10       | 0.5           |
| (1,723) | 1:12:A:LEU:HB3  | 1:13:A:LYS:HG3  | 10       | 0.5           |
| (1,665) | 1:3:A:GLU:HG2   | 1:4:A:CYS:HA    | 9        | 0.5           |
| (1,665) | 1:3:A:GLU:HG3   | 1:4:A:CYS:HA    | 9        | 0.5           |
| (1,618) | 1:10:A:GLN:HE21 | 1:13:A:LYS:HD3  | 6        | 0.5           |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,467) | 1:21:A:ARG:HD2  | 1:21:A:ARG:HG2  | 2        | 0.5           |
| (1,467) | 1:21:A:ARG:HD2  | 1:21:A:ARG:HG3  | 2        | 0.5           |
| (1,464) | 1:21:A:ARG:HB3  | 1:21:A:ARG:HD2  | 3        | 0.5           |
| (1,459) | 1:21:A:ARG:HA   | 1:21:A:ARG:HB3  | 7        | 0.5           |
| (1,425) | 1:13:A:LYS:HB2  | 1:13:A:LYS:HD2  | 6        | 0.5           |
| (1,425) | 1:13:A:LYS:HB3  | 1:13:A:LYS:HD2  | 6        | 0.5           |
| (1,415) | 1:12:A:LEU:HB3  | 1:12:A:LEU:HD11 | 4        | 0.5           |
| (1,415) | 1:12:A:LEU:HB3  | 1:12:A:LEU:HD12 | 4        | 0.5           |
| (1,415) | 1:12:A:LEU:HB3  | 1:12:A:LEU:HD13 | 4        | 0.5           |
| (1,378) | 1:9:A:ILE:HA    | 1:9:A:ILE:HG12  | 2        | 0.5           |
| (1,315) | 1:10:A:GLN:HE22 | 1:13:A:LYS:HE2  | 5        | 0.5           |
| (1,315) | 1:10:A:GLN:HE22 | 1:13:A:LYS:HE3  | 5        | 0.5           |
| (1,259) | 1:4:A:CYS:HB3   | 1:5:A:VAL:H     | 9        | 0.5           |
| (1,232) | 1:11:A:TRP:HE3  | 1:12:A:LEU:HG   | 3        | 0.5           |
| (1,232) | 1:11:A:TRP:HE3  | 1:12:A:LEU:HG   | 4        | 0.5           |
| (1,227) | 1:11:A:TRP:HZ2  | 1:23:A:PRO:HG2  | 3        | 0.5           |
| (1,212) | 1:8:A:TYR:HD1   | 1:9:A:ILE:HG21  | 7        | 0.5           |
| (1,212) | 1:8:A:TYR:HD1   | 1:9:A:ILE:HG22  | 7        | 0.5           |
| (1,212) | 1:8:A:TYR:HD1   | 1:9:A:ILE:HG23  | 7        | 0.5           |
| (1,212) | 1:8:A:TYR:HD2   | 1:9:A:ILE:HG21  | 7        | 0.5           |
| (1,212) | 1:8:A:TYR:HD2   | 1:9:A:ILE:HG22  | 7        | 0.5           |
| (1,212) | 1:8:A:TYR:HD2   | 1:9:A:ILE:HG23  | 7        | 0.5           |
| (1,212) | 1:8:A:TYR:HD1   | 1:9:A:ILE:HG21  | 8        | 0.5           |
| (1,212) | 1:8:A:TYR:HD1   | 1:9:A:ILE:HG22  | 8        | 0.5           |
| (1,212) | 1:8:A:TYR:HD1   | 1:9:A:ILE:HG23  | 8        | 0.5           |
| (1,212) | 1:8:A:TYR:HD2   | 1:9:A:ILE:HG21  | 8        | 0.5           |
| (1,212) | 1:8:A:TYR:HD2   | 1:9:A:ILE:HG22  | 8        | 0.5           |
| (1,212) | 1:8:A:TYR:HD2   | 1:9:A:ILE:HG23  | 8        | 0.5           |
| (1,212) | 1:8:A:TYR:HD1   | 1:9:A:ILE:HG21  | 9        | 0.5           |
| (1,212) | 1:8:A:TYR:HD1   | 1:9:A:ILE:HG22  | 9        | 0.5           |
| (1,212) | 1:8:A:TYR:HD1   | 1:9:A:ILE:HG23  | 9        | 0.5           |
| (1,212) | 1:8:A:TYR:HD2   | 1:9:A:ILE:HG21  | 9        | 0.5           |
| (1,212) | 1:8:A:TYR:HD2   | 1:9:A:ILE:HG22  | 9        | 0.5           |
| (1,212) | 1:8:A:TYR:HD2   | 1:9:A:ILE:HG23  | 9        | 0.5           |
| (1,190) | 1:11:A:TRP:HD1  | 1:24:A:PRO:HD2  | 6        | 0.5           |
| (1,190) | 1:11:A:TRP:HD1  | 1:24:A:PRO:HD2  | 9        | 0.5           |
| (1,185) | 1:11:A:TRP:HB3  | 1:11:A:TRP:HE3  | 1        | 0.5           |
| (1,185) | 1:11:A:TRP:HB3  | 1:11:A:TRP:HE3  | 5        | 0.5           |
| (1,185) | 1:11:A:TRP:HB3  | 1:11:A:TRP:HE3  | 7        | 0.5           |
| (1,185) | 1:11:A:TRP:HB3  | 1:11:A:TRP:HE3  | 9        | 0.5           |
| (1,185) | 1:11:A:TRP:HB3  | 1:11:A:TRP:HE3  | 10       | 0.5           |
| (1,160) | 1:11:A:TRP:HZ2  | 1:22:A:PRO:HA   | 7        | 0.5           |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,140) | 1:9:A:ILE:HA    | 1:12:A:LEU:H    | 8        | 0.5           |
| (1,99)  | 1:11:A:TRP:HE1  | 1:22:A:PRO:HA   | 1        | 0.5           |
| (1,47)  | 1:10:A:GLN:HE21 | 1:10:A:GLN:HG2  | 5        | 0.5           |
| (1,47)  | 1:10:A:GLN:HE21 | 1:10:A:GLN:HG2  | 6        | 0.5           |
| (1,47)  | 1:10:A:GLN:HE21 | 1:10:A:GLN:HG2  | 8        | 0.5           |
| (1,723) | 1:12:A:LEU:HB3  | 1:13:A:LYS:HG2  | 8        | 0.49          |
| (1,723) | 1:12:A:LEU:HB3  | 1:13:A:LYS:HG3  | 8        | 0.49          |
| (1,717) | 1:12:A:LEU:HD11 | 1:16:A:GLY:HA2  | 1        | 0.49          |
| (1,717) | 1:12:A:LEU:HD12 | 1:16:A:GLY:HA2  | 1        | 0.49          |
| (1,717) | 1:12:A:LEU:HD13 | 1:16:A:GLY:HA2  | 1        | 0.49          |
| (1,699) | 1:6:A:ARG:HB3   | 1:7:A:LEU:HD11  | 7        | 0.49          |
| (1,699) | 1:6:A:ARG:HB3   | 1:7:A:LEU:HD12  | 7        | 0.49          |
| (1,699) | 1:6:A:ARG:HB3   | 1:7:A:LEU:HD13  | 7        | 0.49          |
| (1,699) | 1:6:A:ARG:HB3   | 1:7:A:LEU:HD21  | 7        | 0.49          |
| (1,699) | 1:6:A:ARG:HB3   | 1:7:A:LEU:HD22  | 7        | 0.49          |
| (1,699) | 1:6:A:ARG:HB3   | 1:7:A:LEU:HD23  | 7        | 0.49          |
| (1,682) | 1:4:A:CYS:HB2   | 1:5:A:VAL:HG11  | 6        | 0.49          |
| (1,682) | 1:4:A:CYS:HB2   | 1:5:A:VAL:HG12  | 6        | 0.49          |
| (1,682) | 1:4:A:CYS:HB2   | 1:5:A:VAL:HG13  | 6        | 0.49          |
| (1,671) | 1:8:A:TYR:HA    | 1:12:A:LEU:HD21 | 8        | 0.49          |
| (1,671) | 1:8:A:TYR:HA    | 1:12:A:LEU:HD22 | 8        | 0.49          |
| (1,671) | 1:8:A:TYR:HA    | 1:12:A:LEU:HD23 | 8        | 0.49          |
| (1,671) | 1:8:A:TYR:HA    | 1:12:A:LEU:HD21 | 10       | 0.49          |
| (1,671) | 1:8:A:TYR:HA    | 1:12:A:LEU:HD22 | 10       | 0.49          |
| (1,671) | 1:8:A:TYR:HA    | 1:12:A:LEU:HD23 | 10       | 0.49          |
| (1,622) | 1:2:A:GLU:HB3   | 1:5:A:VAL:H     | 5        | 0.49          |
| (1,616) | 1:14:A:ASP:HB3  | 1:16:A:GLY:H    | 4        | 0.49          |
| (1,570) | 1:16:A:GLY:HA3  | 1:17:A:PRO:HD2  | 6        | 0.49          |
| (1,535) | 1:23:A:PRO:HB3  | 1:24:A:PRO:HD2  | 10       | 0.49          |
| (1,467) | 1:21:A:ARG:HD2  | 1:21:A:ARG:HG2  | 8        | 0.49          |
| (1,467) | 1:21:A:ARG:HD2  | 1:21:A:ARG:HG3  | 8        | 0.49          |
| (1,431) | 1:14:A:ASP:HA   | 1:14:A:ASP:HB2  | 3        | 0.49          |
| (1,415) | 1:12:A:LEU:HB3  | 1:12:A:LEU:HD11 | 8        | 0.49          |
| (1,415) | 1:12:A:LEU:HB3  | 1:12:A:LEU:HD12 | 8        | 0.49          |
| (1,415) | 1:12:A:LEU:HB3  | 1:12:A:LEU:HD13 | 8        | 0.49          |
| (1,415) | 1:12:A:LEU:HB3  | 1:12:A:LEU:HD11 | 9        | 0.49          |
| (1,415) | 1:12:A:LEU:HB3  | 1:12:A:LEU:HD12 | 9        | 0.49          |
| (1,415) | 1:12:A:LEU:HB3  | 1:12:A:LEU:HD13 | 9        | 0.49          |
| (1,415) | 1:12:A:LEU:HB3  | 1:12:A:LEU:HD11 | 10       | 0.49          |
| (1,415) | 1:12:A:LEU:HB3  | 1:12:A:LEU:HD12 | 10       | 0.49          |
| (1,415) | 1:12:A:LEU:HB3  | 1:12:A:LEU:HD13 | 10       | 0.49          |
| (1,371) | 1:7:A:LEU:HB2   | 1:7:A:LEU:HG    | 8        | 0.49          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,371) | 1:7:A:LEU:HB2  | 1:7:A:LEU:HG   | 9        | 0.49          |
| (1,368) | 1:7:A:LEU:HA   | 1:7:A:LEU:HD11 | 9        | 0.49          |
| (1,368) | 1:7:A:LEU:HA   | 1:7:A:LEU:HD12 | 9        | 0.49          |
| (1,368) | 1:7:A:LEU:HA   | 1:7:A:LEU:HD13 | 9        | 0.49          |
| (1,368) | 1:7:A:LEU:HA   | 1:7:A:LEU:HD21 | 9        | 0.49          |
| (1,368) | 1:7:A:LEU:HA   | 1:7:A:LEU:HD22 | 9        | 0.49          |
| (1,368) | 1:7:A:LEU:HA   | 1:7:A:LEU:HD23 | 9        | 0.49          |
| (1,353) | 1:6:A:ARG:HB3  | 1:6:A:ARG:HD3  | 1        | 0.49          |
| (1,325) | 1:2:A:GLU:HA   | 1:2:A:GLU:HB2  | 6        | 0.49          |
| (1,238) | 1:8:A:TYR:HE1  | 1:23:A:PRO:HG3 | 1        | 0.49          |
| (1,238) | 1:8:A:TYR:HE2  | 1:23:A:PRO:HG3 | 1        | 0.49          |
| (1,223) | 1:8:A:TYR:HE1  | 1:23:A:PRO:HB2 | 5        | 0.49          |
| (1,223) | 1:8:A:TYR:HE2  | 1:23:A:PRO:HB2 | 5        | 0.49          |
| (1,212) | 1:8:A:TYR:HD1  | 1:9:A:ILE:HG21 | 2        | 0.49          |
| (1,212) | 1:8:A:TYR:HD1  | 1:9:A:ILE:HG22 | 2        | 0.49          |
| (1,212) | 1:8:A:TYR:HD1  | 1:9:A:ILE:HG23 | 2        | 0.49          |
| (1,212) | 1:8:A:TYR:HD2  | 1:9:A:ILE:HG21 | 2        | 0.49          |
| (1,212) | 1:8:A:TYR:HD2  | 1:9:A:ILE:HG22 | 2        | 0.49          |
| (1,212) | 1:8:A:TYR:HD2  | 1:9:A:ILE:HG23 | 2        | 0.49          |
| (1,196) | 1:11:A:TRP:HH2 | 1:23:A:PRO:HB3 | 8        | 0.49          |
| (1,185) | 1:11:A:TRP:HB3 | 1:11:A:TRP:HE3 | 3        | 0.49          |
| (1,185) | 1:11:A:TRP:HB3 | 1:11:A:TRP:HE3 | 8        | 0.49          |
| (1,160) | 1:11:A:TRP:HZ2 | 1:22:A:PRO:HA  | 2        | 0.49          |
| (1,140) | 1:9:A:ILE:HA   | 1:12:A:LEU:H   | 4        | 0.49          |
| (1,723) | 1:12:A:LEU:HB3 | 1:13:A:LYS:HG2 | 7        | 0.48          |
| (1,723) | 1:12:A:LEU:HB3 | 1:13:A:LYS:HG3 | 7        | 0.48          |
| (1,699) | 1:6:A:ARG:HB3  | 1:7:A:LEU:HD11 | 2        | 0.48          |
| (1,699) | 1:6:A:ARG:HB3  | 1:7:A:LEU:HD12 | 2        | 0.48          |
| (1,699) | 1:6:A:ARG:HB3  | 1:7:A:LEU:HD13 | 2        | 0.48          |
| (1,699) | 1:6:A:ARG:HB3  | 1:7:A:LEU:HD21 | 2        | 0.48          |
| (1,699) | 1:6:A:ARG:HB3  | 1:7:A:LEU:HD22 | 2        | 0.48          |
| (1,699) | 1:6:A:ARG:HB3  | 1:7:A:LEU:HD23 | 2        | 0.48          |
| (1,626) | 1:14:A:ASP:HB3 | 1:15:A:GLY:H   | 8        | 0.48          |
| (1,614) | 1:19:A:SER:HG  | 1:20:A:GLY:H   | 7        | 0.48          |
| (1,605) | 1:8:A:TYR:HE1  | 1:11:A:TRP:HZ3 | 4        | 0.48          |
| (1,605) | 1:8:A:TYR:HE2  | 1:11:A:TRP:HZ3 | 4        | 0.48          |
| (1,605) | 1:8:A:TYR:HE1  | 1:11:A:TRP:HZ3 | 10       | 0.48          |
| (1,605) | 1:8:A:TYR:HE2  | 1:11:A:TRP:HZ3 | 10       | 0.48          |
| (1,565) | 1:4:A:CYS:HA   | 1:7:A:LEU:HG   | 8        | 0.48          |
| (1,494) | 1:21:A:ARG:HA  | 1:22:A:PRO:HD3 | 9        | 0.48          |
| (1,472) | 1:22:A:PRO:HA  | 1:22:A:PRO:HD2 | 4        | 0.48          |
| (1,459) | 1:21:A:ARG:HA  | 1:21:A:ARG:HB3 | 4        | 0.48          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,415) | 1:12:A:LEU:HB3  | 1:12:A:LEU:HD11 | 7        | 0.48          |
| (1,415) | 1:12:A:LEU:HB3  | 1:12:A:LEU:HD12 | 7        | 0.48          |
| (1,415) | 1:12:A:LEU:HB3  | 1:12:A:LEU:HD13 | 7        | 0.48          |
| (1,371) | 1:7:A:LEU:HB2   | 1:7:A:LEU:HG    | 1        | 0.48          |
| (1,371) | 1:7:A:LEU:HB2   | 1:7:A:LEU:HG    | 2        | 0.48          |
| (1,371) | 1:7:A:LEU:HB2   | 1:7:A:LEU:HG    | 5        | 0.48          |
| (1,371) | 1:7:A:LEU:HB2   | 1:7:A:LEU:HG    | 7        | 0.48          |
| (1,371) | 1:7:A:LEU:HB2   | 1:7:A:LEU:HG    | 10       | 0.48          |
| (1,353) | 1:6:A:ARG:HB3   | 1:6:A:ARG:HD3   | 8        | 0.48          |
| (1,349) | 1:6:A:ARG:HA    | 1:6:A:ARG:HG2   | 2        | 0.48          |
| (1,321) | 1:11:A:TRP:HB3  | 1:12:A:LEU:H    | 1        | 0.48          |
| (1,321) | 1:11:A:TRP:HB3  | 1:12:A:LEU:H    | 5        | 0.48          |
| (1,270) | 1:8:A:TYR:HD1   | 1:25:A:CYS:H    | 7        | 0.48          |
| (1,270) | 1:8:A:TYR:HD2   | 1:25:A:CYS:H    | 7        | 0.48          |
| (1,270) | 1:8:A:TYR:HD1   | 1:25:A:CYS:H    | 8        | 0.48          |
| (1,270) | 1:8:A:TYR:HD2   | 1:25:A:CYS:H    | 8        | 0.48          |
| (1,270) | 1:8:A:TYR:HD1   | 1:25:A:CYS:H    | 9        | 0.48          |
| (1,270) | 1:8:A:TYR:HD2   | 1:25:A:CYS:H    | 9        | 0.48          |
| (1,232) | 1:11:A:TRP:HE3  | 1:12:A:LEU:HG   | 7        | 0.48          |
| (1,232) | 1:11:A:TRP:HE3  | 1:12:A:LEU:HG   | 9        | 0.48          |
| (1,212) | 1:8:A:TYR:HD1   | 1:9:A:ILE:HG21  | 1        | 0.48          |
| (1,212) | 1:8:A:TYR:HD1   | 1:9:A:ILE:HG22  | 1        | 0.48          |
| (1,212) | 1:8:A:TYR:HD1   | 1:9:A:ILE:HG23  | 1        | 0.48          |
| (1,212) | 1:8:A:TYR:HD2   | 1:9:A:ILE:HG21  | 1        | 0.48          |
| (1,212) | 1:8:A:TYR:HD2   | 1:9:A:ILE:HG22  | 1        | 0.48          |
| (1,212) | 1:8:A:TYR:HD2   | 1:9:A:ILE:HG23  | 1        | 0.48          |
| (1,212) | 1:8:A:TYR:HD1   | 1:9:A:ILE:HG21  | 4        | 0.48          |
| (1,212) | 1:8:A:TYR:HD1   | 1:9:A:ILE:HG22  | 4        | 0.48          |
| (1,212) | 1:8:A:TYR:HD1   | 1:9:A:ILE:HG23  | 4        | 0.48          |
| (1,212) | 1:8:A:TYR:HD2   | 1:9:A:ILE:HG21  | 4        | 0.48          |
| (1,212) | 1:8:A:TYR:HD2   | 1:9:A:ILE:HG22  | 4        | 0.48          |
| (1,212) | 1:8:A:TYR:HD2   | 1:9:A:ILE:HG23  | 4        | 0.48          |
| (1,196) | 1:11:A:TRP:HH2  | 1:23:A:PRO:HB3  | 3        | 0.48          |
| (1,196) | 1:11:A:TRP:HH2  | 1:23:A:PRO:HB3  | 10       | 0.48          |
| (1,185) | 1:11:A:TRP:HB3  | 1:11:A:TRP:HE3  | 4        | 0.48          |
| (1,99)  | 1:11:A:TRP:HE1  | 1:22:A:PRO:HA   | 7        | 0.48          |
| (1,92)  | 1:19:A:SER:H    | 1:19:A:SER:HG   | 6        | 0.48          |
| (1,92)  | 1:19:A:SER:H    | 1:19:A:SER:HG   | 8        | 0.48          |
| (1,47)  | 1:10:A:GLN:HE21 | 1:10:A:GLN:HG2  | 1        | 0.48          |
| (1,47)  | 1:10:A:GLN:HE21 | 1:10:A:GLN:HG2  | 7        | 0.48          |
| (1,682) | 1:4:A:CYS:HB2   | 1:5:A:VAL:HG11  | 4        | 0.47          |
| (1,682) | 1:4:A:CYS:HB2   | 1:5:A:VAL:HG12  | 4        | 0.47          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,682) | 1:4:A:CYS:HB2  | 1:5:A:VAL:HG13 | 4        | 0.47          |
| (1,666) | 1:24:A:PRO:HG2 | 1:25:A:CYS:HB2 | 8        | 0.47          |
| (1,664) | 1:21:A:ARG:HB3 | 1:22:A:PRO:HD2 | 4        | 0.47          |
| (1,662) | 1:17:A:PRO:HB3 | 1:18:A:SER:HB2 | 4        | 0.47          |
| (1,579) | 1:4:A:CYS:HA   | 1:7:A:LEU:HB2  | 1        | 0.47          |
| (1,564) | 1:4:A:CYS:HA   | 1:7:A:LEU:HB3  | 1        | 0.47          |
| (1,512) | 1:23:A:PRO:HB3 | 1:23:A:PRO:HD3 | 1        | 0.47          |
| (1,512) | 1:23:A:PRO:HB3 | 1:23:A:PRO:HD3 | 2        | 0.47          |
| (1,512) | 1:23:A:PRO:HB3 | 1:23:A:PRO:HD3 | 3        | 0.47          |
| (1,459) | 1:21:A:ARG:HA  | 1:21:A:ARG:HB3 | 1        | 0.47          |
| (1,459) | 1:21:A:ARG:HA  | 1:21:A:ARG:HB3 | 5        | 0.47          |
| (1,459) | 1:21:A:ARG:HA  | 1:21:A:ARG:HB3 | 9        | 0.47          |
| (1,425) | 1:13:A:LYS:HB2 | 1:13:A:LYS:HD2 | 8        | 0.47          |
| (1,425) | 1:13:A:LYS:HB3 | 1:13:A:LYS:HD2 | 8        | 0.47          |
| (1,425) | 1:13:A:LYS:HB2 | 1:13:A:LYS:HD2 | 9        | 0.47          |
| (1,425) | 1:13:A:LYS:HB3 | 1:13:A:LYS:HD2 | 9        | 0.47          |
| (1,425) | 1:13:A:LYS:HB2 | 1:13:A:LYS:HD2 | 10       | 0.47          |
| (1,425) | 1:13:A:LYS:HB3 | 1:13:A:LYS:HD2 | 10       | 0.47          |
| (1,371) | 1:7:A:LEU:HB2  | 1:7:A:LEU:HG   | 3        | 0.47          |
| (1,371) | 1:7:A:LEU:HB2  | 1:7:A:LEU:HG   | 4        | 0.47          |
| (1,371) | 1:7:A:LEU:HB2  | 1:7:A:LEU:HG   | 6        | 0.47          |
| (1,357) | 1:6:A:ARG:HD3  | 1:6:A:ARG:HG2  | 8        | 0.47          |
| (1,325) | 1:2:A:GLU:HA   | 1:2:A:GLU:HB2  | 8        | 0.47          |
| (1,277) | 1:20:A:GLY:H   | 1:21:A:ARG:H   | 8        | 0.47          |
| (1,230) | 1:11:A:TRP:HD1 | 1:21:A:ARG:HB2 | 6        | 0.47          |
| (1,212) | 1:8:A:TYR:HD1  | 1:9:A:ILE:HG21 | 10       | 0.47          |
| (1,212) | 1:8:A:TYR:HD1  | 1:9:A:ILE:HG22 | 10       | 0.47          |
| (1,212) | 1:8:A:TYR:HD1  | 1:9:A:ILE:HG23 | 10       | 0.47          |
| (1,212) | 1:8:A:TYR:HD2  | 1:9:A:ILE:HG21 | 10       | 0.47          |
| (1,212) | 1:8:A:TYR:HD2  | 1:9:A:ILE:HG22 | 10       | 0.47          |
| (1,212) | 1:8:A:TYR:HD2  | 1:9:A:ILE:HG23 | 10       | 0.47          |
| (1,160) | 1:11:A:TRP:HZ2 | 1:22:A:PRO:HA  | 3        | 0.47          |
| (1,160) | 1:11:A:TRP:HZ2 | 1:22:A:PRO:HA  | 8        | 0.47          |
| (1,160) | 1:11:A:TRP:HZ2 | 1:22:A:PRO:HA  | 10       | 0.47          |
| (1,140) | 1:9:A:ILE:HA   | 1:12:A:LEU:H   | 2        | 0.47          |
| (1,140) | 1:9:A:ILE:HA   | 1:12:A:LEU:H   | 10       | 0.47          |
| (1,99)  | 1:11:A:TRP:HE1 | 1:22:A:PRO:HA  | 5        | 0.47          |
| (1,92)  | 1:19:A:SER:H   | 1:19:A:SER:HG  | 5        | 0.47          |
| (1,26)  | 1:2:A:GLU:HB2  | 1:3:A:GLU:H    | 3        | 0.47          |
| (1,734) | 1:2:A:GLU:HG3  | 1:5:A:VAL:HB   | 7        | 0.46          |
| (1,719) | 1:9:A:ILE:HG12 | 1:12:A:LEU:HG  | 7        | 0.46          |
| (1,699) | 1:6:A:ARG:HB3  | 1:7:A:LEU:HD11 | 3        | 0.46          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,699) | 1:6:A:ARG:HB3   | 1:7:A:LEU:HD12 | 3        | 0.46          |
| (1,699) | 1:6:A:ARG:HB3   | 1:7:A:LEU:HD13 | 3        | 0.46          |
| (1,699) | 1:6:A:ARG:HB3   | 1:7:A:LEU:HD21 | 3        | 0.46          |
| (1,699) | 1:6:A:ARG:HB3   | 1:7:A:LEU:HD22 | 3        | 0.46          |
| (1,699) | 1:6:A:ARG:HB3   | 1:7:A:LEU:HD23 | 3        | 0.46          |
| (1,622) | 1:2:A:GLU:HB3   | 1:5:A:VAL:H    | 6        | 0.46          |
| (1,564) | 1:4:A:CYS:HA    | 1:7:A:LEU:HB3  | 8        | 0.46          |
| (1,512) | 1:23:A:PRO:HB3  | 1:23:A:PRO:HD3 | 5        | 0.46          |
| (1,512) | 1:23:A:PRO:HB3  | 1:23:A:PRO:HD3 | 6        | 0.46          |
| (1,494) | 1:21:A:ARG:HA   | 1:22:A:PRO:HD3 | 1        | 0.46          |
| (1,492) | 1:22:A:PRO:HB3  | 1:22:A:PRO:HG3 | 2        | 0.46          |
| (1,492) | 1:22:A:PRO:HB3  | 1:22:A:PRO:HG3 | 3        | 0.46          |
| (1,492) | 1:22:A:PRO:HB3  | 1:22:A:PRO:HG3 | 8        | 0.46          |
| (1,492) | 1:22:A:PRO:HB3  | 1:22:A:PRO:HG3 | 9        | 0.46          |
| (1,492) | 1:22:A:PRO:HB3  | 1:22:A:PRO:HG3 | 10       | 0.46          |
| (1,467) | 1:21:A:ARG:HD2  | 1:21:A:ARG:HG2 | 10       | 0.46          |
| (1,467) | 1:21:A:ARG:HD2  | 1:21:A:ARG:HG3 | 10       | 0.46          |
| (1,464) | 1:21:A:ARG:HB3  | 1:21:A:ARG:HD2 | 2        | 0.46          |
| (1,459) | 1:21:A:ARG:HA   | 1:21:A:ARG:HB3 | 6        | 0.46          |
| (1,431) | 1:14:A:ASP:HA   | 1:14:A:ASP:HB2 | 1        | 0.46          |
| (1,431) | 1:14:A:ASP:HA   | 1:14:A:ASP:HB2 | 6        | 0.46          |
| (1,378) | 1:9:A:ILE:HA    | 1:9:A:ILE:HG12 | 3        | 0.46          |
| (1,357) | 1:6:A:ARG:HD3   | 1:6:A:ARG:HG2  | 7        | 0.46          |
| (1,334) | 1:3:A:GLU:HA    | 1:3:A:GLU:HG2  | 5        | 0.46          |
| (1,334) | 1:3:A:GLU:HA    | 1:3:A:GLU:HG3  | 5        | 0.46          |
| (1,325) | 1:2:A:GLU:HA    | 1:2:A:GLU:HB2  | 3        | 0.46          |
| (1,325) | 1:2:A:GLU:HA    | 1:2:A:GLU:HB2  | 9        | 0.46          |
| (1,321) | 1:11:A:TRP:HB3  | 1:12:A:LEU:H   | 2        | 0.46          |
| (1,315) | 1:10:A:GLN:HE22 | 1:13:A:LYS:HE2 | 7        | 0.46          |
| (1,315) | 1:10:A:GLN:HE22 | 1:13:A:LYS:HE3 | 7        | 0.46          |
| (1,259) | 1:4:A:CYS:HB3   | 1:5:A:VAL:H    | 1        | 0.46          |
| (1,172) | 1:11:A:TRP:HZ2  | 1:23:A:PRO:HD3 | 7        | 0.46          |
| (1,140) | 1:9:A:ILE:HA    | 1:12:A:LEU:H   | 7        | 0.46          |
| (1,47)  | 1:10:A:GLN:HE21 | 1:10:A:GLN:HG2 | 2        | 0.46          |
| (1,719) | 1:9:A:ILE:HG12  | 1:12:A:LEU:HG  | 4        | 0.45          |
| (1,699) | 1:6:A:ARG:HB3   | 1:7:A:LEU:HD11 | 9        | 0.45          |
| (1,699) | 1:6:A:ARG:HB3   | 1:7:A:LEU:HD12 | 9        | 0.45          |
| (1,699) | 1:6:A:ARG:HB3   | 1:7:A:LEU:HD13 | 9        | 0.45          |
| (1,699) | 1:6:A:ARG:HB3   | 1:7:A:LEU:HD21 | 9        | 0.45          |
| (1,699) | 1:6:A:ARG:HB3   | 1:7:A:LEU:HD22 | 9        | 0.45          |
| (1,699) | 1:6:A:ARG:HB3   | 1:7:A:LEU:HD23 | 9        | 0.45          |
| (1,665) | 1:3:A:GLU:HG2   | 1:4:A:CYS:HA   | 10       | 0.45          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,665) | 1:3:A:GLU:HG3  | 1:4:A:CYS:HA    | 10       | 0.45          |
| (1,657) | 1:4:A:CYS:HB2  | 1:25:A:CYS:HB3  | 4        | 0.45          |
| (1,571) | 1:14:A:ASP:HB3 | 1:19:A:SER:HB2  | 3        | 0.45          |
| (1,571) | 1:14:A:ASP:HB3 | 1:19:A:SER:HB2  | 10       | 0.45          |
| (1,535) | 1:23:A:PRO:HB3 | 1:24:A:PRO:HD2  | 5        | 0.45          |
| (1,492) | 1:22:A:PRO:HB3 | 1:22:A:PRO:HG3  | 1        | 0.45          |
| (1,492) | 1:22:A:PRO:HB3 | 1:22:A:PRO:HG3  | 5        | 0.45          |
| (1,474) | 1:22:A:PRO:HA  | 1:22:A:PRO:HB3  | 1        | 0.45          |
| (1,474) | 1:22:A:PRO:HA  | 1:22:A:PRO:HB3  | 5        | 0.45          |
| (1,472) | 1:22:A:PRO:HA  | 1:22:A:PRO:HD2  | 7        | 0.45          |
| (1,357) | 1:6:A:ARG:HD3  | 1:6:A:ARG:HG2   | 9        | 0.45          |
| (1,350) | 1:6:A:ARG:HA   | 1:6:A:ARG:HG3   | 7        | 0.45          |
| (1,325) | 1:2:A:GLU:HA   | 1:2:A:GLU:HB2   | 10       | 0.45          |
| (1,273) | 1:18:A:SER:H   | 1:19:A:SER:H    | 6        | 0.45          |
| (1,230) | 1:11:A:TRP:HD1 | 1:21:A:ARG:HB2  | 9        | 0.45          |
| (1,222) | 1:8:A:TYR:HD1  | 1:23:A:PRO:HB2  | 10       | 0.45          |
| (1,222) | 1:8:A:TYR:HD2  | 1:23:A:PRO:HB2  | 10       | 0.45          |
| (1,208) | 1:11:A:TRP:HZ3 | 1:12:A:LEU:HD11 | 1        | 0.45          |
| (1,208) | 1:11:A:TRP:HZ3 | 1:12:A:LEU:HD12 | 1        | 0.45          |
| (1,208) | 1:11:A:TRP:HZ3 | 1:12:A:LEU:HD13 | 1        | 0.45          |
| (1,208) | 1:11:A:TRP:HZ3 | 1:12:A:LEU:HD11 | 2        | 0.45          |
| (1,208) | 1:11:A:TRP:HZ3 | 1:12:A:LEU:HD12 | 2        | 0.45          |
| (1,208) | 1:11:A:TRP:HZ3 | 1:12:A:LEU:HD13 | 2        | 0.45          |
| (1,196) | 1:11:A:TRP:HH2 | 1:23:A:PRO:HB3  | 9        | 0.45          |
| (1,166) | 1:5:A:VAL:HA   | 1:8:A:TYR:HD1   | 9        | 0.45          |
| (1,166) | 1:5:A:VAL:HA   | 1:8:A:TYR:HD2   | 9        | 0.45          |
| (1,111) | 1:10:A:GLN:HB3 | 1:11:A:TRP:H    | 2        | 0.45          |
| (1,108) | 1:14:A:ASP:H   | 1:15:A:GLY:H    | 7        | 0.45          |
| (1,734) | 1:2:A:GLU:HG3  | 1:5:A:VAL:HB    | 9        | 0.44          |
| (1,699) | 1:6:A:ARG:HB3  | 1:7:A:LEU:HD11  | 5        | 0.44          |
| (1,699) | 1:6:A:ARG:HB3  | 1:7:A:LEU:HD12  | 5        | 0.44          |
| (1,699) | 1:6:A:ARG:HB3  | 1:7:A:LEU:HD13  | 5        | 0.44          |
| (1,699) | 1:6:A:ARG:HB3  | 1:7:A:LEU:HD21  | 5        | 0.44          |
| (1,699) | 1:6:A:ARG:HB3  | 1:7:A:LEU:HD22  | 5        | 0.44          |
| (1,699) | 1:6:A:ARG:HB3  | 1:7:A:LEU:HD23  | 5        | 0.44          |
| (1,699) | 1:6:A:ARG:HB3  | 1:7:A:LEU:HD11  | 6        | 0.44          |
| (1,699) | 1:6:A:ARG:HB3  | 1:7:A:LEU:HD12  | 6        | 0.44          |
| (1,699) | 1:6:A:ARG:HB3  | 1:7:A:LEU:HD13  | 6        | 0.44          |
| (1,699) | 1:6:A:ARG:HB3  | 1:7:A:LEU:HD21  | 6        | 0.44          |
| (1,699) | 1:6:A:ARG:HB3  | 1:7:A:LEU:HD22  | 6        | 0.44          |
| (1,699) | 1:6:A:ARG:HB3  | 1:7:A:LEU:HD23  | 6        | 0.44          |
| (1,699) | 1:6:A:ARG:HB3  | 1:7:A:LEU:HD11  | 8        | 0.44          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,699) | 1:6:A:ARG:HB3  | 1:7:A:LEU:HD12  | 8        | 0.44          |
| (1,699) | 1:6:A:ARG:HB3  | 1:7:A:LEU:HD13  | 8        | 0.44          |
| (1,699) | 1:6:A:ARG:HB3  | 1:7:A:LEU:HD21  | 8        | 0.44          |
| (1,699) | 1:6:A:ARG:HB3  | 1:7:A:LEU:HD22  | 8        | 0.44          |
| (1,699) | 1:6:A:ARG:HB3  | 1:7:A:LEU:HD23  | 8        | 0.44          |
| (1,699) | 1:6:A:ARG:HB3  | 1:7:A:LEU:HD11  | 10       | 0.44          |
| (1,699) | 1:6:A:ARG:HB3  | 1:7:A:LEU:HD12  | 10       | 0.44          |
| (1,699) | 1:6:A:ARG:HB3  | 1:7:A:LEU:HD13  | 10       | 0.44          |
| (1,699) | 1:6:A:ARG:HB3  | 1:7:A:LEU:HD21  | 10       | 0.44          |
| (1,699) | 1:6:A:ARG:HB3  | 1:7:A:LEU:HD22  | 10       | 0.44          |
| (1,699) | 1:6:A:ARG:HB3  | 1:7:A:LEU:HD23  | 10       | 0.44          |
| (1,665) | 1:3:A:GLU:HG2  | 1:4:A:CYS:HA    | 8        | 0.44          |
| (1,665) | 1:3:A:GLU:HG3  | 1:4:A:CYS:HA    | 8        | 0.44          |
| (1,626) | 1:14:A:ASP:HB3 | 1:15:A:GLY:H    | 6        | 0.44          |
| (1,616) | 1:14:A:ASP:HB3 | 1:16:A:GLY:H    | 7        | 0.44          |
| (1,569) | 1:8:A:TYR:HA   | 1:11:A:TRP:HB3  | 3        | 0.44          |
| (1,564) | 1:4:A:CYS:HA   | 1:7:A:LEU:HB3   | 5        | 0.44          |
| (1,492) | 1:22:A:PRO:HB3 | 1:22:A:PRO:HG3  | 6        | 0.44          |
| (1,474) | 1:22:A:PRO:HA  | 1:22:A:PRO:HB3  | 3        | 0.44          |
| (1,474) | 1:22:A:PRO:HA  | 1:22:A:PRO:HB3  | 6        | 0.44          |
| (1,474) | 1:22:A:PRO:HA  | 1:22:A:PRO:HB3  | 9        | 0.44          |
| (1,357) | 1:6:A:ARG:HD3  | 1:6:A:ARG:HG2   | 1        | 0.44          |
| (1,280) | 1:4:A:CYS:H    | 1:5:A:VAL:H     | 8        | 0.44          |
| (1,276) | 1:19:A:SER:H   | 1:20:A:GLY:H    | 6        | 0.44          |
| (1,208) | 1:11:A:TRP:HZ3 | 1:12:A:LEU:HD11 | 5        | 0.44          |
| (1,208) | 1:11:A:TRP:HZ3 | 1:12:A:LEU:HD12 | 5        | 0.44          |
| (1,208) | 1:11:A:TRP:HZ3 | 1:12:A:LEU:HD13 | 5        | 0.44          |
| (1,201) | 1:8:A:TYR:HE1  | 1:23:A:PRO:HB3  | 9        | 0.44          |
| (1,201) | 1:8:A:TYR:HE2  | 1:23:A:PRO:HB3  | 9        | 0.44          |
| (1,173) | 1:11:A:TRP:HH2 | 1:17:A:PRO:HD3  | 9        | 0.44          |
| (1,166) | 1:5:A:VAL:HA   | 1:8:A:TYR:HD1   | 10       | 0.44          |
| (1,166) | 1:5:A:VAL:HA   | 1:8:A:TYR:HD2   | 10       | 0.44          |
| (1,160) | 1:11:A:TRP:HZ2 | 1:22:A:PRO:HA   | 4        | 0.44          |
| (1,140) | 1:9:A:ILE:HA   | 1:12:A:LEU:H    | 9        | 0.44          |
| (1,736) | 1:23:A:PRO:HA  | 1:24:A:PRO:HD3  | 3        | 0.43          |
| (1,723) | 1:12:A:LEU:HB3 | 1:13:A:LYS:HG2  | 4        | 0.43          |
| (1,723) | 1:12:A:LEU:HB3 | 1:13:A:LYS:HG3  | 4        | 0.43          |
| (1,716) | 1:9:A:ILE:HG12 | 1:12:A:LEU:HD11 | 6        | 0.43          |
| (1,716) | 1:9:A:ILE:HG12 | 1:12:A:LEU:HD12 | 6        | 0.43          |
| (1,716) | 1:9:A:ILE:HG12 | 1:12:A:LEU:HD13 | 6        | 0.43          |
| (1,682) | 1:4:A:CYS:HB2  | 1:5:A:VAL:HG11  | 2        | 0.43          |
| (1,682) | 1:4:A:CYS:HB2  | 1:5:A:VAL:HG12  | 2        | 0.43          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,682) | 1:4:A:CYS:HB2  | 1:5:A:VAL:HG13 | 2        | 0.43          |
| (1,682) | 1:4:A:CYS:HB2  | 1:5:A:VAL:HG11 | 5        | 0.43          |
| (1,682) | 1:4:A:CYS:HB2  | 1:5:A:VAL:HG12 | 5        | 0.43          |
| (1,682) | 1:4:A:CYS:HB2  | 1:5:A:VAL:HG13 | 5        | 0.43          |
| (1,640) | 1:11:A:TRP:HE3 | 1:24:A:PRO:HD2 | 4        | 0.43          |
| (1,631) | 1:5:A:VAL:HG11 | 1:8:A:TYR:HD1  | 5        | 0.43          |
| (1,631) | 1:5:A:VAL:HG11 | 1:8:A:TYR:HD2  | 5        | 0.43          |
| (1,631) | 1:5:A:VAL:HG12 | 1:8:A:TYR:HD1  | 5        | 0.43          |
| (1,631) | 1:5:A:VAL:HG12 | 1:8:A:TYR:HD2  | 5        | 0.43          |
| (1,631) | 1:5:A:VAL:HG13 | 1:8:A:TYR:HD1  | 5        | 0.43          |
| (1,631) | 1:5:A:VAL:HG13 | 1:8:A:TYR:HD2  | 5        | 0.43          |
| (1,631) | 1:5:A:VAL:HG11 | 1:8:A:TYR:HD1  | 8        | 0.43          |
| (1,631) | 1:5:A:VAL:HG11 | 1:8:A:TYR:HD2  | 8        | 0.43          |
| (1,631) | 1:5:A:VAL:HG12 | 1:8:A:TYR:HD1  | 8        | 0.43          |
| (1,631) | 1:5:A:VAL:HG12 | 1:8:A:TYR:HD2  | 8        | 0.43          |
| (1,631) | 1:5:A:VAL:HG13 | 1:8:A:TYR:HD1  | 8        | 0.43          |
| (1,631) | 1:5:A:VAL:HG13 | 1:8:A:TYR:HD2  | 8        | 0.43          |
| (1,622) | 1:2:A:GLU:HB3  | 1:5:A:VAL:H    | 4        | 0.43          |
| (1,546) | 1:13:A:LYS:HD3 | 1:13:A:LYS:HE2 | 1        | 0.43          |
| (1,546) | 1:13:A:LYS:HD3 | 1:13:A:LYS:HE3 | 1        | 0.43          |
| (1,535) | 1:23:A:PRO:HB3 | 1:24:A:PRO:HD2 | 1        | 0.43          |
| (1,492) | 1:22:A:PRO:HB3 | 1:22:A:PRO:HG3 | 4        | 0.43          |
| (1,474) | 1:22:A:PRO:HA  | 1:22:A:PRO:HB3 | 8        | 0.43          |
| (1,474) | 1:22:A:PRO:HA  | 1:22:A:PRO:HB3 | 10       | 0.43          |
| (1,467) | 1:21:A:ARG:HD2 | 1:21:A:ARG:HG2 | 6        | 0.43          |
| (1,467) | 1:21:A:ARG:HD2 | 1:21:A:ARG:HG3 | 6        | 0.43          |
| (1,431) | 1:14:A:ASP:HA  | 1:14:A:ASP:HB2 | 2        | 0.43          |
| (1,369) | 1:7:A:LEU:HB3  | 1:7:A:LEU:HD11 | 4        | 0.43          |
| (1,369) | 1:7:A:LEU:HB3  | 1:7:A:LEU:HD12 | 4        | 0.43          |
| (1,369) | 1:7:A:LEU:HB3  | 1:7:A:LEU:HD13 | 4        | 0.43          |
| (1,369) | 1:7:A:LEU:HB3  | 1:7:A:LEU:HD21 | 4        | 0.43          |
| (1,369) | 1:7:A:LEU:HB3  | 1:7:A:LEU:HD22 | 4        | 0.43          |
| (1,369) | 1:7:A:LEU:HB3  | 1:7:A:LEU:HD23 | 4        | 0.43          |
| (1,368) | 1:7:A:LEU:HA   | 1:7:A:LEU:HD11 | 8        | 0.43          |
| (1,368) | 1:7:A:LEU:HA   | 1:7:A:LEU:HD12 | 8        | 0.43          |
| (1,368) | 1:7:A:LEU:HA   | 1:7:A:LEU:HD13 | 8        | 0.43          |
| (1,368) | 1:7:A:LEU:HA   | 1:7:A:LEU:HD21 | 8        | 0.43          |
| (1,368) | 1:7:A:LEU:HA   | 1:7:A:LEU:HD22 | 8        | 0.43          |
| (1,368) | 1:7:A:LEU:HA   | 1:7:A:LEU:HD23 | 8        | 0.43          |
| (1,357) | 1:6:A:ARG:HD3  | 1:6:A:ARG:HG2  | 2        | 0.43          |
| (1,325) | 1:2:A:GLU:HA   | 1:2:A:GLU:HB2  | 7        | 0.43          |
| (1,277) | 1:20:A:GLY:H   | 1:21:A:ARG:H   | 10       | 0.43          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,273) | 1:18:A:SER:H    | 1:19:A:SER:H   | 4        | 0.43          |
| (1,259) | 1:4:A:CYS:HB3   | 1:5:A:VAL:H    | 8        | 0.43          |
| (1,140) | 1:9:A:ILE:HA    | 1:12:A:LEU:H   | 1        | 0.43          |
| (1,111) | 1:10:A:GLN:HB3  | 1:11:A:TRP:H   | 10       | 0.43          |
| (1,92)  | 1:19:A:SER:H    | 1:19:A:SER:HG  | 7        | 0.43          |
| (1,734) | 1:2:A:GLU:HG3   | 1:5:A:VAL:HB   | 8        | 0.42          |
| (1,717) | 1:12:A:LEU:HD11 | 1:16:A:GLY:HA2 | 3        | 0.42          |
| (1,717) | 1:12:A:LEU:HD12 | 1:16:A:GLY:HA2 | 3        | 0.42          |
| (1,717) | 1:12:A:LEU:HD13 | 1:16:A:GLY:HA2 | 3        | 0.42          |
| (1,711) | 1:12:A:LEU:HD21 | 1:23:A:PRO:HB2 | 8        | 0.42          |
| (1,711) | 1:12:A:LEU:HD22 | 1:23:A:PRO:HB2 | 8        | 0.42          |
| (1,711) | 1:12:A:LEU:HD23 | 1:23:A:PRO:HB2 | 8        | 0.42          |
| (1,711) | 1:12:A:LEU:HD21 | 1:23:A:PRO:HB2 | 9        | 0.42          |
| (1,711) | 1:12:A:LEU:HD22 | 1:23:A:PRO:HB2 | 9        | 0.42          |
| (1,711) | 1:12:A:LEU:HD23 | 1:23:A:PRO:HB2 | 9        | 0.42          |
| (1,705) | 1:9:A:ILE:HG21  | 1:13:A:LYS:HD2 | 5        | 0.42          |
| (1,705) | 1:9:A:ILE:HG22  | 1:13:A:LYS:HD2 | 5        | 0.42          |
| (1,705) | 1:9:A:ILE:HG23  | 1:13:A:LYS:HD2 | 5        | 0.42          |
| (1,699) | 1:6:A:ARG:HB3   | 1:7:A:LEU:HD11 | 1        | 0.42          |
| (1,699) | 1:6:A:ARG:HB3   | 1:7:A:LEU:HD12 | 1        | 0.42          |
| (1,699) | 1:6:A:ARG:HB3   | 1:7:A:LEU:HD13 | 1        | 0.42          |
| (1,699) | 1:6:A:ARG:HB3   | 1:7:A:LEU:HD21 | 1        | 0.42          |
| (1,699) | 1:6:A:ARG:HB3   | 1:7:A:LEU:HD22 | 1        | 0.42          |
| (1,699) | 1:6:A:ARG:HB3   | 1:7:A:LEU:HD23 | 1        | 0.42          |
| (1,699) | 1:6:A:ARG:HB3   | 1:7:A:LEU:HD11 | 4        | 0.42          |
| (1,699) | 1:6:A:ARG:HB3   | 1:7:A:LEU:HD12 | 4        | 0.42          |
| (1,699) | 1:6:A:ARG:HB3   | 1:7:A:LEU:HD13 | 4        | 0.42          |
| (1,699) | 1:6:A:ARG:HB3   | 1:7:A:LEU:HD21 | 4        | 0.42          |
| (1,699) | 1:6:A:ARG:HB3   | 1:7:A:LEU:HD22 | 4        | 0.42          |
| (1,699) | 1:6:A:ARG:HB3   | 1:7:A:LEU:HD23 | 4        | 0.42          |
| (1,682) | 1:4:A:CYS:HB2   | 1:5:A:VAL:HG11 | 9        | 0.42          |
| (1,682) | 1:4:A:CYS:HB2   | 1:5:A:VAL:HG12 | 9        | 0.42          |
| (1,682) | 1:4:A:CYS:HB2   | 1:5:A:VAL:HG13 | 9        | 0.42          |
| (1,661) | 1:17:A:PRO:HB3  | 1:18:A:SER:HB3 | 2        | 0.42          |
| (1,651) | 1:3:A:GLU:HA    | 1:6:A:ARG:HD2  | 7        | 0.42          |
| (1,640) | 1:11:A:TRP:HE3  | 1:24:A:PRO:HD2 | 7        | 0.42          |
| (1,616) | 1:14:A:ASP:HB3  | 1:16:A:GLY:H   | 9        | 0.42          |
| (1,615) | 1:16:A:GLY:H    | 1:19:A:SER:HB3 | 7        | 0.42          |
| (1,579) | 1:4:A:CYS:HA    | 1:7:A:LEU:HB2  | 8        | 0.42          |
| (1,546) | 1:13:A:LYS:HD3  | 1:13:A:LYS:HE2 | 3        | 0.42          |
| (1,546) | 1:13:A:LYS:HD3  | 1:13:A:LYS:HE3 | 3        | 0.42          |
| (1,546) | 1:13:A:LYS:HD3  | 1:13:A:LYS:HE2 | 5        | 0.42          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,546) | 1:13:A:LYS:HD3 | 1:13:A:LYS:HE3 | 5        | 0.42          |
| (1,546) | 1:13:A:LYS:HD3 | 1:13:A:LYS:HE2 | 6        | 0.42          |
| (1,546) | 1:13:A:LYS:HD3 | 1:13:A:LYS:HE3 | 6        | 0.42          |
| (1,546) | 1:13:A:LYS:HD3 | 1:13:A:LYS:HE2 | 8        | 0.42          |
| (1,546) | 1:13:A:LYS:HD3 | 1:13:A:LYS:HE3 | 8        | 0.42          |
| (1,546) | 1:13:A:LYS:HD3 | 1:13:A:LYS:HE2 | 10       | 0.42          |
| (1,546) | 1:13:A:LYS:HD3 | 1:13:A:LYS:HE3 | 10       | 0.42          |
| (1,494) | 1:21:A:ARG:HA  | 1:22:A:PRO:HD3 | 5        | 0.42          |
| (1,492) | 1:22:A:PRO:HB3 | 1:22:A:PRO:HG3 | 7        | 0.42          |
| (1,485) | 1:22:A:PRO:HD3 | 1:22:A:PRO:HG3 | 4        | 0.42          |
| (1,476) | 1:22:A:PRO:HA  | 1:22:A:PRO:HG3 | 4        | 0.42          |
| (1,474) | 1:22:A:PRO:HA  | 1:22:A:PRO:HB3 | 2        | 0.42          |
| (1,467) | 1:21:A:ARG:HD2 | 1:21:A:ARG:HG2 | 5        | 0.42          |
| (1,467) | 1:21:A:ARG:HD2 | 1:21:A:ARG:HG3 | 5        | 0.42          |
| (1,369) | 1:7:A:LEU:HB3  | 1:7:A:LEU:HD11 | 1        | 0.42          |
| (1,369) | 1:7:A:LEU:HB3  | 1:7:A:LEU:HD12 | 1        | 0.42          |
| (1,369) | 1:7:A:LEU:HB3  | 1:7:A:LEU:HD13 | 1        | 0.42          |
| (1,369) | 1:7:A:LEU:HB3  | 1:7:A:LEU:HD21 | 1        | 0.42          |
| (1,369) | 1:7:A:LEU:HB3  | 1:7:A:LEU:HD22 | 1        | 0.42          |
| (1,369) | 1:7:A:LEU:HB3  | 1:7:A:LEU:HD23 | 1        | 0.42          |
| (1,369) | 1:7:A:LEU:HB3  | 1:7:A:LEU:HD11 | 5        | 0.42          |
| (1,369) | 1:7:A:LEU:HB3  | 1:7:A:LEU:HD12 | 5        | 0.42          |
| (1,369) | 1:7:A:LEU:HB3  | 1:7:A:LEU:HD13 | 5        | 0.42          |
| (1,369) | 1:7:A:LEU:HB3  | 1:7:A:LEU:HD21 | 5        | 0.42          |
| (1,369) | 1:7:A:LEU:HB3  | 1:7:A:LEU:HD22 | 5        | 0.42          |
| (1,369) | 1:7:A:LEU:HB3  | 1:7:A:LEU:HD23 | 5        | 0.42          |
| (1,369) | 1:7:A:LEU:HB3  | 1:7:A:LEU:HD11 | 6        | 0.42          |
| (1,369) | 1:7:A:LEU:HB3  | 1:7:A:LEU:HD12 | 6        | 0.42          |
| (1,369) | 1:7:A:LEU:HB3  | 1:7:A:LEU:HD13 | 6        | 0.42          |
| (1,369) | 1:7:A:LEU:HB3  | 1:7:A:LEU:HD21 | 6        | 0.42          |
| (1,369) | 1:7:A:LEU:HB3  | 1:7:A:LEU:HD22 | 6        | 0.42          |
| (1,369) | 1:7:A:LEU:HB3  | 1:7:A:LEU:HD23 | 6        | 0.42          |
| (1,369) | 1:7:A:LEU:HB3  | 1:7:A:LEU:HD11 | 7        | 0.42          |
| (1,369) | 1:7:A:LEU:HB3  | 1:7:A:LEU:HD12 | 7        | 0.42          |
| (1,369) | 1:7:A:LEU:HB3  | 1:7:A:LEU:HD13 | 7        | 0.42          |
| (1,369) | 1:7:A:LEU:HB3  | 1:7:A:LEU:HD21 | 7        | 0.42          |
| (1,369) | 1:7:A:LEU:HB3  | 1:7:A:LEU:HD22 | 7        | 0.42          |
| (1,369) | 1:7:A:LEU:HB3  | 1:7:A:LEU:HD23 | 7        | 0.42          |
| (1,369) | 1:7:A:LEU:HB3  | 1:7:A:LEU:HD11 | 10       | 0.42          |
| (1,369) | 1:7:A:LEU:HB3  | 1:7:A:LEU:HD12 | 10       | 0.42          |
| (1,369) | 1:7:A:LEU:HB3  | 1:7:A:LEU:HD13 | 10       | 0.42          |
| (1,369) | 1:7:A:LEU:HB3  | 1:7:A:LEU:HD21 | 10       | 0.42          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,369) | 1:7:A:LEU:HB3  | 1:7:A:LEU:HD22  | 10       | 0.42          |
| (1,369) | 1:7:A:LEU:HB3  | 1:7:A:LEU:HD23  | 10       | 0.42          |
| (1,357) | 1:6:A:ARG:HD3  | 1:6:A:ARG:HG2   | 10       | 0.42          |
| (1,276) | 1:19:A:SER:H   | 1:20:A:GLY:H    | 3        | 0.42          |
| (1,276) | 1:19:A:SER:H   | 1:20:A:GLY:H    | 7        | 0.42          |
| (1,273) | 1:18:A:SER:H   | 1:19:A:SER:H    | 5        | 0.42          |
| (1,208) | 1:11:A:TRP:HZ3 | 1:12:A:LEU:HD11 | 6        | 0.42          |
| (1,208) | 1:11:A:TRP:HZ3 | 1:12:A:LEU:HD12 | 6        | 0.42          |
| (1,208) | 1:11:A:TRP:HZ3 | 1:12:A:LEU:HD13 | 6        | 0.42          |
| (1,173) | 1:11:A:TRP:HH2 | 1:17:A:PRO:HD3  | 4        | 0.42          |
| (1,166) | 1:5:A:VAL:HA   | 1:8:A:TYR:HD1   | 7        | 0.42          |
| (1,166) | 1:5:A:VAL:HA   | 1:8:A:TYR:HD2   | 7        | 0.42          |
| (1,166) | 1:5:A:VAL:HA   | 1:8:A:TYR:HD1   | 8        | 0.42          |
| (1,166) | 1:5:A:VAL:HA   | 1:8:A:TYR:HD2   | 8        | 0.42          |
| (1,118) | 1:12:A:LEU:H   | 1:12:A:LEU:HG   | 9        | 0.42          |
| (1,92)  | 1:19:A:SER:H   | 1:19:A:SER:HG   | 4        | 0.42          |
| (1,735) | 1:2:A:GLU:HB2  | 1:5:A:VAL:HB    | 5        | 0.41          |
| (1,734) | 1:2:A:GLU:HG3  | 1:5:A:VAL:HB    | 10       | 0.41          |
| (1,723) | 1:12:A:LEU:HB3 | 1:13:A:LYS:HG2  | 9        | 0.41          |
| (1,723) | 1:12:A:LEU:HB3 | 1:13:A:LYS:HG3  | 9        | 0.41          |
| (1,716) | 1:9:A:ILE:HG12 | 1:12:A:LEU:HD11 | 2        | 0.41          |
| (1,716) | 1:9:A:ILE:HG12 | 1:12:A:LEU:HD12 | 2        | 0.41          |
| (1,716) | 1:9:A:ILE:HG12 | 1:12:A:LEU:HD13 | 2        | 0.41          |
| (1,716) | 1:9:A:ILE:HG12 | 1:12:A:LEU:HD11 | 5        | 0.41          |
| (1,716) | 1:9:A:ILE:HG12 | 1:12:A:LEU:HD12 | 5        | 0.41          |
| (1,716) | 1:9:A:ILE:HG12 | 1:12:A:LEU:HD13 | 5        | 0.41          |
| (1,704) | 1:9:A:ILE:HG21 | 1:13:A:LYS:HD3  | 3        | 0.41          |
| (1,704) | 1:9:A:ILE:HG22 | 1:13:A:LYS:HD3  | 3        | 0.41          |
| (1,704) | 1:9:A:ILE:HG23 | 1:13:A:LYS:HD3  | 3        | 0.41          |
| (1,631) | 1:5:A:VAL:HG11 | 1:8:A:TYR:HD1   | 6        | 0.41          |
| (1,631) | 1:5:A:VAL:HG11 | 1:8:A:TYR:HD2   | 6        | 0.41          |
| (1,631) | 1:5:A:VAL:HG12 | 1:8:A:TYR:HD1   | 6        | 0.41          |
| (1,631) | 1:5:A:VAL:HG12 | 1:8:A:TYR:HD2   | 6        | 0.41          |
| (1,631) | 1:5:A:VAL:HG13 | 1:8:A:TYR:HD1   | 6        | 0.41          |
| (1,631) | 1:5:A:VAL:HG13 | 1:8:A:TYR:HD2   | 6        | 0.41          |
| (1,631) | 1:5:A:VAL:HG11 | 1:8:A:TYR:HD1   | 7        | 0.41          |
| (1,631) | 1:5:A:VAL:HG11 | 1:8:A:TYR:HD2   | 7        | 0.41          |
| (1,631) | 1:5:A:VAL:HG12 | 1:8:A:TYR:HD1   | 7        | 0.41          |
| (1,631) | 1:5:A:VAL:HG12 | 1:8:A:TYR:HD2   | 7        | 0.41          |
| (1,631) | 1:5:A:VAL:HG13 | 1:8:A:TYR:HD1   | 7        | 0.41          |
| (1,631) | 1:5:A:VAL:HG13 | 1:8:A:TYR:HD2   | 7        | 0.41          |
| (1,631) | 1:5:A:VAL:HG11 | 1:8:A:TYR:HD1   | 10       | 0.41          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,631) | 1:5:A:VAL:HG11 | 1:8:A:TYR:HD2  | 10       | 0.41          |
| (1,631) | 1:5:A:VAL:HG12 | 1:8:A:TYR:HD1  | 10       | 0.41          |
| (1,631) | 1:5:A:VAL:HG12 | 1:8:A:TYR:HD2  | 10       | 0.41          |
| (1,631) | 1:5:A:VAL:HG13 | 1:8:A:TYR:HD1  | 10       | 0.41          |
| (1,631) | 1:5:A:VAL:HG13 | 1:8:A:TYR:HD2  | 10       | 0.41          |
| (1,546) | 1:13:A:LYS:HD3 | 1:13:A:LYS:HE2 | 9        | 0.41          |
| (1,546) | 1:13:A:LYS:HD3 | 1:13:A:LYS:HE3 | 9        | 0.41          |
| (1,542) | 1:7:A:LEU:HB2  | 1:24:A:PRO:HB3 | 3        | 0.41          |
| (1,542) | 1:7:A:LEU:HB2  | 1:24:A:PRO:HB3 | 5        | 0.41          |
| (1,494) | 1:21:A:ARG:HA  | 1:22:A:PRO:HD3 | 6        | 0.41          |
| (1,485) | 1:22:A:PRO:HD3 | 1:22:A:PRO:HG3 | 7        | 0.41          |
| (1,476) | 1:22:A:PRO:HA  | 1:22:A:PRO:HG3 | 7        | 0.41          |
| (1,467) | 1:21:A:ARG:HD2 | 1:21:A:ARG:HG2 | 1        | 0.41          |
| (1,467) | 1:21:A:ARG:HD2 | 1:21:A:ARG:HG3 | 1        | 0.41          |
| (1,467) | 1:21:A:ARG:HD2 | 1:21:A:ARG:HG2 | 9        | 0.41          |
| (1,467) | 1:21:A:ARG:HD2 | 1:21:A:ARG:HG3 | 9        | 0.41          |
| (1,451) | 1:18:A:SER:HA  | 1:18:A:SER:HB2 | 5        | 0.41          |
| (1,369) | 1:7:A:LEU:HB3  | 1:7:A:LEU:HD11 | 2        | 0.41          |
| (1,369) | 1:7:A:LEU:HB3  | 1:7:A:LEU:HD12 | 2        | 0.41          |
| (1,369) | 1:7:A:LEU:HB3  | 1:7:A:LEU:HD13 | 2        | 0.41          |
| (1,369) | 1:7:A:LEU:HB3  | 1:7:A:LEU:HD21 | 2        | 0.41          |
| (1,369) | 1:7:A:LEU:HB3  | 1:7:A:LEU:HD22 | 2        | 0.41          |
| (1,369) | 1:7:A:LEU:HB3  | 1:7:A:LEU:HD23 | 2        | 0.41          |
| (1,369) | 1:7:A:LEU:HB3  | 1:7:A:LEU:HD11 | 3        | 0.41          |
| (1,369) | 1:7:A:LEU:HB3  | 1:7:A:LEU:HD12 | 3        | 0.41          |
| (1,369) | 1:7:A:LEU:HB3  | 1:7:A:LEU:HD13 | 3        | 0.41          |
| (1,369) | 1:7:A:LEU:HB3  | 1:7:A:LEU:HD21 | 3        | 0.41          |
| (1,369) | 1:7:A:LEU:HB3  | 1:7:A:LEU:HD22 | 3        | 0.41          |
| (1,369) | 1:7:A:LEU:HB3  | 1:7:A:LEU:HD23 | 3        | 0.41          |
| (1,369) | 1:7:A:LEU:HB3  | 1:7:A:LEU:HD11 | 8        | 0.41          |
| (1,369) | 1:7:A:LEU:HB3  | 1:7:A:LEU:HD12 | 8        | 0.41          |
| (1,369) | 1:7:A:LEU:HB3  | 1:7:A:LEU:HD13 | 8        | 0.41          |
| (1,369) | 1:7:A:LEU:HB3  | 1:7:A:LEU:HD21 | 8        | 0.41          |
| (1,369) | 1:7:A:LEU:HB3  | 1:7:A:LEU:HD22 | 8        | 0.41          |
| (1,369) | 1:7:A:LEU:HB3  | 1:7:A:LEU:HD23 | 8        | 0.41          |
| (1,369) | 1:7:A:LEU:HB3  | 1:7:A:LEU:HD11 | 9        | 0.41          |
| (1,369) | 1:7:A:LEU:HB3  | 1:7:A:LEU:HD12 | 9        | 0.41          |
| (1,369) | 1:7:A:LEU:HB3  | 1:7:A:LEU:HD13 | 9        | 0.41          |
| (1,369) | 1:7:A:LEU:HB3  | 1:7:A:LEU:HD21 | 9        | 0.41          |
| (1,369) | 1:7:A:LEU:HB3  | 1:7:A:LEU:HD22 | 9        | 0.41          |
| (1,369) | 1:7:A:LEU:HB3  | 1:7:A:LEU:HD23 | 9        | 0.41          |
| (1,368) | 1:7:A:LEU:HA   | 1:7:A:LEU:HD11 | 10       | 0.41          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,368) | 1:7:A:LEU:HA   | 1:7:A:LEU:HD12  | 10       | 0.41          |
| (1,368) | 1:7:A:LEU:HA   | 1:7:A:LEU:HD13  | 10       | 0.41          |
| (1,368) | 1:7:A:LEU:HA   | 1:7:A:LEU:HD21  | 10       | 0.41          |
| (1,368) | 1:7:A:LEU:HA   | 1:7:A:LEU:HD22  | 10       | 0.41          |
| (1,368) | 1:7:A:LEU:HA   | 1:7:A:LEU:HD23  | 10       | 0.41          |
| (1,365) | 1:7:A:LEU:HA   | 1:7:A:LEU:HB3   | 3        | 0.41          |
| (1,357) | 1:6:A:ARG:HD3  | 1:6:A:ARG:HG2   | 4        | 0.41          |
| (1,357) | 1:6:A:ARG:HD3  | 1:6:A:ARG:HG2   | 5        | 0.41          |
| (1,280) | 1:4:A:CYS:H    | 1:5:A:VAL:H     | 1        | 0.41          |
| (1,166) | 1:5:A:VAL:HA   | 1:8:A:TYR:HD1   | 4        | 0.41          |
| (1,166) | 1:5:A:VAL:HA   | 1:8:A:TYR:HD2   | 4        | 0.41          |
| (1,160) | 1:11:A:TRP:HZ2 | 1:22:A:PRO:HA   | 9        | 0.41          |
| (1,118) | 1:12:A:LEU:H   | 1:12:A:LEU:HG   | 5        | 0.41          |
| (1,111) | 1:10:A:GLN:HB3 | 1:11:A:TRP:H    | 8        | 0.41          |
| (1,92)  | 1:19:A:SER:H   | 1:19:A:SER:HG   | 3        | 0.41          |
| (1,734) | 1:2:A:GLU:HG3  | 1:5:A:VAL:HB    | 3        | 0.4           |
| (1,677) | 1:12:A:LEU:HA  | 1:12:A:LEU:HD11 | 3        | 0.4           |
| (1,677) | 1:12:A:LEU:HA  | 1:12:A:LEU:HD12 | 3        | 0.4           |
| (1,677) | 1:12:A:LEU:HA  | 1:12:A:LEU:HD13 | 3        | 0.4           |
| (1,648) | 1:15:A:GLY:HA2 | 1:19:A:SER:HB2  | 2        | 0.4           |
| (1,483) | 1:22:A:PRO:HD2 | 1:22:A:PRO:HG2  | 4        | 0.4           |
| (1,483) | 1:22:A:PRO:HD2 | 1:22:A:PRO:HG2  | 7        | 0.4           |
| (1,467) | 1:21:A:ARG:HD2 | 1:21:A:ARG:HG2  | 3        | 0.4           |
| (1,467) | 1:21:A:ARG:HD2 | 1:21:A:ARG:HG3  | 3        | 0.4           |
| (1,467) | 1:21:A:ARG:HD2 | 1:21:A:ARG:HG2  | 4        | 0.4           |
| (1,467) | 1:21:A:ARG:HD2 | 1:21:A:ARG:HG3  | 4        | 0.4           |
| (1,415) | 1:12:A:LEU:HB3 | 1:12:A:LEU:HD11 | 3        | 0.4           |
| (1,415) | 1:12:A:LEU:HB3 | 1:12:A:LEU:HD12 | 3        | 0.4           |
| (1,415) | 1:12:A:LEU:HB3 | 1:12:A:LEU:HD13 | 3        | 0.4           |
| (1,368) | 1:7:A:LEU:HA   | 1:7:A:LEU:HD11  | 2        | 0.4           |
| (1,368) | 1:7:A:LEU:HA   | 1:7:A:LEU:HD12  | 2        | 0.4           |
| (1,368) | 1:7:A:LEU:HA   | 1:7:A:LEU:HD13  | 2        | 0.4           |
| (1,368) | 1:7:A:LEU:HA   | 1:7:A:LEU:HD21  | 2        | 0.4           |
| (1,368) | 1:7:A:LEU:HA   | 1:7:A:LEU:HD22  | 2        | 0.4           |
| (1,368) | 1:7:A:LEU:HA   | 1:7:A:LEU:HD23  | 2        | 0.4           |
| (1,277) | 1:20:A:GLY:H   | 1:21:A:ARG:H    | 3        | 0.4           |
| (1,273) | 1:18:A:SER:H   | 1:19:A:SER:H    | 9        | 0.4           |
| (1,230) | 1:11:A:TRP:HD1 | 1:21:A:ARG:HB2  | 7        | 0.4           |
| (1,225) | 1:23:A:PRO:HB2 | 1:25:A:CYS:H    | 10       | 0.4           |
| (1,177) | 1:8:A:TYR:HD1  | 1:12:A:LEU:HA   | 1        | 0.4           |
| (1,177) | 1:8:A:TYR:HD2  | 1:12:A:LEU:HA   | 1        | 0.4           |
| (1,173) | 1:11:A:TRP:HH2 | 1:17:A:PRO:HD3  | 3        | 0.4           |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,129) | 1:10:A:GLN:HA   | 1:10:A:GLN:HE21 | 4        | 0.4           |
| (1,118) | 1:12:A:LEU:H    | 1:12:A:LEU:HG   | 4        | 0.4           |
| (1,118) | 1:12:A:LEU:H    | 1:12:A:LEU:HG   | 6        | 0.4           |
| (1,92)  | 1:19:A:SER:H    | 1:19:A:SER:HG   | 1        | 0.4           |
| (1,92)  | 1:19:A:SER:H    | 1:19:A:SER:HG   | 2        | 0.4           |
| (1,92)  | 1:19:A:SER:H    | 1:19:A:SER:HG   | 9        | 0.4           |
| (1,735) | 1:2:A:GLU:HB2   | 1:5:A:VAL:HB    | 6        | 0.39          |
| (1,719) | 1:9:A:ILE:HG12  | 1:12:A:LEU:HG   | 9        | 0.39          |
| (1,717) | 1:12:A:LEU:HD11 | 1:16:A:GLY:HA2  | 2        | 0.39          |
| (1,717) | 1:12:A:LEU:HD12 | 1:16:A:GLY:HA2  | 2        | 0.39          |
| (1,717) | 1:12:A:LEU:HD13 | 1:16:A:GLY:HA2  | 2        | 0.39          |
| (1,716) | 1:9:A:ILE:HG12  | 1:12:A:LEU:HD11 | 1        | 0.39          |
| (1,716) | 1:9:A:ILE:HG12  | 1:12:A:LEU:HD12 | 1        | 0.39          |
| (1,716) | 1:9:A:ILE:HG12  | 1:12:A:LEU:HD13 | 1        | 0.39          |
| (1,665) | 1:3:A:GLU:HG2   | 1:4:A:CYS:HA    | 3        | 0.39          |
| (1,665) | 1:3:A:GLU:HG3   | 1:4:A:CYS:HA    | 3        | 0.39          |
| (1,664) | 1:21:A:ARG:HB3  | 1:22:A:PRO:HD2  | 7        | 0.39          |
| (1,640) | 1:11:A:TRP:HE3  | 1:24:A:PRO:HD2  | 9        | 0.39          |
| (1,631) | 1:5:A:VAL:HG11  | 1:8:A:TYR:HD1   | 1        | 0.39          |
| (1,631) | 1:5:A:VAL:HG11  | 1:8:A:TYR:HD2   | 1        | 0.39          |
| (1,631) | 1:5:A:VAL:HG12  | 1:8:A:TYR:HD1   | 1        | 0.39          |
| (1,631) | 1:5:A:VAL:HG12  | 1:8:A:TYR:HD2   | 1        | 0.39          |
| (1,631) | 1:5:A:VAL:HG13  | 1:8:A:TYR:HD1   | 1        | 0.39          |
| (1,631) | 1:5:A:VAL:HG13  | 1:8:A:TYR:HD2   | 1        | 0.39          |
| (1,625) | 1:10:A:GLN:HE21 | 1:14:A:ASP:HB3  | 8        | 0.39          |
| (1,554) | 1:22:A:PRO:HB3  | 1:23:A:PRO:HD2  | 5        | 0.39          |
| (1,485) | 1:22:A:PRO:HD3  | 1:22:A:PRO:HG3  | 2        | 0.39          |
| (1,485) | 1:22:A:PRO:HD3  | 1:22:A:PRO:HG3  | 3        | 0.39          |
| (1,485) | 1:22:A:PRO:HD3  | 1:22:A:PRO:HG3  | 8        | 0.39          |
| (1,485) | 1:22:A:PRO:HD3  | 1:22:A:PRO:HG3  | 10       | 0.39          |
| (1,415) | 1:12:A:LEU:HB3  | 1:12:A:LEU:HD11 | 2        | 0.39          |
| (1,415) | 1:12:A:LEU:HB3  | 1:12:A:LEU:HD12 | 2        | 0.39          |
| (1,415) | 1:12:A:LEU:HB3  | 1:12:A:LEU:HD13 | 2        | 0.39          |
| (1,273) | 1:18:A:SER:H    | 1:19:A:SER:H    | 2        | 0.39          |
| (1,259) | 1:4:A:CYS:HB3   | 1:5:A:VAL:H     | 2        | 0.39          |
| (1,238) | 1:8:A:TYR:HE1   | 1:23:A:PRO:HG3  | 6        | 0.39          |
| (1,238) | 1:8:A:TYR:HE2   | 1:23:A:PRO:HG3  | 6        | 0.39          |
| (1,177) | 1:8:A:TYR:HD1   | 1:12:A:LEU:HA   | 2        | 0.39          |
| (1,177) | 1:8:A:TYR:HD2   | 1:12:A:LEU:HA   | 2        | 0.39          |
| (1,166) | 1:5:A:VAL:HA    | 1:8:A:TYR:HD1   | 2        | 0.39          |
| (1,166) | 1:5:A:VAL:HA    | 1:8:A:TYR:HD2   | 2        | 0.39          |
| (1,166) | 1:5:A:VAL:HA    | 1:8:A:TYR:HD1   | 5        | 0.39          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,166) | 1:5:A:VAL:HA   | 1:8:A:TYR:HD2   | 5        | 0.39          |
| (1,140) | 1:9:A:ILE:HA   | 1:12:A:LEU:H    | 3        | 0.39          |
| (1,118) | 1:12:A:LEU:H   | 1:12:A:LEU:HG   | 1        | 0.39          |
| (1,118) | 1:12:A:LEU:H   | 1:12:A:LEU:HG   | 2        | 0.39          |
| (1,118) | 1:12:A:LEU:H   | 1:12:A:LEU:HG   | 7        | 0.39          |
| (1,99)  | 1:11:A:TRP:HE1 | 1:22:A:PRO:HA   | 2        | 0.39          |
| (1,93)  | 1:19:A:SER:HG  | 1:21:A:ARG:H    | 4        | 0.39          |
| (1,55)  | 1:21:A:ARG:H   | 1:21:A:ARG:HD2  | 6        | 0.39          |
| (1,735) | 1:2:A:GLU:HB2  | 1:5:A:VAL:HB    | 1        | 0.38          |
| (1,735) | 1:2:A:GLU:HB2  | 1:5:A:VAL:HB    | 2        | 0.38          |
| (1,735) | 1:2:A:GLU:HB2  | 1:5:A:VAL:HB    | 3        | 0.38          |
| (1,735) | 1:2:A:GLU:HB2  | 1:5:A:VAL:HB    | 4        | 0.38          |
| (1,735) | 1:2:A:GLU:HB2  | 1:5:A:VAL:HB    | 10       | 0.38          |
| (1,720) | 1:7:A:LEU:HB2  | 1:24:A:PRO:HB2  | 7        | 0.38          |
| (1,682) | 1:4:A:CYS:HB2  | 1:5:A:VAL:HG11  | 7        | 0.38          |
| (1,682) | 1:4:A:CYS:HB2  | 1:5:A:VAL:HG12  | 7        | 0.38          |
| (1,682) | 1:4:A:CYS:HB2  | 1:5:A:VAL:HG13  | 7        | 0.38          |
| (1,665) | 1:3:A:GLU:HG2  | 1:4:A:CYS:HA    | 4        | 0.38          |
| (1,665) | 1:3:A:GLU:HG3  | 1:4:A:CYS:HA    | 4        | 0.38          |
| (1,631) | 1:5:A:VAL:HG11 | 1:8:A:TYR:HD1   | 4        | 0.38          |
| (1,631) | 1:5:A:VAL:HG11 | 1:8:A:TYR:HD2   | 4        | 0.38          |
| (1,631) | 1:5:A:VAL:HG12 | 1:8:A:TYR:HD1   | 4        | 0.38          |
| (1,631) | 1:5:A:VAL:HG12 | 1:8:A:TYR:HD2   | 4        | 0.38          |
| (1,631) | 1:5:A:VAL:HG13 | 1:8:A:TYR:HD1   | 4        | 0.38          |
| (1,631) | 1:5:A:VAL:HG13 | 1:8:A:TYR:HD2   | 4        | 0.38          |
| (1,593) | 1:11:A:TRP:HA  | 1:14:A:ASP:HB3  | 9        | 0.38          |
| (1,579) | 1:4:A:CYS:HA   | 1:7:A:LEU:HB2   | 2        | 0.38          |
| (1,564) | 1:4:A:CYS:HA   | 1:7:A:LEU:HB3   | 7        | 0.38          |
| (1,564) | 1:4:A:CYS:HA   | 1:7:A:LEU:HB3   | 9        | 0.38          |
| (1,542) | 1:7:A:LEU:HB2  | 1:24:A:PRO:HB3  | 1        | 0.38          |
| (1,485) | 1:22:A:PRO:HD3 | 1:22:A:PRO:HG3  | 1        | 0.38          |
| (1,485) | 1:22:A:PRO:HD3 | 1:22:A:PRO:HG3  | 5        | 0.38          |
| (1,485) | 1:22:A:PRO:HD3 | 1:22:A:PRO:HG3  | 9        | 0.38          |
| (1,477) | 1:22:A:PRO:HA  | 1:22:A:PRO:HB2  | 4        | 0.38          |
| (1,467) | 1:21:A:ARG:HD2 | 1:21:A:ARG:HG2  | 7        | 0.38          |
| (1,467) | 1:21:A:ARG:HD2 | 1:21:A:ARG:HG3  | 7        | 0.38          |
| (1,415) | 1:12:A:LEU:HB3 | 1:12:A:LEU:HD11 | 1        | 0.38          |
| (1,415) | 1:12:A:LEU:HB3 | 1:12:A:LEU:HD12 | 1        | 0.38          |
| (1,415) | 1:12:A:LEU:HB3 | 1:12:A:LEU:HD13 | 1        | 0.38          |
| (1,415) | 1:12:A:LEU:HB3 | 1:12:A:LEU:HD11 | 5        | 0.38          |
| (1,415) | 1:12:A:LEU:HB3 | 1:12:A:LEU:HD12 | 5        | 0.38          |
| (1,415) | 1:12:A:LEU:HB3 | 1:12:A:LEU:HD13 | 5        | 0.38          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,411) | 1:12:A:LEU:HB2 | 1:12:A:LEU:HG   | 10       | 0.38          |
| (1,357) | 1:6:A:ARG:HD3  | 1:6:A:ARG:HG2   | 3        | 0.38          |
| (1,357) | 1:6:A:ARG:HD3  | 1:6:A:ARG:HG2   | 6        | 0.38          |
| (1,325) | 1:2:A:GLU:HA   | 1:2:A:GLU:HB2   | 5        | 0.38          |
| (1,273) | 1:18:A:SER:H   | 1:19:A:SER:H    | 8        | 0.38          |
| (1,230) | 1:11:A:TRP:HD1 | 1:21:A:ARG:HB2  | 1        | 0.38          |
| (1,230) | 1:11:A:TRP:HD1 | 1:21:A:ARG:HB2  | 5        | 0.38          |
| (1,173) | 1:11:A:TRP:HH2 | 1:17:A:PRO:HD3  | 7        | 0.38          |
| (1,172) | 1:11:A:TRP:HZ2 | 1:23:A:PRO:HD3  | 4        | 0.38          |
| (1,93)  | 1:19:A:SER:HG  | 1:21:A:ARG:H    | 7        | 0.38          |
| (1,35)  | 1:10:A:GLN:H   | 1:10:A:GLN:HB2  | 4        | 0.38          |
| (1,10)  | 1:9:A:ILE:H    | 1:12:A:LEU:HD21 | 1        | 0.38          |
| (1,10)  | 1:9:A:ILE:H    | 1:12:A:LEU:HD22 | 1        | 0.38          |
| (1,10)  | 1:9:A:ILE:H    | 1:12:A:LEU:HD23 | 1        | 0.38          |
| (1,10)  | 1:9:A:ILE:H    | 1:12:A:LEU:HD21 | 2        | 0.38          |
| (1,10)  | 1:9:A:ILE:H    | 1:12:A:LEU:HD22 | 2        | 0.38          |
| (1,10)  | 1:9:A:ILE:H    | 1:12:A:LEU:HD23 | 2        | 0.38          |
| (1,10)  | 1:9:A:ILE:H    | 1:12:A:LEU:HD21 | 5        | 0.38          |
| (1,10)  | 1:9:A:ILE:H    | 1:12:A:LEU:HD22 | 5        | 0.38          |
| (1,10)  | 1:9:A:ILE:H    | 1:12:A:LEU:HD23 | 5        | 0.38          |
| (1,10)  | 1:9:A:ILE:H    | 1:12:A:LEU:HD21 | 6        | 0.38          |
| (1,10)  | 1:9:A:ILE:H    | 1:12:A:LEU:HD22 | 6        | 0.38          |
| (1,10)  | 1:9:A:ILE:H    | 1:12:A:LEU:HD23 | 6        | 0.38          |
| (1,735) | 1:2:A:GLU:HB2  | 1:5:A:VAL:HB    | 8        | 0.37          |
| (1,734) | 1:2:A:GLU:HG3  | 1:5:A:VAL:HB    | 1        | 0.37          |
| (1,715) | 1:9:A:ILE:HG21 | 1:12:A:LEU:HB2  | 2        | 0.37          |
| (1,715) | 1:9:A:ILE:HG22 | 1:12:A:LEU:HB2  | 2        | 0.37          |
| (1,715) | 1:9:A:ILE:HG23 | 1:12:A:LEU:HB2  | 2        | 0.37          |
| (1,631) | 1:5:A:VAL:HG11 | 1:8:A:TYR:HD1   | 2        | 0.37          |
| (1,631) | 1:5:A:VAL:HG11 | 1:8:A:TYR:HD2   | 2        | 0.37          |
| (1,631) | 1:5:A:VAL:HG12 | 1:8:A:TYR:HD1   | 2        | 0.37          |
| (1,631) | 1:5:A:VAL:HG12 | 1:8:A:TYR:HD2   | 2        | 0.37          |
| (1,631) | 1:5:A:VAL:HG13 | 1:8:A:TYR:HD1   | 2        | 0.37          |
| (1,631) | 1:5:A:VAL:HG13 | 1:8:A:TYR:HD2   | 2        | 0.37          |
| (1,626) | 1:14:A:ASP:HB3 | 1:15:A:GLY:H    | 5        | 0.37          |
| (1,616) | 1:14:A:ASP:HB3 | 1:16:A:GLY:H    | 2        | 0.37          |
| (1,615) | 1:16:A:GLY:H   | 1:19:A:SER:HB3  | 4        | 0.37          |
| (1,593) | 1:11:A:TRP:HA  | 1:14:A:ASP:HB3  | 1        | 0.37          |
| (1,554) | 1:22:A:PRO:HB3 | 1:23:A:PRO:HD2  | 1        | 0.37          |
| (1,554) | 1:22:A:PRO:HB3 | 1:23:A:PRO:HD2  | 6        | 0.37          |
| (1,485) | 1:22:A:PRO:HD3 | 1:22:A:PRO:HG3  | 6        | 0.37          |
| (1,483) | 1:22:A:PRO:HD2 | 1:22:A:PRO:HG2  | 2        | 0.37          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,483) | 1:22:A:PRO:HD2  | 1:22:A:PRO:HG2  | 3        | 0.37          |
| (1,477) | 1:22:A:PRO:HA   | 1:22:A:PRO:HB2  | 7        | 0.37          |
| (1,424) | 1:13:A:LYS:HB2  | 1:13:A:LYS:HD3  | 2        | 0.37          |
| (1,424) | 1:13:A:LYS:HB3  | 1:13:A:LYS:HD3  | 2        | 0.37          |
| (1,415) | 1:12:A:LEU:HB3  | 1:12:A:LEU:HD11 | 6        | 0.37          |
| (1,415) | 1:12:A:LEU:HB3  | 1:12:A:LEU:HD12 | 6        | 0.37          |
| (1,415) | 1:12:A:LEU:HB3  | 1:12:A:LEU:HD13 | 6        | 0.37          |
| (1,411) | 1:12:A:LEU:HB2  | 1:12:A:LEU:HG   | 4        | 0.37          |
| (1,411) | 1:12:A:LEU:HB2  | 1:12:A:LEU:HG   | 8        | 0.37          |
| (1,368) | 1:7:A:LEU:HA    | 1:7:A:LEU:HD11  | 3        | 0.37          |
| (1,368) | 1:7:A:LEU:HA    | 1:7:A:LEU:HD12  | 3        | 0.37          |
| (1,368) | 1:7:A:LEU:HA    | 1:7:A:LEU:HD13  | 3        | 0.37          |
| (1,368) | 1:7:A:LEU:HA    | 1:7:A:LEU:HD21  | 3        | 0.37          |
| (1,368) | 1:7:A:LEU:HA    | 1:7:A:LEU:HD22  | 3        | 0.37          |
| (1,368) | 1:7:A:LEU:HA    | 1:7:A:LEU:HD23  | 3        | 0.37          |
| (1,365) | 1:7:A:LEU:HA    | 1:7:A:LEU:HB3   | 2        | 0.37          |
| (1,365) | 1:7:A:LEU:HA    | 1:7:A:LEU:HB3   | 4        | 0.37          |
| (1,365) | 1:7:A:LEU:HA    | 1:7:A:LEU:HB3   | 5        | 0.37          |
| (1,365) | 1:7:A:LEU:HA    | 1:7:A:LEU:HB3   | 6        | 0.37          |
| (1,365) | 1:7:A:LEU:HA    | 1:7:A:LEU:HB3   | 8        | 0.37          |
| (1,365) | 1:7:A:LEU:HA    | 1:7:A:LEU:HB3   | 10       | 0.37          |
| (1,280) | 1:4:A:CYS:H     | 1:5:A:VAL:H     | 3        | 0.37          |
| (1,215) | 1:11:A:TRP:HZ3  | 1:12:A:LEU:HD21 | 2        | 0.37          |
| (1,215) | 1:11:A:TRP:HZ3  | 1:12:A:LEU:HD22 | 2        | 0.37          |
| (1,215) | 1:11:A:TRP:HZ3  | 1:12:A:LEU:HD23 | 2        | 0.37          |
| (1,199) | 1:8:A:TYR:HD1   | 1:23:A:PRO:HB3  | 5        | 0.37          |
| (1,199) | 1:8:A:TYR:HD2   | 1:23:A:PRO:HB3  | 5        | 0.37          |
| (1,193) | 1:11:A:TRP:HD1  | 1:24:A:PRO:HD3  | 3        | 0.37          |
| (1,173) | 1:11:A:TRP:HH2  | 1:17:A:PRO:HD3  | 8        | 0.37          |
| (1,172) | 1:11:A:TRP:HZ2  | 1:23:A:PRO:HD3  | 3        | 0.37          |
| (1,140) | 1:9:A:ILE:HA    | 1:12:A:LEU:H    | 5        | 0.37          |
| (1,129) | 1:10:A:GLN:HA   | 1:10:A:GLN:HE21 | 9        | 0.37          |
| (1,93)  | 1:19:A:SER:HG   | 1:21:A:ARG:H    | 10       | 0.37          |
| (1,69)  | 1:18:A:SER:H    | 1:18:A:SER:HA   | 2        | 0.37          |
| (1,40)  | 1:6:A:ARG:H     | 1:6:A:ARG:HB2   | 2        | 0.37          |
| (1,735) | 1:2:A:GLU:HB2   | 1:5:A:VAL:HB    | 7        | 0.36          |
| (1,711) | 1:12:A:LEU:HD21 | 1:23:A:PRO:HB2  | 10       | 0.36          |
| (1,711) | 1:12:A:LEU:HD22 | 1:23:A:PRO:HB2  | 10       | 0.36          |
| (1,711) | 1:12:A:LEU:HD23 | 1:23:A:PRO:HB2  | 10       | 0.36          |
| (1,675) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD21 | 5        | 0.36          |
| (1,675) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD22 | 5        | 0.36          |
| (1,675) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD23 | 5        | 0.36          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,675) | 1:12:A:LEU:HA  | 1:12:A:LEU:HD21 | 6        | 0.36          |
| (1,675) | 1:12:A:LEU:HA  | 1:12:A:LEU:HD22 | 6        | 0.36          |
| (1,675) | 1:12:A:LEU:HA  | 1:12:A:LEU:HD23 | 6        | 0.36          |
| (1,648) | 1:15:A:GLY:HA2 | 1:19:A:SER:HB2  | 3        | 0.36          |
| (1,644) | 1:22:A:PRO:HA  | 1:23:A:PRO:HD2  | 7        | 0.36          |
| (1,631) | 1:5:A:VAL:HG11 | 1:8:A:TYR:HD1   | 9        | 0.36          |
| (1,631) | 1:5:A:VAL:HG11 | 1:8:A:TYR:HD2   | 9        | 0.36          |
| (1,631) | 1:5:A:VAL:HG12 | 1:8:A:TYR:HD1   | 9        | 0.36          |
| (1,631) | 1:5:A:VAL:HG12 | 1:8:A:TYR:HD2   | 9        | 0.36          |
| (1,631) | 1:5:A:VAL:HG13 | 1:8:A:TYR:HD1   | 9        | 0.36          |
| (1,631) | 1:5:A:VAL:HG13 | 1:8:A:TYR:HD2   | 9        | 0.36          |
| (1,535) | 1:23:A:PRO:HB3 | 1:24:A:PRO:HD2  | 6        | 0.36          |
| (1,518) | 1:23:A:PRO:HB2 | 1:23:A:PRO:HB3  | 8        | 0.36          |
| (1,518) | 1:23:A:PRO:HB2 | 1:23:A:PRO:HB3  | 9        | 0.36          |
| (1,518) | 1:23:A:PRO:HB2 | 1:23:A:PRO:HB3  | 10       | 0.36          |
| (1,483) | 1:22:A:PRO:HD2 | 1:22:A:PRO:HG2  | 8        | 0.36          |
| (1,483) | 1:22:A:PRO:HD2 | 1:22:A:PRO:HG2  | 9        | 0.36          |
| (1,483) | 1:22:A:PRO:HD2 | 1:22:A:PRO:HG2  | 10       | 0.36          |
| (1,474) | 1:22:A:PRO:HA  | 1:22:A:PRO:HB3  | 4        | 0.36          |
| (1,461) | 1:21:A:ARG:HA  | 1:21:A:ARG:HG2  | 6        | 0.36          |
| (1,461) | 1:21:A:ARG:HA  | 1:21:A:ARG:HG3  | 6        | 0.36          |
| (1,450) | 1:18:A:SER:HA  | 1:18:A:SER:HB3  | 1        | 0.36          |
| (1,450) | 1:18:A:SER:HA  | 1:18:A:SER:HB3  | 10       | 0.36          |
| (1,411) | 1:12:A:LEU:HB2 | 1:12:A:LEU:HG   | 7        | 0.36          |
| (1,411) | 1:12:A:LEU:HB2 | 1:12:A:LEU:HG   | 9        | 0.36          |
| (1,394) | 1:10:A:GLN:HA  | 1:10:A:GLN:HB2  | 9        | 0.36          |
| (1,365) | 1:7:A:LEU:HA   | 1:7:A:LEU:HB3   | 1        | 0.36          |
| (1,365) | 1:7:A:LEU:HA   | 1:7:A:LEU:HB3   | 7        | 0.36          |
| (1,273) | 1:18:A:SER:H   | 1:19:A:SER:H    | 10       | 0.36          |
| (1,177) | 1:8:A:TYR:HD1  | 1:12:A:LEU:HA   | 5        | 0.36          |
| (1,177) | 1:8:A:TYR:HD2  | 1:12:A:LEU:HA   | 5        | 0.36          |
| (1,172) | 1:11:A:TRP:HZ2 | 1:23:A:PRO:HD3  | 1        | 0.36          |
| (1,118) | 1:12:A:LEU:H   | 1:12:A:LEU:HG   | 8        | 0.36          |
| (1,118) | 1:12:A:LEU:H   | 1:12:A:LEU:HG   | 10       | 0.36          |
| (1,26)  | 1:2:A:GLU:HB2  | 1:3:A:GLU:H     | 7        | 0.36          |
| (1,735) | 1:2:A:GLU:HB2  | 1:5:A:VAL:HB    | 9        | 0.35          |
| (1,728) | 1:2:A:GLU:HG2  | 1:6:A:ARG:HG2   | 1        | 0.35          |
| (1,728) | 1:2:A:GLU:HG2  | 1:6:A:ARG:HG2   | 7        | 0.35          |
| (1,666) | 1:24:A:PRO:HG2 | 1:25:A:CYS:HB2  | 4        | 0.35          |
| (1,623) | 1:2:A:GLU:HB3  | 1:6:A:ARG:H     | 5        | 0.35          |
| (1,621) | 1:2:A:GLU:HB2  | 1:6:A:ARG:H     | 10       | 0.35          |
| (1,579) | 1:4:A:CYS:HA   | 1:7:A:LEU:HB2   | 10       | 0.35          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,576) | 1:22:A:PRO:HA  | 1:23:A:PRO:HD3  | 2        | 0.35          |
| (1,542) | 1:7:A:LEU:HB2  | 1:24:A:PRO:HB3  | 6        | 0.35          |
| (1,542) | 1:7:A:LEU:HB2  | 1:24:A:PRO:HB3  | 8        | 0.35          |
| (1,518) | 1:23:A:PRO:HB2 | 1:23:A:PRO:HB3  | 7        | 0.35          |
| (1,506) | 1:23:A:PRO:HD3 | 1:23:A:PRO:HG3  | 4        | 0.35          |
| (1,506) | 1:23:A:PRO:HD3 | 1:23:A:PRO:HG3  | 7        | 0.35          |
| (1,488) | 1:22:A:PRO:HB2 | 1:22:A:PRO:HB3  | 1        | 0.35          |
| (1,488) | 1:22:A:PRO:HB2 | 1:22:A:PRO:HB3  | 2        | 0.35          |
| (1,488) | 1:22:A:PRO:HB2 | 1:22:A:PRO:HB3  | 3        | 0.35          |
| (1,488) | 1:22:A:PRO:HB2 | 1:22:A:PRO:HB3  | 4        | 0.35          |
| (1,488) | 1:22:A:PRO:HB2 | 1:22:A:PRO:HB3  | 5        | 0.35          |
| (1,488) | 1:22:A:PRO:HB2 | 1:22:A:PRO:HB3  | 6        | 0.35          |
| (1,488) | 1:22:A:PRO:HB2 | 1:22:A:PRO:HB3  | 7        | 0.35          |
| (1,488) | 1:22:A:PRO:HB2 | 1:22:A:PRO:HB3  | 8        | 0.35          |
| (1,488) | 1:22:A:PRO:HB2 | 1:22:A:PRO:HB3  | 9        | 0.35          |
| (1,488) | 1:22:A:PRO:HB2 | 1:22:A:PRO:HB3  | 10       | 0.35          |
| (1,483) | 1:22:A:PRO:HD2 | 1:22:A:PRO:HG2  | 1        | 0.35          |
| (1,483) | 1:22:A:PRO:HD2 | 1:22:A:PRO:HG2  | 5        | 0.35          |
| (1,474) | 1:22:A:PRO:HA  | 1:22:A:PRO:HB3  | 7        | 0.35          |
| (1,465) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD2  | 7        | 0.35          |
| (1,456) | 1:20:A:GLY:HA2 | 1:20:A:GLY:HA3  | 1        | 0.35          |
| (1,456) | 1:20:A:GLY:HA2 | 1:20:A:GLY:HA3  | 5        | 0.35          |
| (1,456) | 1:20:A:GLY:HA2 | 1:20:A:GLY:HA3  | 6        | 0.35          |
| (1,456) | 1:20:A:GLY:HA2 | 1:20:A:GLY:HA3  | 9        | 0.35          |
| (1,450) | 1:18:A:SER:HA  | 1:18:A:SER:HB3  | 3        | 0.35          |
| (1,450) | 1:18:A:SER:HA  | 1:18:A:SER:HB3  | 7        | 0.35          |
| (1,450) | 1:18:A:SER:HA  | 1:18:A:SER:HB3  | 8        | 0.35          |
| (1,391) | 1:10:A:GLN:HA  | 1:10:A:GLN:HG2  | 4        | 0.35          |
| (1,370) | 1:7:A:LEU:HD11 | 1:7:A:LEU:HG    | 4        | 0.35          |
| (1,370) | 1:7:A:LEU:HD12 | 1:7:A:LEU:HG    | 4        | 0.35          |
| (1,370) | 1:7:A:LEU:HD13 | 1:7:A:LEU:HG    | 4        | 0.35          |
| (1,370) | 1:7:A:LEU:HD21 | 1:7:A:LEU:HG    | 4        | 0.35          |
| (1,370) | 1:7:A:LEU:HD22 | 1:7:A:LEU:HG    | 4        | 0.35          |
| (1,370) | 1:7:A:LEU:HD23 | 1:7:A:LEU:HG    | 4        | 0.35          |
| (1,365) | 1:7:A:LEU:HA   | 1:7:A:LEU:HB3   | 9        | 0.35          |
| (1,280) | 1:4:A:CYS:H    | 1:5:A:VAL:H     | 6        | 0.35          |
| (1,276) | 1:19:A:SER:H   | 1:20:A:GLY:H    | 4        | 0.35          |
| (1,276) | 1:19:A:SER:H   | 1:20:A:GLY:H    | 8        | 0.35          |
| (1,222) | 1:8:A:TYR:HD1  | 1:23:A:PRO:HB2  | 8        | 0.35          |
| (1,222) | 1:8:A:TYR:HD2  | 1:23:A:PRO:HB2  | 8        | 0.35          |
| (1,215) | 1:11:A:TRP:HZ3 | 1:12:A:LEU:HD21 | 1        | 0.35          |
| (1,215) | 1:11:A:TRP:HZ3 | 1:12:A:LEU:HD22 | 1        | 0.35          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,215) | 1:11:A:TRP:HZ3 | 1:12:A:LEU:HD23 | 1        | 0.35          |
| (1,173) | 1:11:A:TRP:HH2 | 1:17:A:PRO:HD3  | 10       | 0.35          |
| (1,172) | 1:11:A:TRP:HZ2 | 1:23:A:PRO:HD3  | 6        | 0.35          |
| (1,166) | 1:5:A:VAL:HA   | 1:8:A:TYR:HD1   | 1        | 0.35          |
| (1,166) | 1:5:A:VAL:HA   | 1:8:A:TYR:HD2   | 1        | 0.35          |
| (1,166) | 1:5:A:VAL:HA   | 1:8:A:TYR:HD1   | 6        | 0.35          |
| (1,166) | 1:5:A:VAL:HA   | 1:8:A:TYR:HD2   | 6        | 0.35          |
| (1,99)  | 1:11:A:TRP:HE1 | 1:22:A:PRO:HA   | 9        | 0.35          |
| (1,99)  | 1:11:A:TRP:HE1 | 1:22:A:PRO:HA   | 10       | 0.35          |
| (1,69)  | 1:18:A:SER:H   | 1:18:A:SER:HA   | 5        | 0.35          |
| (1,705) | 1:9:A:ILE:HG21 | 1:13:A:LYS:HD2  | 7        | 0.34          |
| (1,705) | 1:9:A:ILE:HG22 | 1:13:A:LYS:HD2  | 7        | 0.34          |
| (1,705) | 1:9:A:ILE:HG23 | 1:13:A:LYS:HD2  | 7        | 0.34          |
| (1,704) | 1:9:A:ILE:HG21 | 1:13:A:LYS:HD3  | 6        | 0.34          |
| (1,704) | 1:9:A:ILE:HG22 | 1:13:A:LYS:HD3  | 6        | 0.34          |
| (1,704) | 1:9:A:ILE:HG23 | 1:13:A:LYS:HD3  | 6        | 0.34          |
| (1,622) | 1:2:A:GLU:HB3  | 1:5:A:VAL:H     | 7        | 0.34          |
| (1,522) | 1:24:A:PRO:HA  | 1:24:A:PRO:HD3  | 3        | 0.34          |
| (1,518) | 1:23:A:PRO:HB2 | 1:23:A:PRO:HB3  | 1        | 0.34          |
| (1,518) | 1:23:A:PRO:HB2 | 1:23:A:PRO:HB3  | 2        | 0.34          |
| (1,518) | 1:23:A:PRO:HB2 | 1:23:A:PRO:HB3  | 3        | 0.34          |
| (1,518) | 1:23:A:PRO:HB2 | 1:23:A:PRO:HB3  | 4        | 0.34          |
| (1,518) | 1:23:A:PRO:HB2 | 1:23:A:PRO:HB3  | 5        | 0.34          |
| (1,518) | 1:23:A:PRO:HB2 | 1:23:A:PRO:HB3  | 6        | 0.34          |
| (1,498) | 1:23:A:PRO:HA  | 1:23:A:PRO:HB3  | 4        | 0.34          |
| (1,498) | 1:23:A:PRO:HA  | 1:23:A:PRO:HB3  | 7        | 0.34          |
| (1,483) | 1:22:A:PRO:HD2 | 1:22:A:PRO:HG2  | 6        | 0.34          |
| (1,461) | 1:21:A:ARG:HA  | 1:21:A:ARG:HG2  | 4        | 0.34          |
| (1,461) | 1:21:A:ARG:HA  | 1:21:A:ARG:HG3  | 4        | 0.34          |
| (1,461) | 1:21:A:ARG:HA  | 1:21:A:ARG:HG2  | 9        | 0.34          |
| (1,461) | 1:21:A:ARG:HA  | 1:21:A:ARG:HG3  | 9        | 0.34          |
| (1,456) | 1:20:A:GLY:HA2 | 1:20:A:GLY:HA3  | 2        | 0.34          |
| (1,456) | 1:20:A:GLY:HA2 | 1:20:A:GLY:HA3  | 3        | 0.34          |
| (1,456) | 1:20:A:GLY:HA2 | 1:20:A:GLY:HA3  | 4        | 0.34          |
| (1,456) | 1:20:A:GLY:HA2 | 1:20:A:GLY:HA3  | 7        | 0.34          |
| (1,456) | 1:20:A:GLY:HA2 | 1:20:A:GLY:HA3  | 8        | 0.34          |
| (1,456) | 1:20:A:GLY:HA2 | 1:20:A:GLY:HA3  | 10       | 0.34          |
| (1,450) | 1:18:A:SER:HA  | 1:18:A:SER:HB3  | 9        | 0.34          |
| (1,448) | 1:17:A:PRO:HB2 | 1:17:A:PRO:HB3  | 1        | 0.34          |
| (1,448) | 1:17:A:PRO:HB2 | 1:17:A:PRO:HB3  | 2        | 0.34          |
| (1,448) | 1:17:A:PRO:HB2 | 1:17:A:PRO:HB3  | 5        | 0.34          |
| (1,448) | 1:17:A:PRO:HB2 | 1:17:A:PRO:HB3  | 6        | 0.34          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,448) | 1:17:A:PRO:HB2 | 1:17:A:PRO:HB3 | 9        | 0.34          |
| (1,370) | 1:7:A:LEU:HD11 | 1:7:A:LEU:HG   | 1        | 0.34          |
| (1,370) | 1:7:A:LEU:HD12 | 1:7:A:LEU:HG   | 1        | 0.34          |
| (1,370) | 1:7:A:LEU:HD13 | 1:7:A:LEU:HG   | 1        | 0.34          |
| (1,370) | 1:7:A:LEU:HD21 | 1:7:A:LEU:HG   | 1        | 0.34          |
| (1,370) | 1:7:A:LEU:HD22 | 1:7:A:LEU:HG   | 1        | 0.34          |
| (1,370) | 1:7:A:LEU:HD23 | 1:7:A:LEU:HG   | 1        | 0.34          |
| (1,370) | 1:7:A:LEU:HD11 | 1:7:A:LEU:HG   | 2        | 0.34          |
| (1,370) | 1:7:A:LEU:HD12 | 1:7:A:LEU:HG   | 2        | 0.34          |
| (1,370) | 1:7:A:LEU:HD13 | 1:7:A:LEU:HG   | 2        | 0.34          |
| (1,370) | 1:7:A:LEU:HD21 | 1:7:A:LEU:HG   | 2        | 0.34          |
| (1,370) | 1:7:A:LEU:HD22 | 1:7:A:LEU:HG   | 2        | 0.34          |
| (1,370) | 1:7:A:LEU:HD23 | 1:7:A:LEU:HG   | 2        | 0.34          |
| (1,370) | 1:7:A:LEU:HD11 | 1:7:A:LEU:HG   | 3        | 0.34          |
| (1,370) | 1:7:A:LEU:HD12 | 1:7:A:LEU:HG   | 3        | 0.34          |
| (1,370) | 1:7:A:LEU:HD13 | 1:7:A:LEU:HG   | 3        | 0.34          |
| (1,370) | 1:7:A:LEU:HD21 | 1:7:A:LEU:HG   | 3        | 0.34          |
| (1,370) | 1:7:A:LEU:HD22 | 1:7:A:LEU:HG   | 3        | 0.34          |
| (1,370) | 1:7:A:LEU:HD23 | 1:7:A:LEU:HG   | 3        | 0.34          |
| (1,370) | 1:7:A:LEU:HD11 | 1:7:A:LEU:HG   | 5        | 0.34          |
| (1,370) | 1:7:A:LEU:HD12 | 1:7:A:LEU:HG   | 5        | 0.34          |
| (1,370) | 1:7:A:LEU:HD13 | 1:7:A:LEU:HG   | 5        | 0.34          |
| (1,370) | 1:7:A:LEU:HD21 | 1:7:A:LEU:HG   | 5        | 0.34          |
| (1,370) | 1:7:A:LEU:HD22 | 1:7:A:LEU:HG   | 5        | 0.34          |
| (1,370) | 1:7:A:LEU:HD23 | 1:7:A:LEU:HG   | 5        | 0.34          |
| (1,370) | 1:7:A:LEU:HD11 | 1:7:A:LEU:HG   | 6        | 0.34          |
| (1,370) | 1:7:A:LEU:HD12 | 1:7:A:LEU:HG   | 6        | 0.34          |
| (1,370) | 1:7:A:LEU:HD13 | 1:7:A:LEU:HG   | 6        | 0.34          |
| (1,370) | 1:7:A:LEU:HD21 | 1:7:A:LEU:HG   | 6        | 0.34          |
| (1,370) | 1:7:A:LEU:HD22 | 1:7:A:LEU:HG   | 6        | 0.34          |
| (1,370) | 1:7:A:LEU:HD23 | 1:7:A:LEU:HG   | 6        | 0.34          |
| (1,370) | 1:7:A:LEU:HD11 | 1:7:A:LEU:HG   | 7        | 0.34          |
| (1,370) | 1:7:A:LEU:HD12 | 1:7:A:LEU:HG   | 7        | 0.34          |
| (1,370) | 1:7:A:LEU:HD13 | 1:7:A:LEU:HG   | 7        | 0.34          |
| (1,370) | 1:7:A:LEU:HD21 | 1:7:A:LEU:HG   | 7        | 0.34          |
| (1,370) | 1:7:A:LEU:HD22 | 1:7:A:LEU:HG   | 7        | 0.34          |
| (1,370) | 1:7:A:LEU:HD23 | 1:7:A:LEU:HG   | 7        | 0.34          |
| (1,370) | 1:7:A:LEU:HD11 | 1:7:A:LEU:HG   | 8        | 0.34          |
| (1,370) | 1:7:A:LEU:HD12 | 1:7:A:LEU:HG   | 8        | 0.34          |
| (1,370) | 1:7:A:LEU:HD13 | 1:7:A:LEU:HG   | 8        | 0.34          |
| (1,370) | 1:7:A:LEU:HD21 | 1:7:A:LEU:HG   | 8        | 0.34          |
| (1,370) | 1:7:A:LEU:HD22 | 1:7:A:LEU:HG   | 8        | 0.34          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,370) | 1:7:A:LEU:HD23 | 1:7:A:LEU:HG    | 8        | 0.34          |
| (1,370) | 1:7:A:LEU:HD11 | 1:7:A:LEU:HG    | 9        | 0.34          |
| (1,370) | 1:7:A:LEU:HD12 | 1:7:A:LEU:HG    | 9        | 0.34          |
| (1,370) | 1:7:A:LEU:HD13 | 1:7:A:LEU:HG    | 9        | 0.34          |
| (1,370) | 1:7:A:LEU:HD21 | 1:7:A:LEU:HG    | 9        | 0.34          |
| (1,370) | 1:7:A:LEU:HD22 | 1:7:A:LEU:HG    | 9        | 0.34          |
| (1,370) | 1:7:A:LEU:HD23 | 1:7:A:LEU:HG    | 9        | 0.34          |
| (1,370) | 1:7:A:LEU:HD11 | 1:7:A:LEU:HG    | 10       | 0.34          |
| (1,370) | 1:7:A:LEU:HD12 | 1:7:A:LEU:HG    | 10       | 0.34          |
| (1,370) | 1:7:A:LEU:HD13 | 1:7:A:LEU:HG    | 10       | 0.34          |
| (1,370) | 1:7:A:LEU:HD21 | 1:7:A:LEU:HG    | 10       | 0.34          |
| (1,370) | 1:7:A:LEU:HD22 | 1:7:A:LEU:HG    | 10       | 0.34          |
| (1,370) | 1:7:A:LEU:HD23 | 1:7:A:LEU:HG    | 10       | 0.34          |
| (1,280) | 1:4:A:CYS:H    | 1:5:A:VAL:H     | 2        | 0.34          |
| (1,276) | 1:19:A:SER:H   | 1:20:A:GLY:H    | 5        | 0.34          |
| (1,273) | 1:18:A:SER:H   | 1:19:A:SER:H    | 7        | 0.34          |
| (1,262) | 1:10:A:GLN:HA  | 1:10:A:GLN:HE22 | 1        | 0.34          |
| (1,199) | 1:8:A:TYR:HD1  | 1:23:A:PRO:HB3  | 8        | 0.34          |
| (1,199) | 1:8:A:TYR:HD2  | 1:23:A:PRO:HB3  | 8        | 0.34          |
| (1,177) | 1:8:A:TYR:HD1  | 1:12:A:LEU:HA   | 6        | 0.34          |
| (1,177) | 1:8:A:TYR:HD2  | 1:12:A:LEU:HA   | 6        | 0.34          |
| (1,140) | 1:9:A:ILE:HA   | 1:12:A:LEU:H    | 6        | 0.34          |
| (1,99)  | 1:11:A:TRP:HE1 | 1:22:A:PRO:HA   | 3        | 0.34          |
| (1,99)  | 1:11:A:TRP:HE1 | 1:22:A:PRO:HA   | 8        | 0.34          |
| (1,76)  | 1:25:A:CYS:H   | 1:25:A:CYS:HB3  | 3        | 0.34          |
| (1,69)  | 1:18:A:SER:H   | 1:18:A:SER:HA   | 3        | 0.34          |
| (1,40)  | 1:6:A:ARG:H    | 1:6:A:ARG:HB2   | 8        | 0.34          |
| (1,734) | 1:2:A:GLU:HG3  | 1:5:A:VAL:HB    | 2        | 0.33          |
| (1,715) | 1:9:A:ILE:HG21 | 1:12:A:LEU:HB2  | 1        | 0.33          |
| (1,715) | 1:9:A:ILE:HG22 | 1:12:A:LEU:HB2  | 1        | 0.33          |
| (1,715) | 1:9:A:ILE:HG23 | 1:12:A:LEU:HB2  | 1        | 0.33          |
| (1,675) | 1:12:A:LEU:HA  | 1:12:A:LEU:HD21 | 1        | 0.33          |
| (1,675) | 1:12:A:LEU:HA  | 1:12:A:LEU:HD22 | 1        | 0.33          |
| (1,675) | 1:12:A:LEU:HA  | 1:12:A:LEU:HD23 | 1        | 0.33          |
| (1,675) | 1:12:A:LEU:HA  | 1:12:A:LEU:HD21 | 2        | 0.33          |
| (1,675) | 1:12:A:LEU:HA  | 1:12:A:LEU:HD22 | 2        | 0.33          |
| (1,675) | 1:12:A:LEU:HA  | 1:12:A:LEU:HD23 | 2        | 0.33          |
| (1,644) | 1:22:A:PRO:HA  | 1:23:A:PRO:HD2  | 4        | 0.33          |
| (1,626) | 1:14:A:ASP:HB3 | 1:15:A:GLY:H    | 4        | 0.33          |
| (1,626) | 1:14:A:ASP:HB3 | 1:15:A:GLY:H    | 9        | 0.33          |
| (1,569) | 1:8:A:TYR:HA   | 1:11:A:TRP:HB3  | 10       | 0.33          |
| (1,545) | 1:13:A:LYS:HB2 | 1:13:A:LYS:HE2  | 2        | 0.33          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,545) | 1:13:A:LYS:HB2  | 1:13:A:LYS:HE3 | 2        | 0.33          |
| (1,545) | 1:13:A:LYS:HB3  | 1:13:A:LYS:HE2 | 2        | 0.33          |
| (1,545) | 1:13:A:LYS:HB3  | 1:13:A:LYS:HE3 | 2        | 0.33          |
| (1,465) | 1:21:A:ARG:HB2  | 1:21:A:ARG:HD2 | 4        | 0.33          |
| (1,465) | 1:21:A:ARG:HB2  | 1:21:A:ARG:HD2 | 6        | 0.33          |
| (1,465) | 1:21:A:ARG:HB2  | 1:21:A:ARG:HD2 | 9        | 0.33          |
| (1,448) | 1:17:A:PRO:HB2  | 1:17:A:PRO:HB3 | 3        | 0.33          |
| (1,448) | 1:17:A:PRO:HB2  | 1:17:A:PRO:HB3 | 4        | 0.33          |
| (1,448) | 1:17:A:PRO:HB2  | 1:17:A:PRO:HB3 | 7        | 0.33          |
| (1,448) | 1:17:A:PRO:HB2  | 1:17:A:PRO:HB3 | 8        | 0.33          |
| (1,448) | 1:17:A:PRO:HB2  | 1:17:A:PRO:HB3 | 10       | 0.33          |
| (1,359) | 1:6:A:ARG:HD2   | 1:6:A:ARG:HG3  | 3        | 0.33          |
| (1,326) | 1:2:A:GLU:HA    | 1:2:A:GLU:HB3  | 5        | 0.33          |
| (1,276) | 1:19:A:SER:H    | 1:20:A:GLY:H   | 10       | 0.33          |
| (1,225) | 1:23:A:PRO:HB2  | 1:25:A:CYS:H   | 8        | 0.33          |
| (1,225) | 1:23:A:PRO:HB2  | 1:25:A:CYS:H   | 9        | 0.33          |
| (1,196) | 1:11:A:TRP:HH2  | 1:23:A:PRO:HB3 | 4        | 0.33          |
| (1,172) | 1:11:A:TRP:HZ2  | 1:23:A:PRO:HD3 | 5        | 0.33          |
| (1,106) | 1:8:A:TYR:H     | 1:9:A:ILE:H    | 3        | 0.33          |
| (1,69)  | 1:18:A:SER:H    | 1:18:A:SER:HA  | 1        | 0.33          |
| (1,40)  | 1:6:A:ARG:H     | 1:6:A:ARG:HB2  | 1        | 0.33          |
| (1,734) | 1:2:A:GLU:HG3   | 1:5:A:VAL:HB   | 5        | 0.32          |
| (1,715) | 1:9:A:ILE:HG21  | 1:12:A:LEU:HB2 | 4        | 0.32          |
| (1,715) | 1:9:A:ILE:HG22  | 1:12:A:LEU:HB2 | 4        | 0.32          |
| (1,715) | 1:9:A:ILE:HG23  | 1:12:A:LEU:HB2 | 4        | 0.32          |
| (1,661) | 1:17:A:PRO:HB3  | 1:18:A:SER:HB3 | 6        | 0.32          |
| (1,651) | 1:3:A:GLU:HA    | 1:6:A:ARG:HD2  | 5        | 0.32          |
| (1,648) | 1:15:A:GLY:HA2  | 1:19:A:SER:HB2 | 6        | 0.32          |
| (1,625) | 1:10:A:GLN:HE21 | 1:14:A:ASP:HB3 | 10       | 0.32          |
| (1,593) | 1:11:A:TRP:HA   | 1:14:A:ASP:HB3 | 6        | 0.32          |
| (1,542) | 1:7:A:LEU:HB2   | 1:24:A:PRO:HB3 | 9        | 0.32          |
| (1,512) | 1:23:A:PRO:HB3  | 1:23:A:PRO:HD3 | 10       | 0.32          |
| (1,498) | 1:23:A:PRO:HA   | 1:23:A:PRO:HB3 | 9        | 0.32          |
| (1,411) | 1:12:A:LEU:HB2  | 1:12:A:LEU:HG  | 1        | 0.32          |
| (1,411) | 1:12:A:LEU:HB2  | 1:12:A:LEU:HG  | 2        | 0.32          |
| (1,403) | 1:11:A:TRP:HB2  | 1:11:A:TRP:HB3 | 1        | 0.32          |
| (1,403) | 1:11:A:TRP:HB2  | 1:11:A:TRP:HB3 | 3        | 0.32          |
| (1,259) | 1:4:A:CYS:HB3   | 1:5:A:VAL:H    | 5        | 0.32          |
| (1,226) | 1:11:A:TRP:HH2  | 1:23:A:PRO:HG2 | 2        | 0.32          |
| (1,199) | 1:8:A:TYR:HD1   | 1:23:A:PRO:HB3 | 6        | 0.32          |
| (1,199) | 1:8:A:TYR:HD2   | 1:23:A:PRO:HB3 | 6        | 0.32          |
| (1,199) | 1:8:A:TYR:HD1   | 1:23:A:PRO:HB3 | 10       | 0.32          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,199) | 1:8:A:TYR:HD2  | 1:23:A:PRO:HB3  | 10       | 0.32          |
| (1,69)  | 1:18:A:SER:H   | 1:18:A:SER:HA   | 4        | 0.32          |
| (1,69)  | 1:18:A:SER:H   | 1:18:A:SER:HA   | 6        | 0.32          |
| (1,69)  | 1:18:A:SER:H   | 1:18:A:SER:HA   | 8        | 0.32          |
| (1,69)  | 1:18:A:SER:H   | 1:18:A:SER:HA   | 9        | 0.32          |
| (1,69)  | 1:18:A:SER:H   | 1:18:A:SER:HA   | 10       | 0.32          |
| (1,40)  | 1:6:A:ARG:H    | 1:6:A:ARG:HB2   | 10       | 0.32          |
| (1,715) | 1:9:A:ILE:HG21 | 1:12:A:LEU:HB2  | 8        | 0.31          |
| (1,715) | 1:9:A:ILE:HG22 | 1:12:A:LEU:HB2  | 8        | 0.31          |
| (1,715) | 1:9:A:ILE:HG23 | 1:12:A:LEU:HB2  | 8        | 0.31          |
| (1,659) | 1:11:A:TRP:HB3 | 1:24:A:PRO:HD2  | 3        | 0.31          |
| (1,579) | 1:4:A:CYS:HA   | 1:7:A:LEU:HB2   | 3        | 0.31          |
| (1,579) | 1:4:A:CYS:HA   | 1:7:A:LEU:HB2   | 6        | 0.31          |
| (1,498) | 1:23:A:PRO:HA  | 1:23:A:PRO:HB3  | 3        | 0.31          |
| (1,498) | 1:23:A:PRO:HA  | 1:23:A:PRO:HB3  | 8        | 0.31          |
| (1,498) | 1:23:A:PRO:HA  | 1:23:A:PRO:HB3  | 10       | 0.31          |
| (1,424) | 1:13:A:LYS:HB2 | 1:13:A:LYS:HD3  | 1        | 0.31          |
| (1,424) | 1:13:A:LYS:HB3 | 1:13:A:LYS:HD3  | 1        | 0.31          |
| (1,403) | 1:11:A:TRP:HB2 | 1:11:A:TRP:HB3  | 2        | 0.31          |
| (1,403) | 1:11:A:TRP:HB2 | 1:11:A:TRP:HB3  | 4        | 0.31          |
| (1,403) | 1:11:A:TRP:HB2 | 1:11:A:TRP:HB3  | 5        | 0.31          |
| (1,403) | 1:11:A:TRP:HB2 | 1:11:A:TRP:HB3  | 6        | 0.31          |
| (1,403) | 1:11:A:TRP:HB2 | 1:11:A:TRP:HB3  | 7        | 0.31          |
| (1,403) | 1:11:A:TRP:HB2 | 1:11:A:TRP:HB3  | 8        | 0.31          |
| (1,403) | 1:11:A:TRP:HB2 | 1:11:A:TRP:HB3  | 9        | 0.31          |
| (1,403) | 1:11:A:TRP:HB2 | 1:11:A:TRP:HB3  | 10       | 0.31          |
| (1,359) | 1:6:A:ARG:HD2  | 1:6:A:ARG:HG3   | 6        | 0.31          |
| (1,301) | 1:12:A:LEU:H   | 1:12:A:LEU:HB2  | 3        | 0.31          |
| (1,280) | 1:4:A:CYS:H    | 1:5:A:VAL:H     | 7        | 0.31          |
| (1,277) | 1:20:A:GLY:H   | 1:21:A:ARG:H    | 2        | 0.31          |
| (1,277) | 1:20:A:GLY:H   | 1:21:A:ARG:H    | 7        | 0.31          |
| (1,239) | 1:8:A:TYR:HE1  | 1:12:A:LEU:HG   | 9        | 0.31          |
| (1,239) | 1:8:A:TYR:HE2  | 1:12:A:LEU:HG   | 9        | 0.31          |
| (1,222) | 1:8:A:TYR:HD1  | 1:23:A:PRO:HB2  | 9        | 0.31          |
| (1,222) | 1:8:A:TYR:HD2  | 1:23:A:PRO:HB2  | 9        | 0.31          |
| (1,215) | 1:11:A:TRP:HZ3 | 1:12:A:LEU:HD21 | 5        | 0.31          |
| (1,215) | 1:11:A:TRP:HZ3 | 1:12:A:LEU:HD22 | 5        | 0.31          |
| (1,215) | 1:11:A:TRP:HZ3 | 1:12:A:LEU:HD23 | 5        | 0.31          |
| (1,199) | 1:8:A:TYR:HD1  | 1:23:A:PRO:HB3  | 9        | 0.31          |
| (1,199) | 1:8:A:TYR:HD2  | 1:23:A:PRO:HB3  | 9        | 0.31          |
| (1,154) | 1:7:A:LEU:H    | 1:7:A:LEU:HB2   | 4        | 0.31          |
| (1,111) | 1:10:A:GLN:HB3 | 1:11:A:TRP:H    | 4        | 0.31          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,69)  | 1:18:A:SER:H    | 1:18:A:SER:HA   | 7        | 0.31          |
| (1,55)  | 1:21:A:ARG:H    | 1:21:A:ARG:HD2  | 9        | 0.31          |
| (1,40)  | 1:6:A:ARG:H     | 1:6:A:ARG:HB2   | 3        | 0.31          |
| (1,717) | 1:12:A:LEU:HD11 | 1:16:A:GLY:HA2  | 5        | 0.3           |
| (1,717) | 1:12:A:LEU:HD12 | 1:16:A:GLY:HA2  | 5        | 0.3           |
| (1,717) | 1:12:A:LEU:HD13 | 1:16:A:GLY:HA2  | 5        | 0.3           |
| (1,715) | 1:9:A:ILE:HG21  | 1:12:A:LEU:HB2  | 7        | 0.3           |
| (1,715) | 1:9:A:ILE:HG22  | 1:12:A:LEU:HB2  | 7        | 0.3           |
| (1,715) | 1:9:A:ILE:HG23  | 1:12:A:LEU:HB2  | 7        | 0.3           |
| (1,715) | 1:9:A:ILE:HG21  | 1:12:A:LEU:HB2  | 10       | 0.3           |
| (1,715) | 1:9:A:ILE:HG22  | 1:12:A:LEU:HB2  | 10       | 0.3           |
| (1,715) | 1:9:A:ILE:HG23  | 1:12:A:LEU:HB2  | 10       | 0.3           |
| (1,705) | 1:9:A:ILE:HG21  | 1:13:A:LYS:HD2  | 8        | 0.3           |
| (1,705) | 1:9:A:ILE:HG22  | 1:13:A:LYS:HD2  | 8        | 0.3           |
| (1,705) | 1:9:A:ILE:HG23  | 1:13:A:LYS:HD2  | 8        | 0.3           |
| (1,704) | 1:9:A:ILE:HG21  | 1:13:A:LYS:HD3  | 7        | 0.3           |
| (1,704) | 1:9:A:ILE:HG22  | 1:13:A:LYS:HD3  | 7        | 0.3           |
| (1,704) | 1:9:A:ILE:HG23  | 1:13:A:LYS:HD3  | 7        | 0.3           |
| (1,681) | 1:11:A:TRP:HB3  | 1:12:A:LEU:HD21 | 3        | 0.3           |
| (1,681) | 1:11:A:TRP:HB3  | 1:12:A:LEU:HD22 | 3        | 0.3           |
| (1,681) | 1:11:A:TRP:HB3  | 1:12:A:LEU:HD23 | 3        | 0.3           |
| (1,666) | 1:24:A:PRO:HG2  | 1:25:A:CYS:HB2  | 1        | 0.3           |
| (1,648) | 1:15:A:GLY:HA2  | 1:19:A:SER:HB2  | 5        | 0.3           |
| (1,640) | 1:11:A:TRP:HE3  | 1:24:A:PRO:HD2  | 1        | 0.3           |
| (1,626) | 1:14:A:ASP:HB3  | 1:15:A:GLY:H    | 2        | 0.3           |
| (1,576) | 1:22:A:PRO:HA   | 1:23:A:PRO:HD3  | 5        | 0.3           |
| (1,576) | 1:22:A:PRO:HA   | 1:23:A:PRO:HD3  | 8        | 0.3           |
| (1,571) | 1:14:A:ASP:HB3  | 1:19:A:SER:HB2  | 5        | 0.3           |
| (1,569) | 1:8:A:TYR:HA    | 1:11:A:TRP:HB3  | 4        | 0.3           |
| (1,569) | 1:8:A:TYR:HA    | 1:11:A:TRP:HB3  | 8        | 0.3           |
| (1,546) | 1:13:A:LYS:HD3  | 1:13:A:LYS:HE2  | 4        | 0.3           |
| (1,546) | 1:13:A:LYS:HD3  | 1:13:A:LYS:HE3  | 4        | 0.3           |
| (1,498) | 1:23:A:PRO:HA   | 1:23:A:PRO:HB3  | 5        | 0.3           |
| (1,465) | 1:21:A:ARG:HB2  | 1:21:A:ARG:HD2  | 1        | 0.3           |
| (1,465) | 1:21:A:ARG:HB2  | 1:21:A:ARG:HD2  | 10       | 0.3           |
| (1,461) | 1:21:A:ARG:HA   | 1:21:A:ARG:HG2  | 1        | 0.3           |
| (1,461) | 1:21:A:ARG:HA   | 1:21:A:ARG:HG3  | 1        | 0.3           |
| (1,359) | 1:6:A:ARG:HD2   | 1:6:A:ARG:HG3   | 4        | 0.3           |
| (1,301) | 1:12:A:LEU:H    | 1:12:A:LEU:HB2  | 6        | 0.3           |
| (1,215) | 1:11:A:TRP:HZ3  | 1:12:A:LEU:HD21 | 6        | 0.3           |
| (1,215) | 1:11:A:TRP:HZ3  | 1:12:A:LEU:HD22 | 6        | 0.3           |
| (1,215) | 1:11:A:TRP:HZ3  | 1:12:A:LEU:HD23 | 6        | 0.3           |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,199) | 1:8:A:TYR:HD1   | 1:23:A:PRO:HB3  | 1        | 0.3           |
| (1,199) | 1:8:A:TYR:HD2   | 1:23:A:PRO:HB3  | 1        | 0.3           |
| (1,154) | 1:7:A:LEU:H     | 1:7:A:LEU:HB2   | 1        | 0.3           |
| (1,93)  | 1:19:A:SER:HG   | 1:21:A:ARG:H    | 8        | 0.3           |
| (1,40)  | 1:6:A:ARG:H     | 1:6:A:ARG:HB2   | 5        | 0.3           |
| (1,720) | 1:7:A:LEU:HB2   | 1:24:A:PRO:HB2  | 1        | 0.29          |
| (1,709) | 1:12:A:LEU:HD11 | 1:23:A:PRO:HB2  | 3        | 0.29          |
| (1,709) | 1:12:A:LEU:HD12 | 1:23:A:PRO:HB2  | 3        | 0.29          |
| (1,709) | 1:12:A:LEU:HD13 | 1:23:A:PRO:HB2  | 3        | 0.29          |
| (1,677) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD11 | 6        | 0.29          |
| (1,677) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD12 | 6        | 0.29          |
| (1,677) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD13 | 6        | 0.29          |
| (1,600) | 1:1:A:GLU:HB3   | 1:1:A:GLU:HG2   | 1        | 0.29          |
| (1,600) | 1:1:A:GLU:HB3   | 1:1:A:GLU:HG3   | 1        | 0.29          |
| (1,579) | 1:4:A:CYS:HA    | 1:7:A:LEU:HB2   | 4        | 0.29          |
| (1,565) | 1:4:A:CYS:HA    | 1:7:A:LEU:HG    | 2        | 0.29          |
| (1,554) | 1:22:A:PRO:HB3  | 1:23:A:PRO:HD2  | 9        | 0.29          |
| (1,550) | 1:11:A:TRP:HB3  | 1:24:A:PRO:HD3  | 8        | 0.29          |
| (1,550) | 1:11:A:TRP:HB3  | 1:24:A:PRO:HD3  | 10       | 0.29          |
| (1,546) | 1:13:A:LYS:HD3  | 1:13:A:LYS:HE2  | 7        | 0.29          |
| (1,546) | 1:13:A:LYS:HD3  | 1:13:A:LYS:HE3  | 7        | 0.29          |
| (1,535) | 1:23:A:PRO:HB3  | 1:24:A:PRO:HD2  | 2        | 0.29          |
| (1,506) | 1:23:A:PRO:HD3  | 1:23:A:PRO:HG3  | 1        | 0.29          |
| (1,506) | 1:23:A:PRO:HD3  | 1:23:A:PRO:HG3  | 5        | 0.29          |
| (1,506) | 1:23:A:PRO:HD3  | 1:23:A:PRO:HG3  | 6        | 0.29          |
| (1,498) | 1:23:A:PRO:HA   | 1:23:A:PRO:HB3  | 1        | 0.29          |
| (1,498) | 1:23:A:PRO:HA   | 1:23:A:PRO:HB3  | 6        | 0.29          |
| (1,465) | 1:21:A:ARG:HB2  | 1:21:A:ARG:HD2  | 5        | 0.29          |
| (1,450) | 1:18:A:SER:HA   | 1:18:A:SER:HB3  | 4        | 0.29          |
| (1,443) | 1:17:A:PRO:HD2  | 1:17:A:PRO:HG2  | 4        | 0.29          |
| (1,443) | 1:17:A:PRO:HD2  | 1:17:A:PRO:HG3  | 4        | 0.29          |
| (1,443) | 1:17:A:PRO:HD2  | 1:17:A:PRO:HG2  | 5        | 0.29          |
| (1,443) | 1:17:A:PRO:HD2  | 1:17:A:PRO:HG3  | 5        | 0.29          |
| (1,443) | 1:17:A:PRO:HD2  | 1:17:A:PRO:HG2  | 6        | 0.29          |
| (1,443) | 1:17:A:PRO:HD2  | 1:17:A:PRO:HG3  | 6        | 0.29          |
| (1,443) | 1:17:A:PRO:HD2  | 1:17:A:PRO:HG2  | 7        | 0.29          |
| (1,443) | 1:17:A:PRO:HD2  | 1:17:A:PRO:HG3  | 7        | 0.29          |
| (1,443) | 1:17:A:PRO:HD2  | 1:17:A:PRO:HG2  | 9        | 0.29          |
| (1,443) | 1:17:A:PRO:HD2  | 1:17:A:PRO:HG3  | 9        | 0.29          |
| (1,411) | 1:12:A:LEU:HB2  | 1:12:A:LEU:HG   | 5        | 0.29          |
| (1,359) | 1:6:A:ARG:HD2   | 1:6:A:ARG:HG3   | 5        | 0.29          |
| (1,326) | 1:2:A:GLU:HA    | 1:2:A:GLU:HB3   | 7        | 0.29          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,321) | 1:11:A:TRP:HB3  | 1:12:A:LEU:H    | 3        | 0.29          |
| (1,250) | 1:11:A:TRP:HE3  | 1:23:A:PRO:HA   | 6        | 0.29          |
| (1,221) | 1:8:A:TYR:HE1   | 1:12:A:LEU:HB2  | 3        | 0.29          |
| (1,221) | 1:8:A:TYR:HE2   | 1:12:A:LEU:HB2  | 3        | 0.29          |
| (1,154) | 1:7:A:LEU:H     | 1:7:A:LEU:HB2   | 9        | 0.29          |
| (1,40)  | 1:6:A:ARG:H     | 1:6:A:ARG:HB2   | 4        | 0.29          |
| (1,40)  | 1:6:A:ARG:H     | 1:6:A:ARG:HB2   | 6        | 0.29          |
| (1,10)  | 1:9:A:ILE:H     | 1:12:A:LEU:HD21 | 7        | 0.29          |
| (1,10)  | 1:9:A:ILE:H     | 1:12:A:LEU:HD22 | 7        | 0.29          |
| (1,10)  | 1:9:A:ILE:H     | 1:12:A:LEU:HD23 | 7        | 0.29          |
| (1,10)  | 1:9:A:ILE:H     | 1:12:A:LEU:HD21 | 9        | 0.29          |
| (1,10)  | 1:9:A:ILE:H     | 1:12:A:LEU:HD22 | 9        | 0.29          |
| (1,10)  | 1:9:A:ILE:H     | 1:12:A:LEU:HD23 | 9        | 0.29          |
| (1,720) | 1:7:A:LEU:HB2   | 1:24:A:PRO:HB2  | 5        | 0.28          |
| (1,715) | 1:9:A:ILE:HG21  | 1:12:A:LEU:HB2  | 9        | 0.28          |
| (1,715) | 1:9:A:ILE:HG22  | 1:12:A:LEU:HB2  | 9        | 0.28          |
| (1,715) | 1:9:A:ILE:HG23  | 1:12:A:LEU:HB2  | 9        | 0.28          |
| (1,711) | 1:12:A:LEU:HD21 | 1:23:A:PRO:HB2  | 3        | 0.28          |
| (1,711) | 1:12:A:LEU:HD22 | 1:23:A:PRO:HB2  | 3        | 0.28          |
| (1,711) | 1:12:A:LEU:HD23 | 1:23:A:PRO:HB2  | 3        | 0.28          |
| (1,705) | 1:9:A:ILE:HG21  | 1:13:A:LYS:HD2  | 10       | 0.28          |
| (1,705) | 1:9:A:ILE:HG22  | 1:13:A:LYS:HD2  | 10       | 0.28          |
| (1,705) | 1:9:A:ILE:HG23  | 1:13:A:LYS:HD2  | 10       | 0.28          |
| (1,677) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD11 | 5        | 0.28          |
| (1,677) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD12 | 5        | 0.28          |
| (1,677) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD13 | 5        | 0.28          |
| (1,651) | 1:3:A:GLU:HA    | 1:6:A:ARG:HD2   | 10       | 0.28          |
| (1,646) | 1:15:A:GLY:HA2  | 1:18:A:SER:HB3  | 1        | 0.28          |
| (1,640) | 1:11:A:TRP:HE3  | 1:24:A:PRO:HD2  | 2        | 0.28          |
| (1,640) | 1:11:A:TRP:HE3  | 1:24:A:PRO:HD2  | 5        | 0.28          |
| (1,640) | 1:11:A:TRP:HE3  | 1:24:A:PRO:HD2  | 6        | 0.28          |
| (1,623) | 1:2:A:GLU:HB3   | 1:6:A:ARG:H     | 1        | 0.28          |
| (1,581) | 1:5:A:VAL:HG11  | 1:6:A:ARG:HA    | 4        | 0.28          |
| (1,581) | 1:5:A:VAL:HG12  | 1:6:A:ARG:HA    | 4        | 0.28          |
| (1,581) | 1:5:A:VAL:HG13  | 1:6:A:ARG:HA    | 4        | 0.28          |
| (1,581) | 1:5:A:VAL:HG11  | 1:6:A:ARG:HA    | 6        | 0.28          |
| (1,581) | 1:5:A:VAL:HG12  | 1:6:A:ARG:HA    | 6        | 0.28          |
| (1,581) | 1:5:A:VAL:HG13  | 1:6:A:ARG:HA    | 6        | 0.28          |
| (1,576) | 1:22:A:PRO:HA   | 1:23:A:PRO:HD3  | 10       | 0.28          |
| (1,551) | 1:16:A:GLY:HA3  | 1:17:A:PRO:HD3  | 6        | 0.28          |
| (1,542) | 1:7:A:LEU:HB2   | 1:24:A:PRO:HB3  | 4        | 0.28          |
| (1,526) | 1:24:A:PRO:HB3  | 1:24:A:PRO:HD2  | 3        | 0.28          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,512) | 1:23:A:PRO:HB3 | 1:23:A:PRO:HD3  | 9        | 0.28          |
| (1,506) | 1:23:A:PRO:HD3 | 1:23:A:PRO:HG3  | 2        | 0.28          |
| (1,506) | 1:23:A:PRO:HD3 | 1:23:A:PRO:HG3  | 8        | 0.28          |
| (1,506) | 1:23:A:PRO:HD3 | 1:23:A:PRO:HG3  | 9        | 0.28          |
| (1,506) | 1:23:A:PRO:HD3 | 1:23:A:PRO:HG3  | 10       | 0.28          |
| (1,498) | 1:23:A:PRO:HA  | 1:23:A:PRO:HB3  | 2        | 0.28          |
| (1,445) | 1:17:A:PRO:HD3 | 1:17:A:PRO:HG2  | 7        | 0.28          |
| (1,445) | 1:17:A:PRO:HD3 | 1:17:A:PRO:HG3  | 7        | 0.28          |
| (1,443) | 1:17:A:PRO:HD2 | 1:17:A:PRO:HG2  | 1        | 0.28          |
| (1,443) | 1:17:A:PRO:HD2 | 1:17:A:PRO:HG3  | 1        | 0.28          |
| (1,443) | 1:17:A:PRO:HD2 | 1:17:A:PRO:HG2  | 2        | 0.28          |
| (1,443) | 1:17:A:PRO:HD2 | 1:17:A:PRO:HG3  | 2        | 0.28          |
| (1,443) | 1:17:A:PRO:HD2 | 1:17:A:PRO:HG2  | 3        | 0.28          |
| (1,443) | 1:17:A:PRO:HD2 | 1:17:A:PRO:HG3  | 3        | 0.28          |
| (1,443) | 1:17:A:PRO:HD2 | 1:17:A:PRO:HG2  | 8        | 0.28          |
| (1,443) | 1:17:A:PRO:HD2 | 1:17:A:PRO:HG3  | 8        | 0.28          |
| (1,443) | 1:17:A:PRO:HD2 | 1:17:A:PRO:HG2  | 10       | 0.28          |
| (1,443) | 1:17:A:PRO:HD2 | 1:17:A:PRO:HG3  | 10       | 0.28          |
| (1,411) | 1:12:A:LEU:HB2 | 1:12:A:LEU:HG   | 3        | 0.28          |
| (1,411) | 1:12:A:LEU:HB2 | 1:12:A:LEU:HG   | 6        | 0.28          |
| (1,359) | 1:6:A:ARG:HD2  | 1:6:A:ARG:HG3   | 10       | 0.28          |
| (1,338) | 1:4:A:CYS:HA   | 1:4:A:CYS:HB2   | 3        | 0.28          |
| (1,301) | 1:12:A:LEU:H   | 1:12:A:LEU:HB2  | 5        | 0.28          |
| (1,239) | 1:8:A:TYR:HE1  | 1:12:A:LEU:HG   | 5        | 0.28          |
| (1,239) | 1:8:A:TYR:HE2  | 1:12:A:LEU:HG   | 5        | 0.28          |
| (1,226) | 1:11:A:TRP:HH2 | 1:23:A:PRO:HG2  | 3        | 0.28          |
| (1,196) | 1:11:A:TRP:HH2 | 1:23:A:PRO:HB3  | 7        | 0.28          |
| (1,171) | 1:11:A:TRP:HH2 | 1:23:A:PRO:HD3  | 1        | 0.28          |
| (1,154) | 1:7:A:LEU:H    | 1:7:A:LEU:HB2   | 6        | 0.28          |
| (1,108) | 1:14:A:ASP:H   | 1:15:A:GLY:H    | 10       | 0.28          |
| (1,76)  | 1:25:A:CYS:H   | 1:25:A:CYS:HB3  | 4        | 0.28          |
| (1,56)  | 1:21:A:ARG:H   | 1:21:A:ARG:HD3  | 2        | 0.28          |
| (1,56)  | 1:21:A:ARG:H   | 1:21:A:ARG:HD3  | 3        | 0.28          |
| (1,55)  | 1:21:A:ARG:H   | 1:21:A:ARG:HD2  | 5        | 0.28          |
| (1,40)  | 1:6:A:ARG:H    | 1:6:A:ARG:HB2   | 7        | 0.28          |
| (1,10)  | 1:9:A:ILE:H    | 1:12:A:LEU:HD21 | 4        | 0.28          |
| (1,10)  | 1:9:A:ILE:H    | 1:12:A:LEU:HD22 | 4        | 0.28          |
| (1,10)  | 1:9:A:ILE:H    | 1:12:A:LEU:HD23 | 4        | 0.28          |
| (1,728) | 1:2:A:GLU:HG2  | 1:6:A:ARG:HG2   | 3        | 0.27          |
| (1,626) | 1:14:A:ASP:HB3 | 1:15:A:GLY:H    | 7        | 0.27          |
| (1,576) | 1:22:A:PRO:HA  | 1:23:A:PRO:HD3  | 9        | 0.27          |
| (1,512) | 1:23:A:PRO:HB3 | 1:23:A:PRO:HD3  | 8        | 0.27          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,506) | 1:23:A:PRO:HD3  | 1:23:A:PRO:HG3  | 3        | 0.27          |
| (1,494) | 1:21:A:ARG:HA   | 1:22:A:PRO:HD3  | 4        | 0.27          |
| (1,479) | 1:22:A:PRO:HB3  | 1:22:A:PRO:HD3  | 7        | 0.27          |
| (1,461) | 1:21:A:ARG:HA   | 1:21:A:ARG:HG2  | 5        | 0.27          |
| (1,461) | 1:21:A:ARG:HA   | 1:21:A:ARG:HG3  | 5        | 0.27          |
| (1,445) | 1:17:A:PRO:HD3  | 1:17:A:PRO:HG2  | 1        | 0.27          |
| (1,445) | 1:17:A:PRO:HD3  | 1:17:A:PRO:HG3  | 1        | 0.27          |
| (1,445) | 1:17:A:PRO:HD3  | 1:17:A:PRO:HG2  | 2        | 0.27          |
| (1,445) | 1:17:A:PRO:HD3  | 1:17:A:PRO:HG3  | 2        | 0.27          |
| (1,445) | 1:17:A:PRO:HD3  | 1:17:A:PRO:HG2  | 3        | 0.27          |
| (1,445) | 1:17:A:PRO:HD3  | 1:17:A:PRO:HG3  | 3        | 0.27          |
| (1,445) | 1:17:A:PRO:HD3  | 1:17:A:PRO:HG2  | 4        | 0.27          |
| (1,445) | 1:17:A:PRO:HD3  | 1:17:A:PRO:HG3  | 4        | 0.27          |
| (1,445) | 1:17:A:PRO:HD3  | 1:17:A:PRO:HG2  | 5        | 0.27          |
| (1,445) | 1:17:A:PRO:HD3  | 1:17:A:PRO:HG3  | 5        | 0.27          |
| (1,445) | 1:17:A:PRO:HD3  | 1:17:A:PRO:HG2  | 6        | 0.27          |
| (1,445) | 1:17:A:PRO:HD3  | 1:17:A:PRO:HG3  | 6        | 0.27          |
| (1,445) | 1:17:A:PRO:HD3  | 1:17:A:PRO:HG2  | 8        | 0.27          |
| (1,445) | 1:17:A:PRO:HD3  | 1:17:A:PRO:HG3  | 8        | 0.27          |
| (1,445) | 1:17:A:PRO:HD3  | 1:17:A:PRO:HG2  | 9        | 0.27          |
| (1,445) | 1:17:A:PRO:HD3  | 1:17:A:PRO:HG3  | 9        | 0.27          |
| (1,445) | 1:17:A:PRO:HD3  | 1:17:A:PRO:HG2  | 10       | 0.27          |
| (1,445) | 1:17:A:PRO:HD3  | 1:17:A:PRO:HG3  | 10       | 0.27          |
| (1,412) | 1:12:A:LEU:HD21 | 1:12:A:LEU:HG   | 8        | 0.27          |
| (1,412) | 1:12:A:LEU:HD22 | 1:12:A:LEU:HG   | 8        | 0.27          |
| (1,412) | 1:12:A:LEU:HD23 | 1:12:A:LEU:HG   | 8        | 0.27          |
| (1,412) | 1:12:A:LEU:HD21 | 1:12:A:LEU:HG   | 10       | 0.27          |
| (1,412) | 1:12:A:LEU:HD22 | 1:12:A:LEU:HG   | 10       | 0.27          |
| (1,412) | 1:12:A:LEU:HD23 | 1:12:A:LEU:HG   | 10       | 0.27          |
| (1,410) | 1:12:A:LEU:HB2  | 1:12:A:LEU:HB3  | 1        | 0.27          |
| (1,410) | 1:12:A:LEU:HB2  | 1:12:A:LEU:HB3  | 2        | 0.27          |
| (1,391) | 1:10:A:GLN:HA   | 1:10:A:GLN:HG2  | 2        | 0.27          |
| (1,359) | 1:6:A:ARG:HD2   | 1:6:A:ARG:HG3   | 2        | 0.27          |
| (1,359) | 1:6:A:ARG:HD2   | 1:6:A:ARG:HG3   | 9        | 0.27          |
| (1,326) | 1:2:A:GLU:HA    | 1:2:A:GLU:HB3   | 3        | 0.27          |
| (1,326) | 1:2:A:GLU:HA    | 1:2:A:GLU:HB3   | 10       | 0.27          |
| (1,250) | 1:11:A:TRP:HE3  | 1:23:A:PRO:HA   | 1        | 0.27          |
| (1,154) | 1:7:A:LEU:H     | 1:7:A:LEU:HB2   | 5        | 0.27          |
| (1,154) | 1:7:A:LEU:H     | 1:7:A:LEU:HB2   | 7        | 0.27          |
| (1,154) | 1:7:A:LEU:H     | 1:7:A:LEU:HB2   | 8        | 0.27          |
| (1,40)  | 1:6:A:ARG:H     | 1:6:A:ARG:HB2   | 9        | 0.27          |
| (1,10)  | 1:9:A:ILE:H     | 1:12:A:LEU:HD21 | 8        | 0.27          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,10)  | 1:9:A:ILE:H     | 1:12:A:LEU:HD22 | 8        | 0.27          |
| (1,10)  | 1:9:A:ILE:H     | 1:12:A:LEU:HD23 | 8        | 0.27          |
| (1,10)  | 1:9:A:ILE:H     | 1:12:A:LEU:HD21 | 10       | 0.27          |
| (1,10)  | 1:9:A:ILE:H     | 1:12:A:LEU:HD22 | 10       | 0.27          |
| (1,10)  | 1:9:A:ILE:H     | 1:12:A:LEU:HD23 | 10       | 0.27          |
| (1,734) | 1:2:A:GLU:HG3   | 1:5:A:VAL:HB    | 6        | 0.26          |
| (1,728) | 1:2:A:GLU:HG2   | 1:6:A:ARG:HG2   | 2        | 0.26          |
| (1,704) | 1:9:A:ILE:HG21  | 1:13:A:LYS:HD3  | 8        | 0.26          |
| (1,704) | 1:9:A:ILE:HG22  | 1:13:A:LYS:HD3  | 8        | 0.26          |
| (1,704) | 1:9:A:ILE:HG23  | 1:13:A:LYS:HD3  | 8        | 0.26          |
| (1,576) | 1:22:A:PRO:HA   | 1:23:A:PRO:HD3  | 1        | 0.26          |
| (1,569) | 1:8:A:TYR:HA    | 1:11:A:TRP:HB3  | 7        | 0.26          |
| (1,569) | 1:8:A:TYR:HA    | 1:11:A:TRP:HB3  | 9        | 0.26          |
| (1,526) | 1:24:A:PRO:HB3  | 1:24:A:PRO:HD2  | 1        | 0.26          |
| (1,522) | 1:24:A:PRO:HA   | 1:24:A:PRO:HD3  | 1        | 0.26          |
| (1,477) | 1:22:A:PRO:HA   | 1:22:A:PRO:HB2  | 2        | 0.26          |
| (1,412) | 1:12:A:LEU:HD21 | 1:12:A:LEU:HG   | 4        | 0.26          |
| (1,412) | 1:12:A:LEU:HD22 | 1:12:A:LEU:HG   | 4        | 0.26          |
| (1,412) | 1:12:A:LEU:HD23 | 1:12:A:LEU:HG   | 4        | 0.26          |
| (1,412) | 1:12:A:LEU:HD21 | 1:12:A:LEU:HG   | 7        | 0.26          |
| (1,412) | 1:12:A:LEU:HD22 | 1:12:A:LEU:HG   | 7        | 0.26          |
| (1,412) | 1:12:A:LEU:HD23 | 1:12:A:LEU:HG   | 7        | 0.26          |
| (1,412) | 1:12:A:LEU:HD21 | 1:12:A:LEU:HG   | 9        | 0.26          |
| (1,412) | 1:12:A:LEU:HD22 | 1:12:A:LEU:HG   | 9        | 0.26          |
| (1,412) | 1:12:A:LEU:HD23 | 1:12:A:LEU:HG   | 9        | 0.26          |
| (1,410) | 1:12:A:LEU:HB2  | 1:12:A:LEU:HB3  | 3        | 0.26          |
| (1,410) | 1:12:A:LEU:HB2  | 1:12:A:LEU:HB3  | 4        | 0.26          |
| (1,410) | 1:12:A:LEU:HB2  | 1:12:A:LEU:HB3  | 5        | 0.26          |
| (1,410) | 1:12:A:LEU:HB2  | 1:12:A:LEU:HB3  | 6        | 0.26          |
| (1,410) | 1:12:A:LEU:HB2  | 1:12:A:LEU:HB3  | 7        | 0.26          |
| (1,410) | 1:12:A:LEU:HB2  | 1:12:A:LEU:HB3  | 8        | 0.26          |
| (1,410) | 1:12:A:LEU:HB2  | 1:12:A:LEU:HB3  | 9        | 0.26          |
| (1,410) | 1:12:A:LEU:HB2  | 1:12:A:LEU:HB3  | 10       | 0.26          |
| (1,404) | 1:12:A:LEU:HA   | 1:12:A:LEU:HB3  | 1        | 0.26          |
| (1,394) | 1:10:A:GLN:HA   | 1:10:A:GLN:HB2  | 10       | 0.26          |
| (1,359) | 1:6:A:ARG:HD2   | 1:6:A:ARG:HG3   | 1        | 0.26          |
| (1,280) | 1:4:A:CYS:H     | 1:5:A:VAL:H     | 10       | 0.26          |
| (1,277) | 1:20:A:GLY:H    | 1:21:A:ARG:H    | 4        | 0.26          |
| (1,273) | 1:18:A:SER:H    | 1:19:A:SER:H    | 3        | 0.26          |
| (1,263) | 1:18:A:SER:HA   | 1:20:A:GLY:H    | 8        | 0.26          |
| (1,262) | 1:10:A:GLN:HA   | 1:10:A:GLN:HE22 | 2        | 0.26          |
| (1,250) | 1:11:A:TRP:HE3  | 1:23:A:PRO:HA   | 3        | 0.26          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,250) | 1:11:A:TRP:HE3 | 1:23:A:PRO:HA   | 5        | 0.26          |
| (1,239) | 1:8:A:TYR:HE1  | 1:12:A:LEU:HG   | 1        | 0.26          |
| (1,239) | 1:8:A:TYR:HE2  | 1:12:A:LEU:HG   | 1        | 0.26          |
| (1,239) | 1:8:A:TYR:HE1  | 1:12:A:LEU:HG   | 7        | 0.26          |
| (1,239) | 1:8:A:TYR:HE2  | 1:12:A:LEU:HG   | 7        | 0.26          |
| (1,218) | 1:11:A:TRP:HH2 | 1:12:A:LEU:HD21 | 3        | 0.26          |
| (1,218) | 1:11:A:TRP:HH2 | 1:12:A:LEU:HD22 | 3        | 0.26          |
| (1,218) | 1:11:A:TRP:HH2 | 1:12:A:LEU:HD23 | 3        | 0.26          |
| (1,173) | 1:11:A:TRP:HH2 | 1:17:A:PRO:HD3  | 1        | 0.26          |
| (1,173) | 1:11:A:TRP:HH2 | 1:17:A:PRO:HD3  | 2        | 0.26          |
| (1,172) | 1:11:A:TRP:HZ2 | 1:23:A:PRO:HD3  | 2        | 0.26          |
| (1,171) | 1:11:A:TRP:HH2 | 1:23:A:PRO:HD3  | 5        | 0.26          |
| (1,171) | 1:11:A:TRP:HH2 | 1:23:A:PRO:HD3  | 6        | 0.26          |
| (1,108) | 1:14:A:ASP:H   | 1:15:A:GLY:H    | 6        | 0.26          |
| (1,730) | 1:2:A:GLU:HG3  | 1:6:A:ARG:HG3   | 7        | 0.25          |
| (1,720) | 1:7:A:LEU:HB2  | 1:24:A:PRO:HB2  | 8        | 0.25          |
| (1,621) | 1:2:A:GLU:HB2  | 1:6:A:ARG:H     | 7        | 0.25          |
| (1,621) | 1:2:A:GLU:HB2  | 1:6:A:ARG:H     | 9        | 0.25          |
| (1,601) | 1:10:A:GLN:H   | 1:12:A:LEU:H    | 3        | 0.25          |
| (1,601) | 1:10:A:GLN:H   | 1:12:A:LEU:H    | 4        | 0.25          |
| (1,601) | 1:10:A:GLN:H   | 1:12:A:LEU:H    | 9        | 0.25          |
| (1,600) | 1:1:A:GLU:HB3  | 1:1:A:GLU:HG2   | 8        | 0.25          |
| (1,600) | 1:1:A:GLU:HB3  | 1:1:A:GLU:HG3   | 8        | 0.25          |
| (1,581) | 1:5:A:VAL:HG11 | 1:6:A:ARG:HA    | 10       | 0.25          |
| (1,581) | 1:5:A:VAL:HG12 | 1:6:A:ARG:HA    | 10       | 0.25          |
| (1,581) | 1:5:A:VAL:HG13 | 1:6:A:ARG:HA    | 10       | 0.25          |
| (1,576) | 1:22:A:PRO:HA  | 1:23:A:PRO:HD3  | 3        | 0.25          |
| (1,576) | 1:22:A:PRO:HA  | 1:23:A:PRO:HD3  | 6        | 0.25          |
| (1,565) | 1:4:A:CYS:HA   | 1:7:A:LEU:HG    | 1        | 0.25          |
| (1,546) | 1:13:A:LYS:HD3 | 1:13:A:LYS:HE2  | 2        | 0.25          |
| (1,546) | 1:13:A:LYS:HD3 | 1:13:A:LYS:HE3  | 2        | 0.25          |
| (1,537) | 1:23:A:PRO:HB2 | 1:24:A:PRO:HD2  | 1        | 0.25          |
| (1,537) | 1:23:A:PRO:HB2 | 1:24:A:PRO:HD2  | 5        | 0.25          |
| (1,526) | 1:24:A:PRO:HB3 | 1:24:A:PRO:HD2  | 2        | 0.25          |
| (1,526) | 1:24:A:PRO:HB3 | 1:24:A:PRO:HD2  | 6        | 0.25          |
| (1,526) | 1:24:A:PRO:HB3 | 1:24:A:PRO:HD2  | 10       | 0.25          |
| (1,522) | 1:24:A:PRO:HA  | 1:24:A:PRO:HD3  | 2        | 0.25          |
| (1,522) | 1:24:A:PRO:HA  | 1:24:A:PRO:HD3  | 5        | 0.25          |
| (1,522) | 1:24:A:PRO:HA  | 1:24:A:PRO:HD3  | 6        | 0.25          |
| (1,477) | 1:22:A:PRO:HA  | 1:22:A:PRO:HB2  | 3        | 0.25          |
| (1,434) | 1:16:A:GLY:HA2 | 1:16:A:GLY:HA3  | 1        | 0.25          |
| (1,434) | 1:16:A:GLY:HA2 | 1:16:A:GLY:HA3  | 2        | 0.25          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,434) | 1:16:A:GLY:HA2  | 1:16:A:GLY:HA3  | 3        | 0.25          |
| (1,434) | 1:16:A:GLY:HA2  | 1:16:A:GLY:HA3  | 4        | 0.25          |
| (1,434) | 1:16:A:GLY:HA2  | 1:16:A:GLY:HA3  | 5        | 0.25          |
| (1,434) | 1:16:A:GLY:HA2  | 1:16:A:GLY:HA3  | 6        | 0.25          |
| (1,434) | 1:16:A:GLY:HA2  | 1:16:A:GLY:HA3  | 7        | 0.25          |
| (1,434) | 1:16:A:GLY:HA2  | 1:16:A:GLY:HA3  | 8        | 0.25          |
| (1,434) | 1:16:A:GLY:HA2  | 1:16:A:GLY:HA3  | 9        | 0.25          |
| (1,434) | 1:16:A:GLY:HA2  | 1:16:A:GLY:HA3  | 10       | 0.25          |
| (1,412) | 1:12:A:LEU:HD21 | 1:12:A:LEU:HG   | 2        | 0.25          |
| (1,412) | 1:12:A:LEU:HD22 | 1:12:A:LEU:HG   | 2        | 0.25          |
| (1,412) | 1:12:A:LEU:HD23 | 1:12:A:LEU:HG   | 2        | 0.25          |
| (1,412) | 1:12:A:LEU:HD21 | 1:12:A:LEU:HG   | 5        | 0.25          |
| (1,412) | 1:12:A:LEU:HD22 | 1:12:A:LEU:HG   | 5        | 0.25          |
| (1,412) | 1:12:A:LEU:HD23 | 1:12:A:LEU:HG   | 5        | 0.25          |
| (1,412) | 1:12:A:LEU:HD21 | 1:12:A:LEU:HG   | 6        | 0.25          |
| (1,412) | 1:12:A:LEU:HD22 | 1:12:A:LEU:HG   | 6        | 0.25          |
| (1,412) | 1:12:A:LEU:HD23 | 1:12:A:LEU:HG   | 6        | 0.25          |
| (1,404) | 1:12:A:LEU:HA   | 1:12:A:LEU:HB3  | 2        | 0.25          |
| (1,391) | 1:10:A:GLN:HA   | 1:10:A:GLN:HG2  | 8        | 0.25          |
| (1,383) | 1:9:A:ILE:HG12  | 1:9:A:ILE:HG13  | 2        | 0.25          |
| (1,383) | 1:9:A:ILE:HG12  | 1:9:A:ILE:HG13  | 3        | 0.25          |
| (1,383) | 1:9:A:ILE:HG12  | 1:9:A:ILE:HG13  | 5        | 0.25          |
| (1,383) | 1:9:A:ILE:HG12  | 1:9:A:ILE:HG13  | 6        | 0.25          |
| (1,359) | 1:6:A:ARG:HD2   | 1:6:A:ARG:HG3   | 7        | 0.25          |
| (1,301) | 1:12:A:LEU:H    | 1:12:A:LEU:HB2  | 7        | 0.25          |
| (1,301) | 1:12:A:LEU:H    | 1:12:A:LEU:HB2  | 10       | 0.25          |
| (1,293) | 1:11:A:TRP:HE1  | 1:24:A:PRO:HD2  | 2        | 0.25          |
| (1,250) | 1:11:A:TRP:HE3  | 1:23:A:PRO:HA   | 2        | 0.25          |
| (1,239) | 1:8:A:TYR:HE1   | 1:12:A:LEU:HG   | 4        | 0.25          |
| (1,239) | 1:8:A:TYR:HE2   | 1:12:A:LEU:HG   | 4        | 0.25          |
| (1,238) | 1:8:A:TYR:HE1   | 1:23:A:PRO:HG3  | 2        | 0.25          |
| (1,238) | 1:8:A:TYR:HE2   | 1:23:A:PRO:HG3  | 2        | 0.25          |
| (1,177) | 1:8:A:TYR:HD1   | 1:12:A:LEU:HA   | 7        | 0.25          |
| (1,177) | 1:8:A:TYR:HD2   | 1:12:A:LEU:HA   | 7        | 0.25          |
| (1,154) | 1:7:A:LEU:H     | 1:7:A:LEU:HB2   | 2        | 0.25          |
| (1,154) | 1:7:A:LEU:H     | 1:7:A:LEU:HB2   | 10       | 0.25          |
| (1,736) | 1:23:A:PRO:HA   | 1:24:A:PRO:HD3  | 5        | 0.24          |
| (1,734) | 1:2:A:GLU:HG3   | 1:5:A:VAL:HB    | 4        | 0.24          |
| (1,715) | 1:9:A:ILE:HG21  | 1:12:A:LEU:HB2  | 5        | 0.24          |
| (1,715) | 1:9:A:ILE:HG22  | 1:12:A:LEU:HB2  | 5        | 0.24          |
| (1,715) | 1:9:A:ILE:HG23  | 1:12:A:LEU:HB2  | 5        | 0.24          |
| (1,677) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD11 | 1        | 0.24          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,677) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD12 | 1        | 0.24          |
| (1,677) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD13 | 1        | 0.24          |
| (1,677) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD11 | 9        | 0.24          |
| (1,677) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD12 | 9        | 0.24          |
| (1,677) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD13 | 9        | 0.24          |
| (1,654) | 1:14:A:ASP:HB3  | 1:19:A:SER:HB3  | 4        | 0.24          |
| (1,651) | 1:3:A:GLU:HA    | 1:6:A:ARG:HD2   | 6        | 0.24          |
| (1,618) | 1:10:A:GLN:HE21 | 1:13:A:LYS:HD3  | 8        | 0.24          |
| (1,563) | 1:7:A:LEU:HA    | 1:10:A:GLN:HB3  | 9        | 0.24          |
| (1,542) | 1:7:A:LEU:HB2   | 1:24:A:PRO:HB3  | 2        | 0.24          |
| (1,526) | 1:24:A:PRO:HB3  | 1:24:A:PRO:HD2  | 4        | 0.24          |
| (1,526) | 1:24:A:PRO:HB3  | 1:24:A:PRO:HD2  | 5        | 0.24          |
| (1,526) | 1:24:A:PRO:HB3  | 1:24:A:PRO:HD2  | 8        | 0.24          |
| (1,526) | 1:24:A:PRO:HB3  | 1:24:A:PRO:HD2  | 9        | 0.24          |
| (1,477) | 1:22:A:PRO:HA   | 1:22:A:PRO:HB2  | 8        | 0.24          |
| (1,412) | 1:12:A:LEU:HD21 | 1:12:A:LEU:HG   | 1        | 0.24          |
| (1,412) | 1:12:A:LEU:HD22 | 1:12:A:LEU:HG   | 1        | 0.24          |
| (1,412) | 1:12:A:LEU:HD23 | 1:12:A:LEU:HG   | 1        | 0.24          |
| (1,404) | 1:12:A:LEU:HA   | 1:12:A:LEU:HB3  | 3        | 0.24          |
| (1,404) | 1:12:A:LEU:HA   | 1:12:A:LEU:HB3  | 5        | 0.24          |
| (1,394) | 1:10:A:GLN:HA   | 1:10:A:GLN:HB2  | 2        | 0.24          |
| (1,394) | 1:10:A:GLN:HA   | 1:10:A:GLN:HB2  | 8        | 0.24          |
| (1,383) | 1:9:A:ILE:HG12  | 1:9:A:ILE:HG13  | 1        | 0.24          |
| (1,383) | 1:9:A:ILE:HG12  | 1:9:A:ILE:HG13  | 4        | 0.24          |
| (1,383) | 1:9:A:ILE:HG12  | 1:9:A:ILE:HG13  | 7        | 0.24          |
| (1,383) | 1:9:A:ILE:HG12  | 1:9:A:ILE:HG13  | 8        | 0.24          |
| (1,383) | 1:9:A:ILE:HG12  | 1:9:A:ILE:HG13  | 9        | 0.24          |
| (1,383) | 1:9:A:ILE:HG12  | 1:9:A:ILE:HG13  | 10       | 0.24          |
| (1,331) | 1:2:A:GLU:HB2   | 1:2:A:GLU:HG3   | 7        | 0.24          |
| (1,301) | 1:12:A:LEU:H    | 1:12:A:LEU:HB2  | 4        | 0.24          |
| (1,301) | 1:12:A:LEU:H    | 1:12:A:LEU:HB2  | 8        | 0.24          |
| (1,301) | 1:12:A:LEU:H    | 1:12:A:LEU:HB2  | 9        | 0.24          |
| (1,239) | 1:8:A:TYR:HE1   | 1:12:A:LEU:HG   | 2        | 0.24          |
| (1,239) | 1:8:A:TYR:HE2   | 1:12:A:LEU:HG   | 2        | 0.24          |
| (1,239) | 1:8:A:TYR:HE1   | 1:12:A:LEU:HG   | 6        | 0.24          |
| (1,239) | 1:8:A:TYR:HE2   | 1:12:A:LEU:HG   | 6        | 0.24          |
| (1,239) | 1:8:A:TYR:HE1   | 1:12:A:LEU:HG   | 10       | 0.24          |
| (1,239) | 1:8:A:TYR:HE2   | 1:12:A:LEU:HG   | 10       | 0.24          |
| (1,210) | 1:11:A:TRP:HE3  | 1:12:A:LEU:HD11 | 6        | 0.24          |
| (1,210) | 1:11:A:TRP:HE3  | 1:12:A:LEU:HD12 | 6        | 0.24          |
| (1,210) | 1:11:A:TRP:HE3  | 1:12:A:LEU:HD13 | 6        | 0.24          |
| (1,154) | 1:7:A:LEU:H     | 1:7:A:LEU:HB2   | 3        | 0.24          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,35)  | 1:10:A:GLN:H    | 1:10:A:GLN:HB2 | 1        | 0.24          |
| (1,736) | 1:23:A:PRO:HA   | 1:24:A:PRO:HD3 | 2        | 0.23          |
| (1,736) | 1:23:A:PRO:HA   | 1:24:A:PRO:HD3 | 6        | 0.23          |
| (1,728) | 1:2:A:GLU:HG2   | 1:6:A:ARG:HG2  | 4        | 0.23          |
| (1,728) | 1:2:A:GLU:HG2   | 1:6:A:ARG:HG2  | 8        | 0.23          |
| (1,720) | 1:7:A:LEU:HB2   | 1:24:A:PRO:HB2 | 9        | 0.23          |
| (1,666) | 1:24:A:PRO:HG2  | 1:25:A:CYS:HB2 | 6        | 0.23          |
| (1,657) | 1:4:A:CYS:HB2   | 1:25:A:CYS:HB3 | 6        | 0.23          |
| (1,654) | 1:14:A:ASP:HB3  | 1:19:A:SER:HB3 | 9        | 0.23          |
| (1,614) | 1:19:A:SER:HG   | 1:20:A:GLY:H   | 6        | 0.23          |
| (1,605) | 1:8:A:TYR:HE1   | 1:11:A:TRP:HZ3 | 1        | 0.23          |
| (1,605) | 1:8:A:TYR:HE2   | 1:11:A:TRP:HZ3 | 1        | 0.23          |
| (1,600) | 1:1:A:GLU:HB3   | 1:1:A:GLU:HG2  | 4        | 0.23          |
| (1,600) | 1:1:A:GLU:HB3   | 1:1:A:GLU:HG3  | 4        | 0.23          |
| (1,600) | 1:1:A:GLU:HB3   | 1:1:A:GLU:HG2  | 10       | 0.23          |
| (1,600) | 1:1:A:GLU:HB3   | 1:1:A:GLU:HG3  | 10       | 0.23          |
| (1,581) | 1:5:A:VAL:HG11  | 1:6:A:ARG:HA   | 2        | 0.23          |
| (1,581) | 1:5:A:VAL:HG12  | 1:6:A:ARG:HA   | 2        | 0.23          |
| (1,581) | 1:5:A:VAL:HG13  | 1:6:A:ARG:HA   | 2        | 0.23          |
| (1,563) | 1:7:A:LEU:HA    | 1:10:A:GLN:HB3 | 2        | 0.23          |
| (1,563) | 1:7:A:LEU:HA    | 1:10:A:GLN:HB3 | 10       | 0.23          |
| (1,551) | 1:16:A:GLY:HA3  | 1:17:A:PRO:HD3 | 5        | 0.23          |
| (1,526) | 1:24:A:PRO:HB3  | 1:24:A:PRO:HD2 | 7        | 0.23          |
| (1,477) | 1:22:A:PRO:HA   | 1:22:A:PRO:HB2 | 10       | 0.23          |
| (1,461) | 1:21:A:ARG:HA   | 1:21:A:ARG:HG2 | 7        | 0.23          |
| (1,461) | 1:21:A:ARG:HA   | 1:21:A:ARG:HG3 | 7        | 0.23          |
| (1,450) | 1:18:A:SER:HA   | 1:18:A:SER:HB3 | 2        | 0.23          |
| (1,413) | 1:12:A:LEU:HD11 | 1:12:A:LEU:HG  | 3        | 0.23          |
| (1,413) | 1:12:A:LEU:HD12 | 1:12:A:LEU:HG  | 3        | 0.23          |
| (1,413) | 1:12:A:LEU:HD13 | 1:12:A:LEU:HG  | 3        | 0.23          |
| (1,404) | 1:12:A:LEU:HA   | 1:12:A:LEU:HB3 | 6        | 0.23          |
| (1,404) | 1:12:A:LEU:HA   | 1:12:A:LEU:HB3 | 7        | 0.23          |
| (1,391) | 1:10:A:GLN:HA   | 1:10:A:GLN:HG2 | 10       | 0.23          |
| (1,364) | 1:6:A:ARG:HG2   | 1:6:A:ARG:HG3  | 1        | 0.23          |
| (1,364) | 1:6:A:ARG:HG2   | 1:6:A:ARG:HG3  | 2        | 0.23          |
| (1,364) | 1:6:A:ARG:HG2   | 1:6:A:ARG:HG3  | 5        | 0.23          |
| (1,364) | 1:6:A:ARG:HG2   | 1:6:A:ARG:HG3  | 6        | 0.23          |
| (1,364) | 1:6:A:ARG:HG2   | 1:6:A:ARG:HG3  | 7        | 0.23          |
| (1,364) | 1:6:A:ARG:HG2   | 1:6:A:ARG:HG3  | 8        | 0.23          |
| (1,359) | 1:6:A:ARG:HD2   | 1:6:A:ARG:HG3  | 8        | 0.23          |
| (1,326) | 1:2:A:GLU:HA    | 1:2:A:GLU:HB3  | 8        | 0.23          |
| (1,326) | 1:2:A:GLU:HA    | 1:2:A:GLU:HB3  | 9        | 0.23          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,276) | 1:19:A:SER:H   | 1:20:A:GLY:H    | 2        | 0.23          |
| (1,259) | 1:4:A:CYS:HB3  | 1:5:A:VAL:H     | 10       | 0.23          |
| (1,210) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD11 | 5        | 0.23          |
| (1,210) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD12 | 5        | 0.23          |
| (1,210) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD13 | 5        | 0.23          |
| (1,75)  | 1:25:A:CYS:H   | 1:25:A:CYS:HB2  | 5        | 0.23          |
| (1,61)  | 1:11:A:TRP:HB2 | 1:12:A:LEU:H    | 8        | 0.23          |
| (1,61)  | 1:11:A:TRP:HB2 | 1:12:A:LEU:H    | 10       | 0.23          |
| (1,55)  | 1:21:A:ARG:H   | 1:21:A:ARG:HD2  | 1        | 0.23          |
| (1,26)  | 1:2:A:GLU:HB2  | 1:3:A:GLU:H     | 10       | 0.23          |
| (1,728) | 1:2:A:GLU:HG2  | 1:6:A:ARG:HG2   | 6        | 0.22          |
| (1,720) | 1:7:A:LEU:HB2  | 1:24:A:PRO:HB2  | 6        | 0.22          |
| (1,662) | 1:17:A:PRO:HB3 | 1:18:A:SER:HB2  | 5        | 0.22          |
| (1,634) | 1:11:A:TRP:HE3 | 1:23:A:PRO:HB2  | 2        | 0.22          |
| (1,623) | 1:2:A:GLU:HB3  | 1:6:A:ARG:H     | 2        | 0.22          |
| (1,614) | 1:19:A:SER:HG  | 1:20:A:GLY:H    | 5        | 0.22          |
| (1,614) | 1:19:A:SER:HG  | 1:20:A:GLY:H    | 10       | 0.22          |
| (1,550) | 1:11:A:TRP:HB3 | 1:24:A:PRO:HD3  | 7        | 0.22          |
| (1,545) | 1:13:A:LYS:HB2 | 1:13:A:LYS:HE2  | 1        | 0.22          |
| (1,545) | 1:13:A:LYS:HB2 | 1:13:A:LYS:HE3  | 1        | 0.22          |
| (1,545) | 1:13:A:LYS:HB3 | 1:13:A:LYS:HE2  | 1        | 0.22          |
| (1,545) | 1:13:A:LYS:HB3 | 1:13:A:LYS:HE3  | 1        | 0.22          |
| (1,545) | 1:13:A:LYS:HB2 | 1:13:A:LYS:HE2  | 4        | 0.22          |
| (1,545) | 1:13:A:LYS:HB2 | 1:13:A:LYS:HE3  | 4        | 0.22          |
| (1,545) | 1:13:A:LYS:HB3 | 1:13:A:LYS:HE2  | 4        | 0.22          |
| (1,545) | 1:13:A:LYS:HB3 | 1:13:A:LYS:HE3  | 4        | 0.22          |
| (1,489) | 1:22:A:PRO:HB2 | 1:22:A:PRO:HG2  | 3        | 0.22          |
| (1,489) | 1:22:A:PRO:HB2 | 1:22:A:PRO:HG2  | 8        | 0.22          |
| (1,489) | 1:22:A:PRO:HB2 | 1:22:A:PRO:HG2  | 10       | 0.22          |
| (1,465) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HD2  | 8        | 0.22          |
| (1,455) | 1:19:A:SER:HB2 | 1:19:A:SER:HB3  | 1        | 0.22          |
| (1,455) | 1:19:A:SER:HB2 | 1:19:A:SER:HB3  | 2        | 0.22          |
| (1,455) | 1:19:A:SER:HB2 | 1:19:A:SER:HB3  | 4        | 0.22          |
| (1,455) | 1:19:A:SER:HB2 | 1:19:A:SER:HB3  | 5        | 0.22          |
| (1,455) | 1:19:A:SER:HB2 | 1:19:A:SER:HB3  | 6        | 0.22          |
| (1,455) | 1:19:A:SER:HB2 | 1:19:A:SER:HB3  | 7        | 0.22          |
| (1,455) | 1:19:A:SER:HB2 | 1:19:A:SER:HB3  | 8        | 0.22          |
| (1,455) | 1:19:A:SER:HB2 | 1:19:A:SER:HB3  | 9        | 0.22          |
| (1,455) | 1:19:A:SER:HB2 | 1:19:A:SER:HB3  | 10       | 0.22          |
| (1,404) | 1:12:A:LEU:HA  | 1:12:A:LEU:HB3  | 4        | 0.22          |
| (1,404) | 1:12:A:LEU:HA  | 1:12:A:LEU:HB3  | 8        | 0.22          |
| (1,404) | 1:12:A:LEU:HA  | 1:12:A:LEU:HB3  | 9        | 0.22          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,404) | 1:12:A:LEU:HA  | 1:12:A:LEU:HB3  | 10       | 0.22          |
| (1,394) | 1:10:A:GLN:HA  | 1:10:A:GLN:HB2  | 3        | 0.22          |
| (1,385) | 1:9:A:ILE:HD11 | 1:9:A:ILE:HG13  | 4        | 0.22          |
| (1,385) | 1:9:A:ILE:HD12 | 1:9:A:ILE:HG13  | 4        | 0.22          |
| (1,385) | 1:9:A:ILE:HD13 | 1:9:A:ILE:HG13  | 4        | 0.22          |
| (1,385) | 1:9:A:ILE:HD11 | 1:9:A:ILE:HG13  | 7        | 0.22          |
| (1,385) | 1:9:A:ILE:HD12 | 1:9:A:ILE:HG13  | 7        | 0.22          |
| (1,385) | 1:9:A:ILE:HD13 | 1:9:A:ILE:HG13  | 7        | 0.22          |
| (1,385) | 1:9:A:ILE:HD11 | 1:9:A:ILE:HG13  | 8        | 0.22          |
| (1,385) | 1:9:A:ILE:HD12 | 1:9:A:ILE:HG13  | 8        | 0.22          |
| (1,385) | 1:9:A:ILE:HD13 | 1:9:A:ILE:HG13  | 8        | 0.22          |
| (1,385) | 1:9:A:ILE:HD11 | 1:9:A:ILE:HG13  | 9        | 0.22          |
| (1,385) | 1:9:A:ILE:HD12 | 1:9:A:ILE:HG13  | 9        | 0.22          |
| (1,385) | 1:9:A:ILE:HD13 | 1:9:A:ILE:HG13  | 9        | 0.22          |
| (1,385) | 1:9:A:ILE:HD11 | 1:9:A:ILE:HG13  | 10       | 0.22          |
| (1,385) | 1:9:A:ILE:HD12 | 1:9:A:ILE:HG13  | 10       | 0.22          |
| (1,385) | 1:9:A:ILE:HD13 | 1:9:A:ILE:HG13  | 10       | 0.22          |
| (1,364) | 1:6:A:ARG:HG2  | 1:6:A:ARG:HG3   | 3        | 0.22          |
| (1,364) | 1:6:A:ARG:HG2  | 1:6:A:ARG:HG3   | 4        | 0.22          |
| (1,364) | 1:6:A:ARG:HG2  | 1:6:A:ARG:HG3   | 9        | 0.22          |
| (1,364) | 1:6:A:ARG:HG2  | 1:6:A:ARG:HG3   | 10       | 0.22          |
| (1,331) | 1:2:A:GLU:HB2  | 1:2:A:GLU:HG3   | 8        | 0.22          |
| (1,331) | 1:2:A:GLU:HB2  | 1:2:A:GLU:HG3   | 9        | 0.22          |
| (1,326) | 1:2:A:GLU:HA   | 1:2:A:GLU:HB3   | 6        | 0.22          |
| (1,321) | 1:11:A:TRP:HB3 | 1:12:A:LEU:H    | 9        | 0.22          |
| (1,301) | 1:12:A:LEU:H   | 1:12:A:LEU:HB2  | 1        | 0.22          |
| (1,293) | 1:11:A:TRP:HE1 | 1:24:A:PRO:HD2  | 5        | 0.22          |
| (1,284) | 1:2:A:GLU:HA   | 1:3:A:GLU:H     | 10       | 0.22          |
| (1,259) | 1:4:A:CYS:HB3  | 1:5:A:VAL:H     | 7        | 0.22          |
| (1,220) | 1:8:A:TYR:HD1  | 1:9:A:ILE:HG12  | 10       | 0.22          |
| (1,220) | 1:8:A:TYR:HD2  | 1:9:A:ILE:HG12  | 10       | 0.22          |
| (1,210) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD11 | 2        | 0.22          |
| (1,210) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD12 | 2        | 0.22          |
| (1,210) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HD13 | 2        | 0.22          |
| (1,177) | 1:8:A:TYR:HD1  | 1:12:A:LEU:HA   | 8        | 0.22          |
| (1,177) | 1:8:A:TYR:HD2  | 1:12:A:LEU:HA   | 8        | 0.22          |
| (1,177) | 1:8:A:TYR:HD1  | 1:12:A:LEU:HA   | 10       | 0.22          |
| (1,177) | 1:8:A:TYR:HD2  | 1:12:A:LEU:HA   | 10       | 0.22          |
| (1,173) | 1:11:A:TRP:HH2 | 1:17:A:PRO:HD3  | 5        | 0.22          |
| (1,108) | 1:14:A:ASP:H   | 1:15:A:GLY:H    | 8        | 0.22          |
| (1,98)  | 1:11:A:TRP:HE1 | 1:19:A:SER:HG   | 8        | 0.22          |
| (1,98)  | 1:11:A:TRP:HE1 | 1:19:A:SER:HG   | 10       | 0.22          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,75)  | 1:25:A:CYS:H    | 1:25:A:CYS:HB2  | 1        | 0.22          |
| (1,75)  | 1:25:A:CYS:H    | 1:25:A:CYS:HB2  | 3        | 0.22          |
| (1,736) | 1:23:A:PRO:HA   | 1:24:A:PRO:HD3  | 1        | 0.21          |
| (1,717) | 1:12:A:LEU:HD11 | 1:16:A:GLY:HA2  | 6        | 0.21          |
| (1,717) | 1:12:A:LEU:HD12 | 1:16:A:GLY:HA2  | 6        | 0.21          |
| (1,717) | 1:12:A:LEU:HD13 | 1:16:A:GLY:HA2  | 6        | 0.21          |
| (1,715) | 1:9:A:ILE:HG21  | 1:12:A:LEU:HB2  | 6        | 0.21          |
| (1,715) | 1:9:A:ILE:HG22  | 1:12:A:LEU:HB2  | 6        | 0.21          |
| (1,715) | 1:9:A:ILE:HG23  | 1:12:A:LEU:HB2  | 6        | 0.21          |
| (1,704) | 1:9:A:ILE:HG21  | 1:13:A:LYS:HD3  | 5        | 0.21          |
| (1,704) | 1:9:A:ILE:HG22  | 1:13:A:LYS:HD3  | 5        | 0.21          |
| (1,704) | 1:9:A:ILE:HG23  | 1:13:A:LYS:HD3  | 5        | 0.21          |
| (1,704) | 1:9:A:ILE:HG21  | 1:13:A:LYS:HD3  | 10       | 0.21          |
| (1,704) | 1:9:A:ILE:HG22  | 1:13:A:LYS:HD3  | 10       | 0.21          |
| (1,704) | 1:9:A:ILE:HG23  | 1:13:A:LYS:HD3  | 10       | 0.21          |
| (1,680) | 1:11:A:TRP:HB3  | 1:12:A:LEU:HD21 | 3        | 0.21          |
| (1,680) | 1:11:A:TRP:HB3  | 1:12:A:LEU:HD22 | 3        | 0.21          |
| (1,680) | 1:11:A:TRP:HB3  | 1:12:A:LEU:HD23 | 3        | 0.21          |
| (1,677) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD11 | 7        | 0.21          |
| (1,677) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD12 | 7        | 0.21          |
| (1,677) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD13 | 7        | 0.21          |
| (1,647) | 1:15:A:GLY:HA2  | 1:18:A:SER:HB2  | 2        | 0.21          |
| (1,633) | 1:11:A:TRP:HZ3  | 1:23:A:PRO:HB2  | 2        | 0.21          |
| (1,601) | 1:10:A:GLN:H    | 1:12:A:LEU:H    | 7        | 0.21          |
| (1,600) | 1:1:A:GLU:HB3   | 1:1:A:GLU:HG2   | 2        | 0.21          |
| (1,600) | 1:1:A:GLU:HB3   | 1:1:A:GLU:HG3   | 2        | 0.21          |
| (1,600) | 1:1:A:GLU:HB3   | 1:1:A:GLU:HG2   | 6        | 0.21          |
| (1,600) | 1:1:A:GLU:HB3   | 1:1:A:GLU:HG3   | 6        | 0.21          |
| (1,600) | 1:1:A:GLU:HB3   | 1:1:A:GLU:HG2   | 7        | 0.21          |
| (1,600) | 1:1:A:GLU:HB3   | 1:1:A:GLU:HG3   | 7        | 0.21          |
| (1,497) | 1:23:A:PRO:HA   | 1:23:A:PRO:HB2  | 3        | 0.21          |
| (1,489) | 1:22:A:PRO:HB2  | 1:22:A:PRO:HG2  | 1        | 0.21          |
| (1,489) | 1:22:A:PRO:HB2  | 1:22:A:PRO:HG2  | 2        | 0.21          |
| (1,489) | 1:22:A:PRO:HB2  | 1:22:A:PRO:HG2  | 5        | 0.21          |
| (1,489) | 1:22:A:PRO:HB2  | 1:22:A:PRO:HG2  | 9        | 0.21          |
| (1,455) | 1:19:A:SER:HB2  | 1:19:A:SER:HB3  | 3        | 0.21          |
| (1,424) | 1:13:A:LYS:HB2  | 1:13:A:LYS:HD3  | 3        | 0.21          |
| (1,424) | 1:13:A:LYS:HB3  | 1:13:A:LYS:HD3  | 3        | 0.21          |
| (1,418) | 1:12:A:LEU:HD11 | 1:12:A:LEU:HD21 | 8        | 0.21          |
| (1,418) | 1:12:A:LEU:HD11 | 1:12:A:LEU:HD22 | 8        | 0.21          |
| (1,418) | 1:12:A:LEU:HD11 | 1:12:A:LEU:HD23 | 8        | 0.21          |
| (1,418) | 1:12:A:LEU:HD12 | 1:12:A:LEU:HD21 | 8        | 0.21          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,418) | 1:12:A:LEU:HD12 | 1:12:A:LEU:HD22 | 8        | 0.21          |
| (1,418) | 1:12:A:LEU:HD12 | 1:12:A:LEU:HD23 | 8        | 0.21          |
| (1,418) | 1:12:A:LEU:HD13 | 1:12:A:LEU:HD21 | 8        | 0.21          |
| (1,418) | 1:12:A:LEU:HD13 | 1:12:A:LEU:HD22 | 8        | 0.21          |
| (1,418) | 1:12:A:LEU:HD13 | 1:12:A:LEU:HD23 | 8        | 0.21          |
| (1,408) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD11 | 6        | 0.21          |
| (1,408) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD12 | 6        | 0.21          |
| (1,408) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD13 | 6        | 0.21          |
| (1,385) | 1:9:A:ILE:HD11  | 1:9:A:ILE:HG13  | 1        | 0.21          |
| (1,385) | 1:9:A:ILE:HD12  | 1:9:A:ILE:HG13  | 1        | 0.21          |
| (1,385) | 1:9:A:ILE:HD13  | 1:9:A:ILE:HG13  | 1        | 0.21          |
| (1,385) | 1:9:A:ILE:HD11  | 1:9:A:ILE:HG13  | 2        | 0.21          |
| (1,385) | 1:9:A:ILE:HD12  | 1:9:A:ILE:HG13  | 2        | 0.21          |
| (1,385) | 1:9:A:ILE:HD13  | 1:9:A:ILE:HG13  | 2        | 0.21          |
| (1,385) | 1:9:A:ILE:HD11  | 1:9:A:ILE:HG13  | 5        | 0.21          |
| (1,385) | 1:9:A:ILE:HD12  | 1:9:A:ILE:HG13  | 5        | 0.21          |
| (1,385) | 1:9:A:ILE:HD13  | 1:9:A:ILE:HG13  | 5        | 0.21          |
| (1,385) | 1:9:A:ILE:HD11  | 1:9:A:ILE:HG13  | 6        | 0.21          |
| (1,385) | 1:9:A:ILE:HD12  | 1:9:A:ILE:HG13  | 6        | 0.21          |
| (1,385) | 1:9:A:ILE:HD13  | 1:9:A:ILE:HG13  | 6        | 0.21          |
| (1,352) | 1:6:A:ARG:HB3   | 1:6:A:ARG:HD2   | 7        | 0.21          |
| (1,331) | 1:2:A:GLU:HB2   | 1:2:A:GLU:HG3   | 10       | 0.21          |
| (1,321) | 1:11:A:TRP:HB3  | 1:12:A:LEU:H    | 7        | 0.21          |
| (1,301) | 1:12:A:LEU:H    | 1:12:A:LEU:HB2  | 2        | 0.21          |
| (1,293) | 1:11:A:TRP:HE1  | 1:24:A:PRO:HD2  | 1        | 0.21          |
| (1,273) | 1:18:A:SER:H    | 1:19:A:SER:H    | 1        | 0.21          |
| (1,239) | 1:8:A:TYR:HE1   | 1:12:A:LEU:HG   | 8        | 0.21          |
| (1,239) | 1:8:A:TYR:HE2   | 1:12:A:LEU:HG   | 8        | 0.21          |
| (1,200) | 1:11:A:TRP:HE3  | 1:23:A:PRO:HB3  | 3        | 0.21          |
| (1,155) | 1:7:A:LEU:H     | 1:7:A:LEU:HD11  | 10       | 0.21          |
| (1,155) | 1:7:A:LEU:H     | 1:7:A:LEU:HD12  | 10       | 0.21          |
| (1,155) | 1:7:A:LEU:H     | 1:7:A:LEU:HD13  | 10       | 0.21          |
| (1,155) | 1:7:A:LEU:H     | 1:7:A:LEU:HD21  | 10       | 0.21          |
| (1,155) | 1:7:A:LEU:H     | 1:7:A:LEU:HD22  | 10       | 0.21          |
| (1,155) | 1:7:A:LEU:H     | 1:7:A:LEU:HD23  | 10       | 0.21          |
| (1,93)  | 1:19:A:SER:HG   | 1:21:A:ARG:H    | 3        | 0.21          |
| (1,75)  | 1:25:A:CYS:H    | 1:25:A:CYS:HB2  | 2        | 0.21          |
| (1,61)  | 1:11:A:TRP:HB2  | 1:12:A:LEU:H    | 4        | 0.21          |
| (1,16)  | 1:5:A:VAL:H     | 1:5:A:VAL:HG21  | 3        | 0.21          |
| (1,16)  | 1:5:A:VAL:H     | 1:5:A:VAL:HG22  | 3        | 0.21          |
| (1,16)  | 1:5:A:VAL:H     | 1:5:A:VAL:HG23  | 3        | 0.21          |
| (1,8)   | 1:5:A:VAL:H     | 1:5:A:VAL:HG21  | 3        | 0.21          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,8)   | 1:5:A:VAL:H     | 1:5:A:VAL:HG22  | 3        | 0.21          |
| (1,8)   | 1:5:A:VAL:H     | 1:5:A:VAL:HG23  | 3        | 0.21          |
| (1,736) | 1:23:A:PRO:HA   | 1:24:A:PRO:HD3  | 4        | 0.2           |
| (1,736) | 1:23:A:PRO:HA   | 1:24:A:PRO:HD3  | 7        | 0.2           |
| (1,728) | 1:2:A:GLU:HG2   | 1:6:A:ARG:HG2   | 10       | 0.2           |
| (1,716) | 1:9:A:ILE:HG12  | 1:12:A:LEU:HD11 | 9        | 0.2           |
| (1,716) | 1:9:A:ILE:HG12  | 1:12:A:LEU:HD12 | 9        | 0.2           |
| (1,716) | 1:9:A:ILE:HG12  | 1:12:A:LEU:HD13 | 9        | 0.2           |
| (1,715) | 1:9:A:ILE:HG21  | 1:12:A:LEU:HB2  | 3        | 0.2           |
| (1,715) | 1:9:A:ILE:HG22  | 1:12:A:LEU:HB2  | 3        | 0.2           |
| (1,715) | 1:9:A:ILE:HG23  | 1:12:A:LEU:HB2  | 3        | 0.2           |
| (1,677) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD11 | 4        | 0.2           |
| (1,677) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD12 | 4        | 0.2           |
| (1,677) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD13 | 4        | 0.2           |
| (1,634) | 1:11:A:TRP:HE3  | 1:23:A:PRO:HB2  | 1        | 0.2           |
| (1,634) | 1:11:A:TRP:HE3  | 1:23:A:PRO:HB2  | 5        | 0.2           |
| (1,621) | 1:2:A:GLU:HB2   | 1:6:A:ARG:H     | 3        | 0.2           |
| (1,618) | 1:10:A:GLN:HE21 | 1:13:A:LYS:HD3  | 10       | 0.2           |
| (1,601) | 1:10:A:GLN:H    | 1:12:A:LEU:H    | 10       | 0.2           |
| (1,600) | 1:1:A:GLU:HB3   | 1:1:A:GLU:HG2   | 3        | 0.2           |
| (1,600) | 1:1:A:GLU:HB3   | 1:1:A:GLU:HG3   | 3        | 0.2           |
| (1,597) | 1:1:A:GLU:HA    | 1:1:A:GLU:HB2   | 1        | 0.2           |
| (1,597) | 1:1:A:GLU:HA    | 1:1:A:GLU:HB2   | 3        | 0.2           |
| (1,597) | 1:1:A:GLU:HA    | 1:1:A:GLU:HB2   | 4        | 0.2           |
| (1,597) | 1:1:A:GLU:HA    | 1:1:A:GLU:HB2   | 5        | 0.2           |
| (1,597) | 1:1:A:GLU:HA    | 1:1:A:GLU:HB2   | 6        | 0.2           |
| (1,597) | 1:1:A:GLU:HA    | 1:1:A:GLU:HB2   | 8        | 0.2           |
| (1,565) | 1:4:A:CYS:HA    | 1:7:A:LEU:HG    | 5        | 0.2           |
| (1,551) | 1:16:A:GLY:HA3  | 1:17:A:PRO:HD3  | 2        | 0.2           |
| (1,522) | 1:24:A:PRO:HA   | 1:24:A:PRO:HD3  | 10       | 0.2           |
| (1,489) | 1:22:A:PRO:HB2  | 1:22:A:PRO:HG2  | 6        | 0.2           |
| (1,450) | 1:18:A:SER:HA   | 1:18:A:SER:HB3  | 6        | 0.2           |
| (1,418) | 1:12:A:LEU:HD11 | 1:12:A:LEU:HD21 | 10       | 0.2           |
| (1,418) | 1:12:A:LEU:HD11 | 1:12:A:LEU:HD22 | 10       | 0.2           |
| (1,418) | 1:12:A:LEU:HD11 | 1:12:A:LEU:HD23 | 10       | 0.2           |
| (1,418) | 1:12:A:LEU:HD12 | 1:12:A:LEU:HD21 | 10       | 0.2           |
| (1,418) | 1:12:A:LEU:HD12 | 1:12:A:LEU:HD22 | 10       | 0.2           |
| (1,418) | 1:12:A:LEU:HD12 | 1:12:A:LEU:HD23 | 10       | 0.2           |
| (1,418) | 1:12:A:LEU:HD13 | 1:12:A:LEU:HD21 | 10       | 0.2           |
| (1,418) | 1:12:A:LEU:HD13 | 1:12:A:LEU:HD22 | 10       | 0.2           |
| (1,418) | 1:12:A:LEU:HD13 | 1:12:A:LEU:HD23 | 10       | 0.2           |
| (1,408) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD11 | 5        | 0.2           |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,408) | 1:12:A:LEU:HA  | 1:12:A:LEU:HD12 | 5        | 0.2           |
| (1,408) | 1:12:A:LEU:HA  | 1:12:A:LEU:HD13 | 5        | 0.2           |
| (1,405) | 1:12:A:LEU:HA  | 1:12:A:LEU:HG   | 3        | 0.2           |
| (1,385) | 1:9:A:ILE:HD11 | 1:9:A:ILE:HG13  | 3        | 0.2           |
| (1,385) | 1:9:A:ILE:HD12 | 1:9:A:ILE:HG13  | 3        | 0.2           |
| (1,385) | 1:9:A:ILE:HD13 | 1:9:A:ILE:HG13  | 3        | 0.2           |
| (1,333) | 1:2:A:GLU:HB2  | 1:2:A:GLU:HB3   | 1        | 0.2           |
| (1,333) | 1:2:A:GLU:HB2  | 1:2:A:GLU:HB3   | 2        | 0.2           |
| (1,333) | 1:2:A:GLU:HB2  | 1:2:A:GLU:HB3   | 3        | 0.2           |
| (1,333) | 1:2:A:GLU:HB2  | 1:2:A:GLU:HB3   | 4        | 0.2           |
| (1,333) | 1:2:A:GLU:HB2  | 1:2:A:GLU:HB3   | 5        | 0.2           |
| (1,333) | 1:2:A:GLU:HB2  | 1:2:A:GLU:HB3   | 6        | 0.2           |
| (1,333) | 1:2:A:GLU:HB2  | 1:2:A:GLU:HB3   | 7        | 0.2           |
| (1,333) | 1:2:A:GLU:HB2  | 1:2:A:GLU:HB3   | 8        | 0.2           |
| (1,333) | 1:2:A:GLU:HB2  | 1:2:A:GLU:HB3   | 9        | 0.2           |
| (1,248) | 1:8:A:TYR:HD1  | 1:23:A:PRO:HA   | 6        | 0.2           |
| (1,248) | 1:8:A:TYR:HD2  | 1:23:A:PRO:HA   | 6        | 0.2           |
| (1,232) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HG   | 2        | 0.2           |
| (1,220) | 1:8:A:TYR:HD1  | 1:9:A:ILE:HG12  | 4        | 0.2           |
| (1,220) | 1:8:A:TYR:HD2  | 1:9:A:ILE:HG12  | 4        | 0.2           |
| (1,208) | 1:11:A:TRP:HZ3 | 1:12:A:LEU:HD11 | 9        | 0.2           |
| (1,208) | 1:11:A:TRP:HZ3 | 1:12:A:LEU:HD12 | 9        | 0.2           |
| (1,208) | 1:11:A:TRP:HZ3 | 1:12:A:LEU:HD13 | 9        | 0.2           |
| (1,195) | 1:8:A:TYR:HE1  | 1:24:A:PRO:HD3  | 8        | 0.2           |
| (1,195) | 1:8:A:TYR:HE2  | 1:24:A:PRO:HD3  | 8        | 0.2           |
| (1,180) | 1:11:A:TRP:HB2 | 1:11:A:TRP:HE3  | 4        | 0.2           |
| (1,179) | 1:11:A:TRP:HB2 | 1:11:A:TRP:HD1  | 4        | 0.2           |
| (1,179) | 1:11:A:TRP:HB2 | 1:11:A:TRP:HD1  | 7        | 0.2           |
| (1,155) | 1:7:A:LEU:H    | 1:7:A:LEU:HD11  | 2        | 0.2           |
| (1,155) | 1:7:A:LEU:H    | 1:7:A:LEU:HD12  | 2        | 0.2           |
| (1,155) | 1:7:A:LEU:H    | 1:7:A:LEU:HD13  | 2        | 0.2           |
| (1,155) | 1:7:A:LEU:H    | 1:7:A:LEU:HD21  | 2        | 0.2           |
| (1,155) | 1:7:A:LEU:H    | 1:7:A:LEU:HD22  | 2        | 0.2           |
| (1,155) | 1:7:A:LEU:H    | 1:7:A:LEU:HD23  | 2        | 0.2           |
| (1,98)  | 1:11:A:TRP:HE1 | 1:19:A:SER:HG   | 1        | 0.2           |
| (1,76)  | 1:25:A:CYS:H   | 1:25:A:CYS:HB3  | 6        | 0.2           |
| (1,61)  | 1:11:A:TRP:HB2 | 1:12:A:LEU:H    | 7        | 0.2           |
| (1,61)  | 1:11:A:TRP:HB2 | 1:12:A:LEU:H    | 9        | 0.2           |
| (1,55)  | 1:21:A:ARG:H   | 1:21:A:ARG:HD2  | 4        | 0.2           |
| (1,26)  | 1:2:A:GLU:HB2  | 1:3:A:GLU:H     | 9        | 0.2           |
| (1,736) | 1:23:A:PRO:HA  | 1:24:A:PRO:HD3  | 9        | 0.19          |
| (1,704) | 1:9:A:ILE:HG21 | 1:13:A:LYS:HD3  | 1        | 0.19          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,704) | 1:9:A:ILE:HG22  | 1:13:A:LYS:HD3  | 1        | 0.19          |
| (1,704) | 1:9:A:ILE:HG23  | 1:13:A:LYS:HD3  | 1        | 0.19          |
| (1,704) | 1:9:A:ILE:HG21  | 1:13:A:LYS:HD3  | 4        | 0.19          |
| (1,704) | 1:9:A:ILE:HG22  | 1:13:A:LYS:HD3  | 4        | 0.19          |
| (1,704) | 1:9:A:ILE:HG23  | 1:13:A:LYS:HD3  | 4        | 0.19          |
| (1,704) | 1:9:A:ILE:HG21  | 1:13:A:LYS:HD3  | 9        | 0.19          |
| (1,704) | 1:9:A:ILE:HG22  | 1:13:A:LYS:HD3  | 9        | 0.19          |
| (1,704) | 1:9:A:ILE:HG23  | 1:13:A:LYS:HD3  | 9        | 0.19          |
| (1,677) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD11 | 2        | 0.19          |
| (1,677) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD12 | 2        | 0.19          |
| (1,677) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD13 | 2        | 0.19          |
| (1,666) | 1:24:A:PRO:HG2  | 1:25:A:CYS:HB2  | 10       | 0.19          |
| (1,654) | 1:14:A:ASP:HB3  | 1:19:A:SER:HB3  | 7        | 0.19          |
| (1,653) | 1:4:A:CYS:HB3   | 1:25:A:CYS:HB2  | 10       | 0.19          |
| (1,652) | 1:3:A:GLU:HA    | 1:6:A:ARG:HD3   | 2        | 0.19          |
| (1,633) | 1:11:A:TRP:HZ3  | 1:23:A:PRO:HB2  | 1        | 0.19          |
| (1,622) | 1:2:A:GLU:HB3   | 1:5:A:VAL:H     | 9        | 0.19          |
| (1,601) | 1:10:A:GLN:H    | 1:12:A:LEU:H    | 8        | 0.19          |
| (1,600) | 1:1:A:GLU:HB3   | 1:1:A:GLU:HG2   | 9        | 0.19          |
| (1,600) | 1:1:A:GLU:HB3   | 1:1:A:GLU:HG3   | 9        | 0.19          |
| (1,545) | 1:13:A:LYS:HB2  | 1:13:A:LYS:HE2  | 7        | 0.19          |
| (1,545) | 1:13:A:LYS:HB2  | 1:13:A:LYS:HE3  | 7        | 0.19          |
| (1,545) | 1:13:A:LYS:HB3  | 1:13:A:LYS:HE2  | 7        | 0.19          |
| (1,545) | 1:13:A:LYS:HB3  | 1:13:A:LYS:HE3  | 7        | 0.19          |
| (1,531) | 1:24:A:PRO:HB2  | 1:24:A:PRO:HB3  | 3        | 0.19          |
| (1,522) | 1:24:A:PRO:HA   | 1:24:A:PRO:HD3  | 8        | 0.19          |
| (1,479) | 1:22:A:PRO:HB3  | 1:22:A:PRO:HD3  | 4        | 0.19          |
| (1,477) | 1:22:A:PRO:HA   | 1:22:A:PRO:HB2  | 1        | 0.19          |
| (1,418) | 1:12:A:LEU:HD11 | 1:12:A:LEU:HD21 | 7        | 0.19          |
| (1,418) | 1:12:A:LEU:HD11 | 1:12:A:LEU:HD22 | 7        | 0.19          |
| (1,418) | 1:12:A:LEU:HD11 | 1:12:A:LEU:HD23 | 7        | 0.19          |
| (1,418) | 1:12:A:LEU:HD12 | 1:12:A:LEU:HD21 | 7        | 0.19          |
| (1,418) | 1:12:A:LEU:HD12 | 1:12:A:LEU:HD22 | 7        | 0.19          |
| (1,418) | 1:12:A:LEU:HD12 | 1:12:A:LEU:HD23 | 7        | 0.19          |
| (1,418) | 1:12:A:LEU:HD13 | 1:12:A:LEU:HD21 | 7        | 0.19          |
| (1,418) | 1:12:A:LEU:HD13 | 1:12:A:LEU:HD22 | 7        | 0.19          |
| (1,418) | 1:12:A:LEU:HD13 | 1:12:A:LEU:HD23 | 7        | 0.19          |
| (1,417) | 1:12:A:LEU:HB2  | 1:12:A:LEU:HD11 | 3        | 0.19          |
| (1,417) | 1:12:A:LEU:HB2  | 1:12:A:LEU:HD12 | 3        | 0.19          |
| (1,417) | 1:12:A:LEU:HB2  | 1:12:A:LEU:HD13 | 3        | 0.19          |
| (1,412) | 1:12:A:LEU:HD21 | 1:12:A:LEU:HG   | 3        | 0.19          |
| (1,412) | 1:12:A:LEU:HD22 | 1:12:A:LEU:HG   | 3        | 0.19          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,412) | 1:12:A:LEU:HD23 | 1:12:A:LEU:HG   | 3        | 0.19          |
| (1,397) | 1:10:A:GLN:HB2  | 1:10:A:GLN:HG2  | 2        | 0.19          |
| (1,397) | 1:10:A:GLN:HB2  | 1:10:A:GLN:HG2  | 10       | 0.19          |
| (1,375) | 1:8:A:TYR:HA    | 1:8:A:TYR:HB2   | 3        | 0.19          |
| (1,375) | 1:8:A:TYR:HA    | 1:8:A:TYR:HB3   | 3        | 0.19          |
| (1,375) | 1:8:A:TYR:HA    | 1:8:A:TYR:HB2   | 8        | 0.19          |
| (1,375) | 1:8:A:TYR:HA    | 1:8:A:TYR:HB3   | 8        | 0.19          |
| (1,375) | 1:8:A:TYR:HA    | 1:8:A:TYR:HB2   | 9        | 0.19          |
| (1,375) | 1:8:A:TYR:HA    | 1:8:A:TYR:HB3   | 9        | 0.19          |
| (1,337) | 1:4:A:CYS:HA    | 1:4:A:CYS:HB3   | 3        | 0.19          |
| (1,333) | 1:2:A:GLU:HB2   | 1:2:A:GLU:HB3   | 10       | 0.19          |
| (1,331) | 1:2:A:GLU:HB2   | 1:2:A:GLU:HG3   | 1        | 0.19          |
| (1,331) | 1:2:A:GLU:HB2   | 1:2:A:GLU:HG3   | 3        | 0.19          |
| (1,326) | 1:2:A:GLU:HA    | 1:2:A:GLU:HB3   | 2        | 0.19          |
| (1,326) | 1:2:A:GLU:HA    | 1:2:A:GLU:HB3   | 4        | 0.19          |
| (1,321) | 1:11:A:TRP:HB3  | 1:12:A:LEU:H    | 4        | 0.19          |
| (1,293) | 1:11:A:TRP:HE1  | 1:24:A:PRO:HD2  | 6        | 0.19          |
| (1,284) | 1:2:A:GLU:HA    | 1:3:A:GLU:H     | 7        | 0.19          |
| (1,284) | 1:2:A:GLU:HA    | 1:3:A:GLU:H     | 9        | 0.19          |
| (1,226) | 1:11:A:TRP:HH2  | 1:23:A:PRO:HG2  | 5        | 0.19          |
| (1,225) | 1:23:A:PRO:HB2  | 1:25:A:CYS:H    | 1        | 0.19          |
| (1,210) | 1:11:A:TRP:HE3  | 1:12:A:LEU:HD11 | 1        | 0.19          |
| (1,210) | 1:11:A:TRP:HE3  | 1:12:A:LEU:HD12 | 1        | 0.19          |
| (1,210) | 1:11:A:TRP:HE3  | 1:12:A:LEU:HD13 | 1        | 0.19          |
| (1,180) | 1:11:A:TRP:HB2  | 1:11:A:TRP:HE3  | 3        | 0.19          |
| (1,180) | 1:11:A:TRP:HB2  | 1:11:A:TRP:HE3  | 7        | 0.19          |
| (1,180) | 1:11:A:TRP:HB2  | 1:11:A:TRP:HE3  | 8        | 0.19          |
| (1,180) | 1:11:A:TRP:HB2  | 1:11:A:TRP:HE3  | 9        | 0.19          |
| (1,180) | 1:11:A:TRP:HB2  | 1:11:A:TRP:HE3  | 10       | 0.19          |
| (1,179) | 1:11:A:TRP:HB2  | 1:11:A:TRP:HD1  | 3        | 0.19          |
| (1,179) | 1:11:A:TRP:HB2  | 1:11:A:TRP:HD1  | 8        | 0.19          |
| (1,179) | 1:11:A:TRP:HB2  | 1:11:A:TRP:HD1  | 9        | 0.19          |
| (1,177) | 1:8:A:TYR:HD1   | 1:12:A:LEU:HA   | 9        | 0.19          |
| (1,177) | 1:8:A:TYR:HD2   | 1:12:A:LEU:HA   | 9        | 0.19          |
| (1,173) | 1:11:A:TRP:HH2  | 1:17:A:PRO:HD3  | 6        | 0.19          |
| (1,164) | 1:8:A:TYR:HA    | 1:8:A:TYR:HD1   | 3        | 0.19          |
| (1,164) | 1:8:A:TYR:HA    | 1:8:A:TYR:HD2   | 3        | 0.19          |
| (1,155) | 1:7:A:LEU:H     | 1:7:A:LEU:HD11  | 7        | 0.19          |
| (1,155) | 1:7:A:LEU:H     | 1:7:A:LEU:HD12  | 7        | 0.19          |
| (1,155) | 1:7:A:LEU:H     | 1:7:A:LEU:HD13  | 7        | 0.19          |
| (1,155) | 1:7:A:LEU:H     | 1:7:A:LEU:HD21  | 7        | 0.19          |
| (1,155) | 1:7:A:LEU:H     | 1:7:A:LEU:HD22  | 7        | 0.19          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,155) | 1:7:A:LEU:H     | 1:7:A:LEU:HD23  | 7        | 0.19          |
| (1,155) | 1:7:A:LEU:H     | 1:7:A:LEU:HD11  | 8        | 0.19          |
| (1,155) | 1:7:A:LEU:H     | 1:7:A:LEU:HD12  | 8        | 0.19          |
| (1,155) | 1:7:A:LEU:H     | 1:7:A:LEU:HD13  | 8        | 0.19          |
| (1,155) | 1:7:A:LEU:H     | 1:7:A:LEU:HD21  | 8        | 0.19          |
| (1,155) | 1:7:A:LEU:H     | 1:7:A:LEU:HD22  | 8        | 0.19          |
| (1,155) | 1:7:A:LEU:H     | 1:7:A:LEU:HD23  | 8        | 0.19          |
| (1,152) | 1:8:A:TYR:HB2   | 1:9:A:ILE:H     | 5        | 0.19          |
| (1,152) | 1:8:A:TYR:HB3   | 1:9:A:ILE:H     | 5        | 0.19          |
| (1,115) | 1:9:A:ILE:H     | 1:9:A:ILE:HG13  | 1        | 0.19          |
| (1,35)  | 1:10:A:GLN:H    | 1:10:A:GLN:HB2  | 5        | 0.19          |
| (1,35)  | 1:10:A:GLN:H    | 1:10:A:GLN:HB2  | 7        | 0.19          |
| (1,736) | 1:23:A:PRO:HA   | 1:24:A:PRO:HD3  | 8        | 0.18          |
| (1,717) | 1:12:A:LEU:HD11 | 1:16:A:GLY:HA2  | 8        | 0.18          |
| (1,717) | 1:12:A:LEU:HD12 | 1:16:A:GLY:HA2  | 8        | 0.18          |
| (1,717) | 1:12:A:LEU:HD13 | 1:16:A:GLY:HA2  | 8        | 0.18          |
| (1,695) | 1:5:A:VAL:HG11  | 1:9:A:ILE:HB    | 6        | 0.18          |
| (1,695) | 1:5:A:VAL:HG12  | 1:9:A:ILE:HB    | 6        | 0.18          |
| (1,695) | 1:5:A:VAL:HG13  | 1:9:A:ILE:HB    | 6        | 0.18          |
| (1,677) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD11 | 8        | 0.18          |
| (1,677) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD12 | 8        | 0.18          |
| (1,677) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD13 | 8        | 0.18          |
| (1,648) | 1:15:A:GLY:HA2  | 1:19:A:SER:HB2  | 1        | 0.18          |
| (1,647) | 1:15:A:GLY:HA2  | 1:18:A:SER:HB2  | 6        | 0.18          |
| (1,625) | 1:10:A:GLN:HE21 | 1:14:A:ASP:HB3  | 6        | 0.18          |
| (1,623) | 1:2:A:GLU:HB3   | 1:6:A:ARG:H     | 8        | 0.18          |
| (1,622) | 1:2:A:GLU:HB3   | 1:5:A:VAL:H     | 3        | 0.18          |
| (1,614) | 1:19:A:SER:HG   | 1:20:A:GLY:H    | 1        | 0.18          |
| (1,605) | 1:8:A:TYR:HE1   | 1:11:A:TRP:HZ3  | 2        | 0.18          |
| (1,605) | 1:8:A:TYR:HE2   | 1:11:A:TRP:HZ3  | 2        | 0.18          |
| (1,605) | 1:8:A:TYR:HE1   | 1:11:A:TRP:HZ3  | 5        | 0.18          |
| (1,605) | 1:8:A:TYR:HE2   | 1:11:A:TRP:HZ3  | 5        | 0.18          |
| (1,605) | 1:8:A:TYR:HE1   | 1:11:A:TRP:HZ3  | 6        | 0.18          |
| (1,605) | 1:8:A:TYR:HE2   | 1:11:A:TRP:HZ3  | 6        | 0.18          |
| (1,600) | 1:1:A:GLU:HB3   | 1:1:A:GLU:HG2   | 5        | 0.18          |
| (1,600) | 1:1:A:GLU:HB3   | 1:1:A:GLU:HG3   | 5        | 0.18          |
| (1,581) | 1:5:A:VAL:HG11  | 1:6:A:ARG:HA    | 8        | 0.18          |
| (1,581) | 1:5:A:VAL:HG12  | 1:6:A:ARG:HA    | 8        | 0.18          |
| (1,581) | 1:5:A:VAL:HG13  | 1:6:A:ARG:HA    | 8        | 0.18          |
| (1,550) | 1:11:A:TRP:HB3  | 1:24:A:PRO:HD3  | 4        | 0.18          |
| (1,550) | 1:11:A:TRP:HB3  | 1:24:A:PRO:HD3  | 9        | 0.18          |
| (1,540) | 1:25:A:CYS:HB2  | 1:25:A:CYS:HB3  | 1        | 0.18          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,540) | 1:25:A:CYS:HB2  | 1:25:A:CYS:HB3  | 2        | 0.18          |
| (1,540) | 1:25:A:CYS:HB2  | 1:25:A:CYS:HB3  | 5        | 0.18          |
| (1,522) | 1:24:A:PRO:HA   | 1:24:A:PRO:HD3  | 4        | 0.18          |
| (1,522) | 1:24:A:PRO:HA   | 1:24:A:PRO:HD3  | 9        | 0.18          |
| (1,494) | 1:21:A:ARG:HA   | 1:22:A:PRO:HD3  | 7        | 0.18          |
| (1,477) | 1:22:A:PRO:HA   | 1:22:A:PRO:HB2  | 5        | 0.18          |
| (1,477) | 1:22:A:PRO:HA   | 1:22:A:PRO:HB2  | 6        | 0.18          |
| (1,440) | 1:17:A:PRO:HD2  | 1:17:A:PRO:HD3  | 1        | 0.18          |
| (1,440) | 1:17:A:PRO:HD2  | 1:17:A:PRO:HD3  | 2        | 0.18          |
| (1,440) | 1:17:A:PRO:HD2  | 1:17:A:PRO:HD3  | 3        | 0.18          |
| (1,440) | 1:17:A:PRO:HD2  | 1:17:A:PRO:HD3  | 4        | 0.18          |
| (1,440) | 1:17:A:PRO:HD2  | 1:17:A:PRO:HD3  | 5        | 0.18          |
| (1,440) | 1:17:A:PRO:HD2  | 1:17:A:PRO:HD3  | 6        | 0.18          |
| (1,440) | 1:17:A:PRO:HD2  | 1:17:A:PRO:HD3  | 7        | 0.18          |
| (1,440) | 1:17:A:PRO:HD2  | 1:17:A:PRO:HD3  | 8        | 0.18          |
| (1,440) | 1:17:A:PRO:HD2  | 1:17:A:PRO:HD3  | 9        | 0.18          |
| (1,440) | 1:17:A:PRO:HD2  | 1:17:A:PRO:HD3  | 10       | 0.18          |
| (1,432) | 1:14:A:ASP:HB2  | 1:14:A:ASP:HB3  | 3        | 0.18          |
| (1,432) | 1:14:A:ASP:HB2  | 1:14:A:ASP:HB3  | 4        | 0.18          |
| (1,432) | 1:14:A:ASP:HB2  | 1:14:A:ASP:HB3  | 7        | 0.18          |
| (1,432) | 1:14:A:ASP:HB2  | 1:14:A:ASP:HB3  | 8        | 0.18          |
| (1,432) | 1:14:A:ASP:HB2  | 1:14:A:ASP:HB3  | 10       | 0.18          |
| (1,418) | 1:12:A:LEU:HD11 | 1:12:A:LEU:HD21 | 1        | 0.18          |
| (1,418) | 1:12:A:LEU:HD11 | 1:12:A:LEU:HD22 | 1        | 0.18          |
| (1,418) | 1:12:A:LEU:HD11 | 1:12:A:LEU:HD23 | 1        | 0.18          |
| (1,418) | 1:12:A:LEU:HD12 | 1:12:A:LEU:HD21 | 1        | 0.18          |
| (1,418) | 1:12:A:LEU:HD12 | 1:12:A:LEU:HD22 | 1        | 0.18          |
| (1,418) | 1:12:A:LEU:HD12 | 1:12:A:LEU:HD23 | 1        | 0.18          |
| (1,418) | 1:12:A:LEU:HD13 | 1:12:A:LEU:HD21 | 1        | 0.18          |
| (1,418) | 1:12:A:LEU:HD13 | 1:12:A:LEU:HD22 | 1        | 0.18          |
| (1,418) | 1:12:A:LEU:HD13 | 1:12:A:LEU:HD23 | 1        | 0.18          |
| (1,418) | 1:12:A:LEU:HD11 | 1:12:A:LEU:HD21 | 2        | 0.18          |
| (1,418) | 1:12:A:LEU:HD11 | 1:12:A:LEU:HD22 | 2        | 0.18          |
| (1,418) | 1:12:A:LEU:HD11 | 1:12:A:LEU:HD23 | 2        | 0.18          |
| (1,418) | 1:12:A:LEU:HD12 | 1:12:A:LEU:HD21 | 2        | 0.18          |
| (1,418) | 1:12:A:LEU:HD12 | 1:12:A:LEU:HD22 | 2        | 0.18          |
| (1,418) | 1:12:A:LEU:HD12 | 1:12:A:LEU:HD23 | 2        | 0.18          |
| (1,418) | 1:12:A:LEU:HD13 | 1:12:A:LEU:HD21 | 2        | 0.18          |
| (1,418) | 1:12:A:LEU:HD13 | 1:12:A:LEU:HD22 | 2        | 0.18          |
| (1,418) | 1:12:A:LEU:HD13 | 1:12:A:LEU:HD23 | 2        | 0.18          |
| (1,418) | 1:12:A:LEU:HD11 | 1:12:A:LEU:HD21 | 3        | 0.18          |
| (1,418) | 1:12:A:LEU:HD11 | 1:12:A:LEU:HD22 | 3        | 0.18          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,418) | 1:12:A:LEU:HD11 | 1:12:A:LEU:HD23 | 3        | 0.18          |
| (1,418) | 1:12:A:LEU:HD12 | 1:12:A:LEU:HD21 | 3        | 0.18          |
| (1,418) | 1:12:A:LEU:HD12 | 1:12:A:LEU:HD22 | 3        | 0.18          |
| (1,418) | 1:12:A:LEU:HD12 | 1:12:A:LEU:HD23 | 3        | 0.18          |
| (1,418) | 1:12:A:LEU:HD13 | 1:12:A:LEU:HD21 | 3        | 0.18          |
| (1,418) | 1:12:A:LEU:HD13 | 1:12:A:LEU:HD22 | 3        | 0.18          |
| (1,418) | 1:12:A:LEU:HD13 | 1:12:A:LEU:HD23 | 3        | 0.18          |
| (1,418) | 1:12:A:LEU:HD11 | 1:12:A:LEU:HD21 | 4        | 0.18          |
| (1,418) | 1:12:A:LEU:HD11 | 1:12:A:LEU:HD22 | 4        | 0.18          |
| (1,418) | 1:12:A:LEU:HD11 | 1:12:A:LEU:HD23 | 4        | 0.18          |
| (1,418) | 1:12:A:LEU:HD12 | 1:12:A:LEU:HD21 | 4        | 0.18          |
| (1,418) | 1:12:A:LEU:HD12 | 1:12:A:LEU:HD22 | 4        | 0.18          |
| (1,418) | 1:12:A:LEU:HD12 | 1:12:A:LEU:HD23 | 4        | 0.18          |
| (1,418) | 1:12:A:LEU:HD13 | 1:12:A:LEU:HD21 | 4        | 0.18          |
| (1,418) | 1:12:A:LEU:HD13 | 1:12:A:LEU:HD22 | 4        | 0.18          |
| (1,418) | 1:12:A:LEU:HD13 | 1:12:A:LEU:HD23 | 4        | 0.18          |
| (1,418) | 1:12:A:LEU:HD11 | 1:12:A:LEU:HD21 | 9        | 0.18          |
| (1,418) | 1:12:A:LEU:HD11 | 1:12:A:LEU:HD22 | 9        | 0.18          |
| (1,418) | 1:12:A:LEU:HD11 | 1:12:A:LEU:HD23 | 9        | 0.18          |
| (1,418) | 1:12:A:LEU:HD12 | 1:12:A:LEU:HD21 | 9        | 0.18          |
| (1,418) | 1:12:A:LEU:HD12 | 1:12:A:LEU:HD22 | 9        | 0.18          |
| (1,418) | 1:12:A:LEU:HD12 | 1:12:A:LEU:HD23 | 9        | 0.18          |
| (1,418) | 1:12:A:LEU:HD13 | 1:12:A:LEU:HD21 | 9        | 0.18          |
| (1,418) | 1:12:A:LEU:HD13 | 1:12:A:LEU:HD22 | 9        | 0.18          |
| (1,418) | 1:12:A:LEU:HD13 | 1:12:A:LEU:HD23 | 9        | 0.18          |
| (1,397) | 1:10:A:GLN:HB2  | 1:10:A:GLN:HG2  | 8        | 0.18          |
| (1,377) | 1:9:A:ILE:HA    | 1:9:A:ILE:HG13  | 5        | 0.18          |
| (1,377) | 1:9:A:ILE:HA    | 1:9:A:ILE:HG13  | 6        | 0.18          |
| (1,375) | 1:8:A:TYR:HA    | 1:8:A:TYR:HB2   | 4        | 0.18          |
| (1,375) | 1:8:A:TYR:HA    | 1:8:A:TYR:HB3   | 4        | 0.18          |
| (1,375) | 1:8:A:TYR:HA    | 1:8:A:TYR:HB2   | 7        | 0.18          |
| (1,375) | 1:8:A:TYR:HA    | 1:8:A:TYR:HB3   | 7        | 0.18          |
| (1,375) | 1:8:A:TYR:HA    | 1:8:A:TYR:HB2   | 10       | 0.18          |
| (1,375) | 1:8:A:TYR:HA    | 1:8:A:TYR:HB3   | 10       | 0.18          |
| (1,339) | 1:4:A:CYS:HB2   | 1:4:A:CYS:HB3   | 4        | 0.18          |
| (1,339) | 1:4:A:CYS:HB2   | 1:4:A:CYS:HB3   | 6        | 0.18          |
| (1,331) | 1:2:A:GLU:HB2   | 1:2:A:GLU:HG3   | 2        | 0.18          |
| (1,331) | 1:2:A:GLU:HB2   | 1:2:A:GLU:HG3   | 5        | 0.18          |
| (1,326) | 1:2:A:GLU:HA    | 1:2:A:GLU:HB3   | 1        | 0.18          |
| (1,321) | 1:11:A:TRP:HB3  | 1:12:A:LEU:H    | 8        | 0.18          |
| (1,321) | 1:11:A:TRP:HB3  | 1:12:A:LEU:H    | 10       | 0.18          |
| (1,280) | 1:4:A:CYS:H     | 1:5:A:VAL:H     | 4        | 0.18          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,280) | 1:4:A:CYS:H    | 1:5:A:VAL:H     | 5        | 0.18          |
| (1,262) | 1:10:A:GLN:HA  | 1:10:A:GLN:HE22 | 4        | 0.18          |
| (1,262) | 1:10:A:GLN:HA  | 1:10:A:GLN:HE22 | 6        | 0.18          |
| (1,232) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HG   | 1        | 0.18          |
| (1,232) | 1:11:A:TRP:HE3 | 1:12:A:LEU:HG   | 5        | 0.18          |
| (1,220) | 1:8:A:TYR:HD1  | 1:9:A:ILE:HG12  | 1        | 0.18          |
| (1,220) | 1:8:A:TYR:HD2  | 1:9:A:ILE:HG12  | 1        | 0.18          |
| (1,214) | 1:8:A:TYR:HD1  | 1:12:A:LEU:HD21 | 3        | 0.18          |
| (1,214) | 1:8:A:TYR:HD1  | 1:12:A:LEU:HD22 | 3        | 0.18          |
| (1,214) | 1:8:A:TYR:HD1  | 1:12:A:LEU:HD23 | 3        | 0.18          |
| (1,214) | 1:8:A:TYR:HD2  | 1:12:A:LEU:HD21 | 3        | 0.18          |
| (1,214) | 1:8:A:TYR:HD2  | 1:12:A:LEU:HD22 | 3        | 0.18          |
| (1,214) | 1:8:A:TYR:HD2  | 1:12:A:LEU:HD23 | 3        | 0.18          |
| (1,208) | 1:11:A:TRP:HZ3 | 1:12:A:LEU:HD11 | 7        | 0.18          |
| (1,208) | 1:11:A:TRP:HZ3 | 1:12:A:LEU:HD12 | 7        | 0.18          |
| (1,208) | 1:11:A:TRP:HZ3 | 1:12:A:LEU:HD13 | 7        | 0.18          |
| (1,195) | 1:8:A:TYR:HE1  | 1:24:A:PRO:HD3  | 5        | 0.18          |
| (1,195) | 1:8:A:TYR:HE2  | 1:24:A:PRO:HD3  | 5        | 0.18          |
| (1,179) | 1:11:A:TRP:HB2 | 1:11:A:TRP:HD1  | 10       | 0.18          |
| (1,115) | 1:9:A:ILE:H    | 1:9:A:ILE:HG13  | 2        | 0.18          |
| (1,115) | 1:9:A:ILE:H    | 1:9:A:ILE:HG13  | 3        | 0.18          |
| (1,115) | 1:9:A:ILE:H    | 1:9:A:ILE:HG13  | 5        | 0.18          |
| (1,736) | 1:23:A:PRO:HA  | 1:24:A:PRO:HD3  | 10       | 0.17          |
| (1,654) | 1:14:A:ASP:HB3 | 1:19:A:SER:HB3  | 5        | 0.17          |
| (1,642) | 1:8:A:TYR:HD1  | 1:25:A:CYS:HB2  | 1        | 0.17          |
| (1,642) | 1:8:A:TYR:HD2  | 1:25:A:CYS:HB2  | 1        | 0.17          |
| (1,633) | 1:11:A:TRP:HZ3 | 1:23:A:PRO:HB2  | 6        | 0.17          |
| (1,615) | 1:16:A:GLY:H   | 1:19:A:SER:HB3  | 9        | 0.17          |
| (1,596) | 1:1:A:GLU:HA   | 1:1:A:GLU:HG2   | 4        | 0.17          |
| (1,596) | 1:1:A:GLU:HA   | 1:1:A:GLU:HG3   | 4        | 0.17          |
| (1,581) | 1:5:A:VAL:HG11 | 1:6:A:ARG:HA    | 9        | 0.17          |
| (1,581) | 1:5:A:VAL:HG12 | 1:6:A:ARG:HA    | 9        | 0.17          |
| (1,581) | 1:5:A:VAL:HG13 | 1:6:A:ARG:HA    | 9        | 0.17          |
| (1,563) | 1:7:A:LEU:HA   | 1:10:A:GLN:HB3  | 8        | 0.17          |
| (1,540) | 1:25:A:CYS:HB2 | 1:25:A:CYS:HB3  | 3        | 0.17          |
| (1,540) | 1:25:A:CYS:HB2 | 1:25:A:CYS:HB3  | 7        | 0.17          |
| (1,540) | 1:25:A:CYS:HB2 | 1:25:A:CYS:HB3  | 8        | 0.17          |
| (1,540) | 1:25:A:CYS:HB2 | 1:25:A:CYS:HB3  | 9        | 0.17          |
| (1,540) | 1:25:A:CYS:HB2 | 1:25:A:CYS:HB3  | 10       | 0.17          |
| (1,537) | 1:23:A:PRO:HB2 | 1:24:A:PRO:HD2  | 2        | 0.17          |
| (1,531) | 1:24:A:PRO:HB2 | 1:24:A:PRO:HB3  | 1        | 0.17          |
| (1,531) | 1:24:A:PRO:HB2 | 1:24:A:PRO:HB3  | 2        | 0.17          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,531) | 1:24:A:PRO:HB2 | 1:24:A:PRO:HB3  | 4        | 0.17          |
| (1,531) | 1:24:A:PRO:HB2 | 1:24:A:PRO:HB3  | 5        | 0.17          |
| (1,531) | 1:24:A:PRO:HB2 | 1:24:A:PRO:HB3  | 6        | 0.17          |
| (1,531) | 1:24:A:PRO:HB2 | 1:24:A:PRO:HB3  | 7        | 0.17          |
| (1,531) | 1:24:A:PRO:HB2 | 1:24:A:PRO:HB3  | 8        | 0.17          |
| (1,531) | 1:24:A:PRO:HB2 | 1:24:A:PRO:HB3  | 9        | 0.17          |
| (1,531) | 1:24:A:PRO:HB2 | 1:24:A:PRO:HB3  | 10       | 0.17          |
| (1,522) | 1:24:A:PRO:HA  | 1:24:A:PRO:HD3  | 7        | 0.17          |
| (1,497) | 1:23:A:PRO:HA  | 1:23:A:PRO:HB2  | 2        | 0.17          |
| (1,489) | 1:22:A:PRO:HB2 | 1:22:A:PRO:HG2  | 4        | 0.17          |
| (1,489) | 1:22:A:PRO:HB2 | 1:22:A:PRO:HG2  | 7        | 0.17          |
| (1,471) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HG2  | 10       | 0.17          |
| (1,471) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HG3  | 10       | 0.17          |
| (1,432) | 1:14:A:ASP:HB2 | 1:14:A:ASP:HB3  | 1        | 0.17          |
| (1,432) | 1:14:A:ASP:HB2 | 1:14:A:ASP:HB3  | 2        | 0.17          |
| (1,432) | 1:14:A:ASP:HB2 | 1:14:A:ASP:HB3  | 5        | 0.17          |
| (1,432) | 1:14:A:ASP:HB2 | 1:14:A:ASP:HB3  | 6        | 0.17          |
| (1,432) | 1:14:A:ASP:HB2 | 1:14:A:ASP:HB3  | 9        | 0.17          |
| (1,375) | 1:8:A:TYR:HA   | 1:8:A:TYR:HB2   | 1        | 0.17          |
| (1,375) | 1:8:A:TYR:HA   | 1:8:A:TYR:HB3   | 1        | 0.17          |
| (1,375) | 1:8:A:TYR:HA   | 1:8:A:TYR:HB2   | 2        | 0.17          |
| (1,375) | 1:8:A:TYR:HA   | 1:8:A:TYR:HB3   | 2        | 0.17          |
| (1,375) | 1:8:A:TYR:HA   | 1:8:A:TYR:HB2   | 5        | 0.17          |
| (1,375) | 1:8:A:TYR:HA   | 1:8:A:TYR:HB3   | 5        | 0.17          |
| (1,353) | 1:6:A:ARG:HB3  | 1:6:A:ARG:HD3   | 9        | 0.17          |
| (1,341) | 1:5:A:VAL:HA   | 1:5:A:VAL:HG21  | 9        | 0.17          |
| (1,341) | 1:5:A:VAL:HA   | 1:5:A:VAL:HG22  | 9        | 0.17          |
| (1,341) | 1:5:A:VAL:HA   | 1:5:A:VAL:HG23  | 9        | 0.17          |
| (1,339) | 1:4:A:CYS:HB2  | 1:4:A:CYS:HB3   | 3        | 0.17          |
| (1,339) | 1:4:A:CYS:HB2  | 1:4:A:CYS:HB3   | 10       | 0.17          |
| (1,335) | 1:3:A:GLU:HA   | 1:3:A:GLU:HB2   | 2        | 0.17          |
| (1,335) | 1:3:A:GLU:HA   | 1:3:A:GLU:HB3   | 2        | 0.17          |
| (1,331) | 1:2:A:GLU:HB2  | 1:2:A:GLU:HG3   | 6        | 0.17          |
| (1,284) | 1:2:A:GLU:HA   | 1:3:A:GLU:H     | 3        | 0.17          |
| (1,262) | 1:10:A:GLN:HA  | 1:10:A:GLN:HE22 | 9        | 0.17          |
| (1,220) | 1:8:A:TYR:HD1  | 1:9:A:ILE:HG12  | 7        | 0.17          |
| (1,220) | 1:8:A:TYR:HD2  | 1:9:A:ILE:HG12  | 7        | 0.17          |
| (1,220) | 1:8:A:TYR:HD1  | 1:9:A:ILE:HG12  | 8        | 0.17          |
| (1,220) | 1:8:A:TYR:HD2  | 1:9:A:ILE:HG12  | 8        | 0.17          |
| (1,220) | 1:8:A:TYR:HD1  | 1:9:A:ILE:HG12  | 9        | 0.17          |
| (1,220) | 1:8:A:TYR:HD2  | 1:9:A:ILE:HG12  | 9        | 0.17          |
| (1,208) | 1:11:A:TRP:HZ3 | 1:12:A:LEU:HD11 | 4        | 0.17          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,208) | 1:11:A:TRP:HZ3 | 1:12:A:LEU:HD12 | 4        | 0.17          |
| (1,208) | 1:11:A:TRP:HZ3 | 1:12:A:LEU:HD13 | 4        | 0.17          |
| (1,195) | 1:8:A:TYR:HE1  | 1:24:A:PRO:HD3  | 6        | 0.17          |
| (1,195) | 1:8:A:TYR:HE2  | 1:24:A:PRO:HD3  | 6        | 0.17          |
| (1,152) | 1:8:A:TYR:HB2  | 1:9:A:ILE:H     | 1        | 0.17          |
| (1,152) | 1:8:A:TYR:HB3  | 1:9:A:ILE:H     | 1        | 0.17          |
| (1,152) | 1:8:A:TYR:HB2  | 1:9:A:ILE:H     | 2        | 0.17          |
| (1,152) | 1:8:A:TYR:HB3  | 1:9:A:ILE:H     | 2        | 0.17          |
| (1,152) | 1:8:A:TYR:HB2  | 1:9:A:ILE:H     | 6        | 0.17          |
| (1,152) | 1:8:A:TYR:HB3  | 1:9:A:ILE:H     | 6        | 0.17          |
| (1,123) | 1:24:A:PRO:HG2 | 1:25:A:CYS:H    | 7        | 0.17          |
| (1,115) | 1:9:A:ILE:H    | 1:9:A:ILE:HG13  | 6        | 0.17          |
| (1,98)  | 1:11:A:TRP:HE1 | 1:19:A:SER:HG   | 3        | 0.17          |
| (1,94)  | 1:20:A:GLY:HA3 | 1:21:A:ARG:H    | 6        | 0.17          |
| (1,94)  | 1:20:A:GLY:HA3 | 1:21:A:ARG:H    | 9        | 0.17          |
| (1,93)  | 1:19:A:SER:HG  | 1:21:A:ARG:H    | 2        | 0.17          |
| (1,35)  | 1:10:A:GLN:H   | 1:10:A:GLN:HB2  | 6        | 0.17          |
| (1,719) | 1:9:A:ILE:HG12 | 1:12:A:LEU:HG   | 1        | 0.16          |
| (1,716) | 1:9:A:ILE:HG12 | 1:12:A:LEU:HD11 | 4        | 0.16          |
| (1,716) | 1:9:A:ILE:HG12 | 1:12:A:LEU:HD12 | 4        | 0.16          |
| (1,716) | 1:9:A:ILE:HG12 | 1:12:A:LEU:HD13 | 4        | 0.16          |
| (1,706) | 1:6:A:ARG:HG3  | 1:7:A:LEU:HD11  | 1        | 0.16          |
| (1,706) | 1:6:A:ARG:HG3  | 1:7:A:LEU:HD12  | 1        | 0.16          |
| (1,706) | 1:6:A:ARG:HG3  | 1:7:A:LEU:HD13  | 1        | 0.16          |
| (1,706) | 1:6:A:ARG:HG3  | 1:7:A:LEU:HD21  | 1        | 0.16          |
| (1,706) | 1:6:A:ARG:HG3  | 1:7:A:LEU:HD22  | 1        | 0.16          |
| (1,706) | 1:6:A:ARG:HG3  | 1:7:A:LEU:HD23  | 1        | 0.16          |
| (1,705) | 1:9:A:ILE:HG21 | 1:13:A:LYS:HD2  | 4        | 0.16          |
| (1,705) | 1:9:A:ILE:HG22 | 1:13:A:LYS:HD2  | 4        | 0.16          |
| (1,705) | 1:9:A:ILE:HG23 | 1:13:A:LYS:HD2  | 4        | 0.16          |
| (1,695) | 1:5:A:VAL:HG11 | 1:9:A:ILE:HB    | 8        | 0.16          |
| (1,695) | 1:5:A:VAL:HG12 | 1:9:A:ILE:HB    | 8        | 0.16          |
| (1,695) | 1:5:A:VAL:HG13 | 1:9:A:ILE:HB    | 8        | 0.16          |
| (1,641) | 1:8:A:TYR:HD1  | 1:25:A:CYS:HB3  | 2        | 0.16          |
| (1,641) | 1:8:A:TYR:HD2  | 1:25:A:CYS:HB3  | 2        | 0.16          |
| (1,621) | 1:2:A:GLU:HB2  | 1:6:A:ARG:H     | 4        | 0.16          |
| (1,621) | 1:2:A:GLU:HB2  | 1:6:A:ARG:H     | 6        | 0.16          |
| (1,614) | 1:19:A:SER:HG  | 1:20:A:GLY:H    | 8        | 0.16          |
| (1,542) | 1:7:A:LEU:HB2  | 1:24:A:PRO:HB3  | 10       | 0.16          |
| (1,540) | 1:25:A:CYS:HB2 | 1:25:A:CYS:HB3  | 4        | 0.16          |
| (1,540) | 1:25:A:CYS:HB2 | 1:25:A:CYS:HB3  | 6        | 0.16          |
| (1,524) | 1:24:A:PRO:HD2 | 1:24:A:PRO:HD3  | 1        | 0.16          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,524) | 1:24:A:PRO:HD2  | 1:24:A:PRO:HD3  | 2        | 0.16          |
| (1,524) | 1:24:A:PRO:HD2  | 1:24:A:PRO:HD3  | 5        | 0.16          |
| (1,524) | 1:24:A:PRO:HD2  | 1:24:A:PRO:HD3  | 8        | 0.16          |
| (1,497) | 1:23:A:PRO:HA   | 1:23:A:PRO:HB2  | 1        | 0.16          |
| (1,497) | 1:23:A:PRO:HA   | 1:23:A:PRO:HB2  | 6        | 0.16          |
| (1,477) | 1:22:A:PRO:HA   | 1:22:A:PRO:HB2  | 9        | 0.16          |
| (1,418) | 1:12:A:LEU:HD11 | 1:12:A:LEU:HD21 | 5        | 0.16          |
| (1,418) | 1:12:A:LEU:HD11 | 1:12:A:LEU:HD22 | 5        | 0.16          |
| (1,418) | 1:12:A:LEU:HD11 | 1:12:A:LEU:HD23 | 5        | 0.16          |
| (1,418) | 1:12:A:LEU:HD12 | 1:12:A:LEU:HD21 | 5        | 0.16          |
| (1,418) | 1:12:A:LEU:HD12 | 1:12:A:LEU:HD22 | 5        | 0.16          |
| (1,418) | 1:12:A:LEU:HD12 | 1:12:A:LEU:HD23 | 5        | 0.16          |
| (1,418) | 1:12:A:LEU:HD13 | 1:12:A:LEU:HD21 | 5        | 0.16          |
| (1,418) | 1:12:A:LEU:HD13 | 1:12:A:LEU:HD22 | 5        | 0.16          |
| (1,418) | 1:12:A:LEU:HD13 | 1:12:A:LEU:HD23 | 5        | 0.16          |
| (1,408) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD11 | 1        | 0.16          |
| (1,408) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD12 | 1        | 0.16          |
| (1,408) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD13 | 1        | 0.16          |
| (1,408) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD11 | 9        | 0.16          |
| (1,408) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD12 | 9        | 0.16          |
| (1,408) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD13 | 9        | 0.16          |
| (1,397) | 1:10:A:GLN:HB2  | 1:10:A:GLN:HG2  | 4        | 0.16          |
| (1,375) | 1:8:A:TYR:HA    | 1:8:A:TYR:HB2   | 6        | 0.16          |
| (1,375) | 1:8:A:TYR:HA    | 1:8:A:TYR:HB3   | 6        | 0.16          |
| (1,372) | 1:7:A:LEU:HB2   | 1:7:A:LEU:HB3   | 3        | 0.16          |
| (1,372) | 1:7:A:LEU:HB2   | 1:7:A:LEU:HB3   | 10       | 0.16          |
| (1,341) | 1:5:A:VAL:HA    | 1:5:A:VAL:HG21  | 1        | 0.16          |
| (1,341) | 1:5:A:VAL:HA    | 1:5:A:VAL:HG22  | 1        | 0.16          |
| (1,341) | 1:5:A:VAL:HA    | 1:5:A:VAL:HG23  | 1        | 0.16          |
| (1,341) | 1:5:A:VAL:HA    | 1:5:A:VAL:HG21  | 3        | 0.16          |
| (1,341) | 1:5:A:VAL:HA    | 1:5:A:VAL:HG22  | 3        | 0.16          |
| (1,341) | 1:5:A:VAL:HA    | 1:5:A:VAL:HG23  | 3        | 0.16          |
| (1,341) | 1:5:A:VAL:HA    | 1:5:A:VAL:HG21  | 5        | 0.16          |
| (1,341) | 1:5:A:VAL:HA    | 1:5:A:VAL:HG22  | 5        | 0.16          |
| (1,341) | 1:5:A:VAL:HA    | 1:5:A:VAL:HG23  | 5        | 0.16          |
| (1,341) | 1:5:A:VAL:HA    | 1:5:A:VAL:HG21  | 7        | 0.16          |
| (1,341) | 1:5:A:VAL:HA    | 1:5:A:VAL:HG22  | 7        | 0.16          |
| (1,341) | 1:5:A:VAL:HA    | 1:5:A:VAL:HG23  | 7        | 0.16          |
| (1,339) | 1:4:A:CYS:HB2   | 1:4:A:CYS:HB3   | 1        | 0.16          |
| (1,339) | 1:4:A:CYS:HB2   | 1:4:A:CYS:HB3   | 2        | 0.16          |
| (1,339) | 1:4:A:CYS:HB2   | 1:4:A:CYS:HB3   | 5        | 0.16          |
| (1,339) | 1:4:A:CYS:HB2   | 1:4:A:CYS:HB3   | 7        | 0.16          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,339) | 1:4:A:CYS:HB2   | 1:4:A:CYS:HB3  | 8        | 0.16          |
| (1,339) | 1:4:A:CYS:HB2   | 1:4:A:CYS:HB3  | 9        | 0.16          |
| (1,335) | 1:3:A:GLU:HA    | 1:3:A:GLU:HB2  | 1        | 0.16          |
| (1,335) | 1:3:A:GLU:HA    | 1:3:A:GLU:HB3  | 1        | 0.16          |
| (1,335) | 1:3:A:GLU:HA    | 1:3:A:GLU:HB2  | 6        | 0.16          |
| (1,335) | 1:3:A:GLU:HA    | 1:3:A:GLU:HB3  | 6        | 0.16          |
| (1,335) | 1:3:A:GLU:HA    | 1:3:A:GLU:HB2  | 7        | 0.16          |
| (1,335) | 1:3:A:GLU:HA    | 1:3:A:GLU:HB3  | 7        | 0.16          |
| (1,335) | 1:3:A:GLU:HA    | 1:3:A:GLU:HB2  | 10       | 0.16          |
| (1,335) | 1:3:A:GLU:HA    | 1:3:A:GLU:HB3  | 10       | 0.16          |
| (1,331) | 1:2:A:GLU:HB2   | 1:2:A:GLU:HG3  | 4        | 0.16          |
| (1,255) | 1:11:A:TRP:HH2  | 1:17:A:PRO:HB2 | 6        | 0.16          |
| (1,254) | 1:11:A:TRP:HZ2  | 1:17:A:PRO:HB2 | 9        | 0.16          |
| (1,254) | 1:11:A:TRP:HZ2  | 1:17:A:PRO:HB2 | 10       | 0.16          |
| (1,232) | 1:11:A:TRP:HE3  | 1:12:A:LEU:HG  | 6        | 0.16          |
| (1,226) | 1:11:A:TRP:HH2  | 1:23:A:PRO:HG2 | 6        | 0.16          |
| (1,195) | 1:8:A:TYR:HE1   | 1:24:A:PRO:HD3 | 1        | 0.16          |
| (1,195) | 1:8:A:TYR:HE2   | 1:24:A:PRO:HD3 | 1        | 0.16          |
| (1,195) | 1:8:A:TYR:HE1   | 1:24:A:PRO:HD3 | 2        | 0.16          |
| (1,195) | 1:8:A:TYR:HE2   | 1:24:A:PRO:HD3 | 2        | 0.16          |
| (1,195) | 1:8:A:TYR:HE1   | 1:24:A:PRO:HD3 | 9        | 0.16          |
| (1,195) | 1:8:A:TYR:HE2   | 1:24:A:PRO:HD3 | 9        | 0.16          |
| (1,177) | 1:8:A:TYR:HD1   | 1:12:A:LEU:HA  | 4        | 0.16          |
| (1,177) | 1:8:A:TYR:HD2   | 1:12:A:LEU:HA  | 4        | 0.16          |
| (1,155) | 1:7:A:LEU:H     | 1:7:A:LEU:HD11 | 5        | 0.16          |
| (1,155) | 1:7:A:LEU:H     | 1:7:A:LEU:HD12 | 5        | 0.16          |
| (1,155) | 1:7:A:LEU:H     | 1:7:A:LEU:HD13 | 5        | 0.16          |
| (1,155) | 1:7:A:LEU:H     | 1:7:A:LEU:HD21 | 5        | 0.16          |
| (1,155) | 1:7:A:LEU:H     | 1:7:A:LEU:HD22 | 5        | 0.16          |
| (1,155) | 1:7:A:LEU:H     | 1:7:A:LEU:HD23 | 5        | 0.16          |
| (1,115) | 1:9:A:ILE:H     | 1:9:A:ILE:HG13 | 4        | 0.16          |
| (1,98)  | 1:11:A:TRP:HE1  | 1:19:A:SER:HG  | 4        | 0.16          |
| (1,21)  | 1:12:A:LEU:HB2  | 1:13:A:LYS:H   | 4        | 0.16          |
| (1,21)  | 1:12:A:LEU:HB2  | 1:13:A:LYS:H   | 7        | 0.16          |
| (1,21)  | 1:12:A:LEU:HB2  | 1:13:A:LYS:H   | 10       | 0.16          |
| (1,720) | 1:7:A:LEU:HB2   | 1:24:A:PRO:HB2 | 2        | 0.15          |
| (1,720) | 1:7:A:LEU:HB2   | 1:24:A:PRO:HB2 | 4        | 0.15          |
| (1,717) | 1:12:A:LEU:HD11 | 1:16:A:GLY:HA2 | 7        | 0.15          |
| (1,717) | 1:12:A:LEU:HD12 | 1:16:A:GLY:HA2 | 7        | 0.15          |
| (1,717) | 1:12:A:LEU:HD13 | 1:16:A:GLY:HA2 | 7        | 0.15          |
| (1,717) | 1:12:A:LEU:HD11 | 1:16:A:GLY:HA2 | 10       | 0.15          |
| (1,717) | 1:12:A:LEU:HD12 | 1:16:A:GLY:HA2 | 10       | 0.15          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,717) | 1:12:A:LEU:HD13 | 1:16:A:GLY:HA2  | 10       | 0.15          |
| (1,706) | 1:6:A:ARG:HG3   | 1:7:A:LEU:HD11  | 5        | 0.15          |
| (1,706) | 1:6:A:ARG:HG3   | 1:7:A:LEU:HD12  | 5        | 0.15          |
| (1,706) | 1:6:A:ARG:HG3   | 1:7:A:LEU:HD13  | 5        | 0.15          |
| (1,706) | 1:6:A:ARG:HG3   | 1:7:A:LEU:HD21  | 5        | 0.15          |
| (1,706) | 1:6:A:ARG:HG3   | 1:7:A:LEU:HD22  | 5        | 0.15          |
| (1,706) | 1:6:A:ARG:HG3   | 1:7:A:LEU:HD23  | 5        | 0.15          |
| (1,706) | 1:6:A:ARG:HG3   | 1:7:A:LEU:HD11  | 8        | 0.15          |
| (1,706) | 1:6:A:ARG:HG3   | 1:7:A:LEU:HD12  | 8        | 0.15          |
| (1,706) | 1:6:A:ARG:HG3   | 1:7:A:LEU:HD13  | 8        | 0.15          |
| (1,706) | 1:6:A:ARG:HG3   | 1:7:A:LEU:HD21  | 8        | 0.15          |
| (1,706) | 1:6:A:ARG:HG3   | 1:7:A:LEU:HD22  | 8        | 0.15          |
| (1,706) | 1:6:A:ARG:HG3   | 1:7:A:LEU:HD23  | 8        | 0.15          |
| (1,695) | 1:5:A:VAL:HG11  | 1:9:A:ILE:HB    | 7        | 0.15          |
| (1,695) | 1:5:A:VAL:HG12  | 1:9:A:ILE:HB    | 7        | 0.15          |
| (1,695) | 1:5:A:VAL:HG13  | 1:9:A:ILE:HB    | 7        | 0.15          |
| (1,694) | 1:9:A:ILE:HG21  | 1:12:A:LEU:HB3  | 3        | 0.15          |
| (1,694) | 1:9:A:ILE:HG22  | 1:12:A:LEU:HB3  | 3        | 0.15          |
| (1,694) | 1:9:A:ILE:HG23  | 1:12:A:LEU:HB3  | 3        | 0.15          |
| (1,677) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD11 | 10       | 0.15          |
| (1,677) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD12 | 10       | 0.15          |
| (1,677) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD13 | 10       | 0.15          |
| (1,641) | 1:8:A:TYR:HD1   | 1:25:A:CYS:HB3  | 5        | 0.15          |
| (1,641) | 1:8:A:TYR:HD2   | 1:25:A:CYS:HB3  | 5        | 0.15          |
| (1,601) | 1:10:A:GLN:H    | 1:12:A:LEU:H    | 2        | 0.15          |
| (1,601) | 1:10:A:GLN:H    | 1:12:A:LEU:H    | 5        | 0.15          |
| (1,581) | 1:5:A:VAL:HG11  | 1:6:A:ARG:HA    | 1        | 0.15          |
| (1,581) | 1:5:A:VAL:HG12  | 1:6:A:ARG:HA    | 1        | 0.15          |
| (1,581) | 1:5:A:VAL:HG13  | 1:6:A:ARG:HA    | 1        | 0.15          |
| (1,552) | 1:11:A:TRP:HB2  | 1:24:A:PRO:HD2  | 5        | 0.15          |
| (1,552) | 1:11:A:TRP:HB2  | 1:24:A:PRO:HD2  | 6        | 0.15          |
| (1,537) | 1:23:A:PRO:HB2  | 1:24:A:PRO:HD2  | 10       | 0.15          |
| (1,524) | 1:24:A:PRO:HD2  | 1:24:A:PRO:HD3  | 3        | 0.15          |
| (1,524) | 1:24:A:PRO:HD2  | 1:24:A:PRO:HD3  | 4        | 0.15          |
| (1,524) | 1:24:A:PRO:HD2  | 1:24:A:PRO:HD3  | 6        | 0.15          |
| (1,524) | 1:24:A:PRO:HD2  | 1:24:A:PRO:HD3  | 7        | 0.15          |
| (1,524) | 1:24:A:PRO:HD2  | 1:24:A:PRO:HD3  | 9        | 0.15          |
| (1,524) | 1:24:A:PRO:HD2  | 1:24:A:PRO:HD3  | 10       | 0.15          |
| (1,520) | 1:24:A:PRO:HA   | 1:24:A:PRO:HB3  | 1        | 0.15          |
| (1,520) | 1:24:A:PRO:HA   | 1:24:A:PRO:HB3  | 2        | 0.15          |
| (1,520) | 1:24:A:PRO:HA   | 1:24:A:PRO:HB3  | 5        | 0.15          |
| (1,520) | 1:24:A:PRO:HA   | 1:24:A:PRO:HB3  | 6        | 0.15          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,520) | 1:24:A:PRO:HA   | 1:24:A:PRO:HB3  | 10       | 0.15          |
| (1,497) | 1:23:A:PRO:HA   | 1:23:A:PRO:HB2  | 5        | 0.15          |
| (1,497) | 1:23:A:PRO:HA   | 1:23:A:PRO:HB2  | 8        | 0.15          |
| (1,497) | 1:23:A:PRO:HA   | 1:23:A:PRO:HB2  | 10       | 0.15          |
| (1,478) | 1:22:A:PRO:HD2  | 1:22:A:PRO:HD3  | 3        | 0.15          |
| (1,478) | 1:22:A:PRO:HD2  | 1:22:A:PRO:HD3  | 8        | 0.15          |
| (1,478) | 1:22:A:PRO:HD2  | 1:22:A:PRO:HD3  | 10       | 0.15          |
| (1,418) | 1:12:A:LEU:HD11 | 1:12:A:LEU:HD21 | 6        | 0.15          |
| (1,418) | 1:12:A:LEU:HD11 | 1:12:A:LEU:HD22 | 6        | 0.15          |
| (1,418) | 1:12:A:LEU:HD11 | 1:12:A:LEU:HD23 | 6        | 0.15          |
| (1,418) | 1:12:A:LEU:HD12 | 1:12:A:LEU:HD21 | 6        | 0.15          |
| (1,418) | 1:12:A:LEU:HD12 | 1:12:A:LEU:HD22 | 6        | 0.15          |
| (1,418) | 1:12:A:LEU:HD12 | 1:12:A:LEU:HD23 | 6        | 0.15          |
| (1,418) | 1:12:A:LEU:HD13 | 1:12:A:LEU:HD21 | 6        | 0.15          |
| (1,418) | 1:12:A:LEU:HD13 | 1:12:A:LEU:HD22 | 6        | 0.15          |
| (1,418) | 1:12:A:LEU:HD13 | 1:12:A:LEU:HD23 | 6        | 0.15          |
| (1,372) | 1:7:A:LEU:HB2   | 1:7:A:LEU:HB3   | 1        | 0.15          |
| (1,372) | 1:7:A:LEU:HB2   | 1:7:A:LEU:HB3   | 2        | 0.15          |
| (1,372) | 1:7:A:LEU:HB2   | 1:7:A:LEU:HB3   | 4        | 0.15          |
| (1,372) | 1:7:A:LEU:HB2   | 1:7:A:LEU:HB3   | 5        | 0.15          |
| (1,372) | 1:7:A:LEU:HB2   | 1:7:A:LEU:HB3   | 6        | 0.15          |
| (1,372) | 1:7:A:LEU:HB2   | 1:7:A:LEU:HB3   | 7        | 0.15          |
| (1,372) | 1:7:A:LEU:HB2   | 1:7:A:LEU:HB3   | 8        | 0.15          |
| (1,372) | 1:7:A:LEU:HB2   | 1:7:A:LEU:HB3   | 9        | 0.15          |
| (1,341) | 1:5:A:VAL:HA    | 1:5:A:VAL:HG21  | 10       | 0.15          |
| (1,341) | 1:5:A:VAL:HA    | 1:5:A:VAL:HG22  | 10       | 0.15          |
| (1,341) | 1:5:A:VAL:HA    | 1:5:A:VAL:HG23  | 10       | 0.15          |
| (1,335) | 1:3:A:GLU:HA    | 1:3:A:GLU:HB2   | 8        | 0.15          |
| (1,335) | 1:3:A:GLU:HA    | 1:3:A:GLU:HB3   | 8        | 0.15          |
| (1,263) | 1:18:A:SER:HA   | 1:20:A:GLY:H    | 10       | 0.15          |
| (1,254) | 1:11:A:TRP:HZ2  | 1:17:A:PRO:HB2  | 6        | 0.15          |
| (1,254) | 1:11:A:TRP:HZ2  | 1:17:A:PRO:HB2  | 7        | 0.15          |
| (1,226) | 1:11:A:TRP:HH2  | 1:23:A:PRO:HG2  | 1        | 0.15          |
| (1,220) | 1:8:A:TYR:HD1   | 1:9:A:ILE:HG12  | 2        | 0.15          |
| (1,220) | 1:8:A:TYR:HD2   | 1:9:A:ILE:HG12  | 2        | 0.15          |
| (1,195) | 1:8:A:TYR:HE1   | 1:24:A:PRO:HD3  | 4        | 0.15          |
| (1,195) | 1:8:A:TYR:HE2   | 1:24:A:PRO:HD3  | 4        | 0.15          |
| (1,108) | 1:14:A:ASP:H    | 1:15:A:GLY:H    | 5        | 0.15          |
| (1,94)  | 1:20:A:GLY:HA3  | 1:21:A:ARG:H    | 1        | 0.15          |
| (1,65)  | 1:20:A:GLY:H    | 1:20:A:GLY:HA2  | 2        | 0.15          |
| (1,21)  | 1:12:A:LEU:HB2  | 1:13:A:LYS:H    | 6        | 0.15          |
| (1,21)  | 1:12:A:LEU:HB2  | 1:13:A:LYS:H    | 8        | 0.15          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,719) | 1:9:A:ILE:HG12  | 1:12:A:LEU:HG   | 2        | 0.14          |
| (1,717) | 1:12:A:LEU:HD11 | 1:16:A:GLY:HA2  | 4        | 0.14          |
| (1,717) | 1:12:A:LEU:HD12 | 1:16:A:GLY:HA2  | 4        | 0.14          |
| (1,717) | 1:12:A:LEU:HD13 | 1:16:A:GLY:HA2  | 4        | 0.14          |
| (1,716) | 1:9:A:ILE:HG12  | 1:12:A:LEU:HD11 | 7        | 0.14          |
| (1,716) | 1:9:A:ILE:HG12  | 1:12:A:LEU:HD12 | 7        | 0.14          |
| (1,716) | 1:9:A:ILE:HG12  | 1:12:A:LEU:HD13 | 7        | 0.14          |
| (1,706) | 1:6:A:ARG:HG3   | 1:7:A:LEU:HD11  | 6        | 0.14          |
| (1,706) | 1:6:A:ARG:HG3   | 1:7:A:LEU:HD12  | 6        | 0.14          |
| (1,706) | 1:6:A:ARG:HG3   | 1:7:A:LEU:HD13  | 6        | 0.14          |
| (1,706) | 1:6:A:ARG:HG3   | 1:7:A:LEU:HD21  | 6        | 0.14          |
| (1,706) | 1:6:A:ARG:HG3   | 1:7:A:LEU:HD22  | 6        | 0.14          |
| (1,706) | 1:6:A:ARG:HG3   | 1:7:A:LEU:HD23  | 6        | 0.14          |
| (1,706) | 1:6:A:ARG:HG3   | 1:7:A:LEU:HD11  | 10       | 0.14          |
| (1,706) | 1:6:A:ARG:HG3   | 1:7:A:LEU:HD12  | 10       | 0.14          |
| (1,706) | 1:6:A:ARG:HG3   | 1:7:A:LEU:HD13  | 10       | 0.14          |
| (1,706) | 1:6:A:ARG:HG3   | 1:7:A:LEU:HD21  | 10       | 0.14          |
| (1,706) | 1:6:A:ARG:HG3   | 1:7:A:LEU:HD22  | 10       | 0.14          |
| (1,706) | 1:6:A:ARG:HG3   | 1:7:A:LEU:HD23  | 10       | 0.14          |
| (1,646) | 1:15:A:GLY:HA2  | 1:18:A:SER:HB3  | 5        | 0.14          |
| (1,642) | 1:8:A:TYR:HD1   | 1:25:A:CYS:HB2  | 8        | 0.14          |
| (1,642) | 1:8:A:TYR:HD2   | 1:25:A:CYS:HB2  | 8        | 0.14          |
| (1,641) | 1:8:A:TYR:HD1   | 1:25:A:CYS:HB3  | 1        | 0.14          |
| (1,641) | 1:8:A:TYR:HD2   | 1:25:A:CYS:HB3  | 1        | 0.14          |
| (1,634) | 1:11:A:TRP:HE3  | 1:23:A:PRO:HB2  | 6        | 0.14          |
| (1,614) | 1:19:A:SER:HG   | 1:20:A:GLY:H    | 3        | 0.14          |
| (1,601) | 1:10:A:GLN:H    | 1:12:A:LEU:H    | 1        | 0.14          |
| (1,601) | 1:10:A:GLN:H    | 1:12:A:LEU:H    | 6        | 0.14          |
| (1,593) | 1:11:A:TRP:HA   | 1:14:A:ASP:HB3  | 2        | 0.14          |
| (1,581) | 1:5:A:VAL:HG11  | 1:6:A:ARG:HA    | 7        | 0.14          |
| (1,581) | 1:5:A:VAL:HG12  | 1:6:A:ARG:HA    | 7        | 0.14          |
| (1,581) | 1:5:A:VAL:HG13  | 1:6:A:ARG:HA    | 7        | 0.14          |
| (1,552) | 1:11:A:TRP:HB2  | 1:24:A:PRO:HD2  | 2        | 0.14          |
| (1,537) | 1:23:A:PRO:HB2  | 1:24:A:PRO:HD2  | 9        | 0.14          |
| (1,520) | 1:24:A:PRO:HA   | 1:24:A:PRO:HB3  | 4        | 0.14          |
| (1,520) | 1:24:A:PRO:HA   | 1:24:A:PRO:HB3  | 8        | 0.14          |
| (1,520) | 1:24:A:PRO:HA   | 1:24:A:PRO:HB3  | 9        | 0.14          |
| (1,515) | 1:23:A:PRO:HB2  | 1:23:A:PRO:HG2  | 4        | 0.14          |
| (1,515) | 1:23:A:PRO:HB2  | 1:23:A:PRO:HG2  | 7        | 0.14          |
| (1,497) | 1:23:A:PRO:HA   | 1:23:A:PRO:HB2  | 9        | 0.14          |
| (1,478) | 1:22:A:PRO:HD2  | 1:22:A:PRO:HD3  | 1        | 0.14          |
| (1,478) | 1:22:A:PRO:HD2  | 1:22:A:PRO:HD3  | 2        | 0.14          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,478) | 1:22:A:PRO:HD2 | 1:22:A:PRO:HD3 | 4        | 0.14          |
| (1,478) | 1:22:A:PRO:HD2 | 1:22:A:PRO:HD3 | 5        | 0.14          |
| (1,478) | 1:22:A:PRO:HD2 | 1:22:A:PRO:HD3 | 6        | 0.14          |
| (1,478) | 1:22:A:PRO:HD2 | 1:22:A:PRO:HD3 | 7        | 0.14          |
| (1,478) | 1:22:A:PRO:HD2 | 1:22:A:PRO:HD3 | 9        | 0.14          |
| (1,471) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HG2 | 3        | 0.14          |
| (1,471) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HG3 | 3        | 0.14          |
| (1,471) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HG2 | 8        | 0.14          |
| (1,471) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HG3 | 8        | 0.14          |
| (1,453) | 1:19:A:SER:HA  | 1:19:A:SER:HB2 | 5        | 0.14          |
| (1,453) | 1:19:A:SER:HA  | 1:19:A:SER:HB2 | 6        | 0.14          |
| (1,390) | 1:9:A:ILE:HG12 | 1:9:A:ILE:HG21 | 5        | 0.14          |
| (1,390) | 1:9:A:ILE:HG12 | 1:9:A:ILE:HG22 | 5        | 0.14          |
| (1,390) | 1:9:A:ILE:HG12 | 1:9:A:ILE:HG23 | 5        | 0.14          |
| (1,341) | 1:5:A:VAL:HA   | 1:5:A:VAL:HG21 | 4        | 0.14          |
| (1,341) | 1:5:A:VAL:HA   | 1:5:A:VAL:HG22 | 4        | 0.14          |
| (1,341) | 1:5:A:VAL:HA   | 1:5:A:VAL:HG23 | 4        | 0.14          |
| (1,341) | 1:5:A:VAL:HA   | 1:5:A:VAL:HG21 | 8        | 0.14          |
| (1,341) | 1:5:A:VAL:HA   | 1:5:A:VAL:HG22 | 8        | 0.14          |
| (1,341) | 1:5:A:VAL:HA   | 1:5:A:VAL:HG23 | 8        | 0.14          |
| (1,335) | 1:3:A:GLU:HA   | 1:3:A:GLU:HB2  | 4        | 0.14          |
| (1,335) | 1:3:A:GLU:HA   | 1:3:A:GLU:HB3  | 4        | 0.14          |
| (1,335) | 1:3:A:GLU:HA   | 1:3:A:GLU:HB2  | 9        | 0.14          |
| (1,335) | 1:3:A:GLU:HA   | 1:3:A:GLU:HB3  | 9        | 0.14          |
| (1,254) | 1:11:A:TRP:HZ2 | 1:17:A:PRO:HB2 | 4        | 0.14          |
| (1,251) | 1:8:A:TYR:HE1  | 1:23:A:PRO:HA  | 3        | 0.14          |
| (1,251) | 1:8:A:TYR:HE2  | 1:23:A:PRO:HA  | 3        | 0.14          |
| (1,195) | 1:8:A:TYR:HE1  | 1:24:A:PRO:HD3 | 7        | 0.14          |
| (1,195) | 1:8:A:TYR:HE2  | 1:24:A:PRO:HD3 | 7        | 0.14          |
| (1,195) | 1:8:A:TYR:HE1  | 1:24:A:PRO:HD3 | 10       | 0.14          |
| (1,195) | 1:8:A:TYR:HE2  | 1:24:A:PRO:HD3 | 10       | 0.14          |
| (1,155) | 1:7:A:LEU:H    | 1:7:A:LEU:HD11 | 1        | 0.14          |
| (1,155) | 1:7:A:LEU:H    | 1:7:A:LEU:HD12 | 1        | 0.14          |
| (1,155) | 1:7:A:LEU:H    | 1:7:A:LEU:HD13 | 1        | 0.14          |
| (1,155) | 1:7:A:LEU:H    | 1:7:A:LEU:HD21 | 1        | 0.14          |
| (1,155) | 1:7:A:LEU:H    | 1:7:A:LEU:HD22 | 1        | 0.14          |
| (1,155) | 1:7:A:LEU:H    | 1:7:A:LEU:HD23 | 1        | 0.14          |
| (1,155) | 1:7:A:LEU:H    | 1:7:A:LEU:HD11 | 9        | 0.14          |
| (1,155) | 1:7:A:LEU:H    | 1:7:A:LEU:HD12 | 9        | 0.14          |
| (1,155) | 1:7:A:LEU:H    | 1:7:A:LEU:HD13 | 9        | 0.14          |
| (1,155) | 1:7:A:LEU:H    | 1:7:A:LEU:HD21 | 9        | 0.14          |
| (1,155) | 1:7:A:LEU:H    | 1:7:A:LEU:HD22 | 9        | 0.14          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,155) | 1:7:A:LEU:H    | 1:7:A:LEU:HD23  | 9        | 0.14          |
| (1,152) | 1:8:A:TYR:HB2  | 1:9:A:ILE:H     | 3        | 0.14          |
| (1,152) | 1:8:A:TYR:HB3  | 1:9:A:ILE:H     | 3        | 0.14          |
| (1,115) | 1:9:A:ILE:H    | 1:9:A:ILE:HG13  | 9        | 0.14          |
| (1,75)  | 1:25:A:CYS:H   | 1:25:A:CYS:HB2  | 7        | 0.14          |
| (1,21)  | 1:12:A:LEU:HB2 | 1:13:A:LYS:H    | 3        | 0.14          |
| (1,21)  | 1:12:A:LEU:HB2 | 1:13:A:LYS:H    | 5        | 0.14          |
| (1,21)  | 1:12:A:LEU:HB2 | 1:13:A:LYS:H    | 9        | 0.14          |
| (1,719) | 1:9:A:ILE:HG12 | 1:12:A:LEU:HG   | 5        | 0.13          |
| (1,706) | 1:6:A:ARG:HG3  | 1:7:A:LEU:HD11  | 4        | 0.13          |
| (1,706) | 1:6:A:ARG:HG3  | 1:7:A:LEU:HD12  | 4        | 0.13          |
| (1,706) | 1:6:A:ARG:HG3  | 1:7:A:LEU:HD13  | 4        | 0.13          |
| (1,706) | 1:6:A:ARG:HG3  | 1:7:A:LEU:HD21  | 4        | 0.13          |
| (1,706) | 1:6:A:ARG:HG3  | 1:7:A:LEU:HD22  | 4        | 0.13          |
| (1,706) | 1:6:A:ARG:HG3  | 1:7:A:LEU:HD23  | 4        | 0.13          |
| (1,633) | 1:11:A:TRP:HZ3 | 1:23:A:PRO:HB2  | 3        | 0.13          |
| (1,615) | 1:16:A:GLY:H   | 1:19:A:SER:HB3  | 6        | 0.13          |
| (1,615) | 1:16:A:GLY:H   | 1:19:A:SER:HB3  | 8        | 0.13          |
| (1,598) | 1:1:A:GLU:HA   | 1:1:A:GLU:HB3   | 7        | 0.13          |
| (1,598) | 1:1:A:GLU:HA   | 1:1:A:GLU:HB3   | 9        | 0.13          |
| (1,581) | 1:5:A:VAL:HG11 | 1:6:A:ARG:HA    | 5        | 0.13          |
| (1,581) | 1:5:A:VAL:HG12 | 1:6:A:ARG:HA    | 5        | 0.13          |
| (1,581) | 1:5:A:VAL:HG13 | 1:6:A:ARG:HA    | 5        | 0.13          |
| (1,551) | 1:16:A:GLY:HA3 | 1:17:A:PRO:HD3  | 1        | 0.13          |
| (1,551) | 1:16:A:GLY:HA3 | 1:17:A:PRO:HD3  | 9        | 0.13          |
| (1,537) | 1:23:A:PRO:HB2 | 1:24:A:PRO:HD2  | 6        | 0.13          |
| (1,520) | 1:24:A:PRO:HA  | 1:24:A:PRO:HB3  | 7        | 0.13          |
| (1,469) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HB3  | 1        | 0.13          |
| (1,469) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HB3  | 4        | 0.13          |
| (1,469) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HB3  | 7        | 0.13          |
| (1,464) | 1:21:A:ARG:HB3 | 1:21:A:ARG:HD2  | 7        | 0.13          |
| (1,453) | 1:19:A:SER:HA  | 1:19:A:SER:HB2  | 1        | 0.13          |
| (1,435) | 1:17:A:PRO:HA  | 1:17:A:PRO:HD2  | 1        | 0.13          |
| (1,435) | 1:17:A:PRO:HA  | 1:17:A:PRO:HD2  | 2        | 0.13          |
| (1,435) | 1:17:A:PRO:HA  | 1:17:A:PRO:HD2  | 3        | 0.13          |
| (1,435) | 1:17:A:PRO:HA  | 1:17:A:PRO:HD2  | 4        | 0.13          |
| (1,435) | 1:17:A:PRO:HA  | 1:17:A:PRO:HD2  | 6        | 0.13          |
| (1,435) | 1:17:A:PRO:HA  | 1:17:A:PRO:HD2  | 7        | 0.13          |
| (1,435) | 1:17:A:PRO:HA  | 1:17:A:PRO:HD2  | 8        | 0.13          |
| (1,435) | 1:17:A:PRO:HA  | 1:17:A:PRO:HD2  | 10       | 0.13          |
| (1,408) | 1:12:A:LEU:HA  | 1:12:A:LEU:HD11 | 4        | 0.13          |
| (1,408) | 1:12:A:LEU:HA  | 1:12:A:LEU:HD12 | 4        | 0.13          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,408) | 1:12:A:LEU:HA  | 1:12:A:LEU:HD13 | 4        | 0.13          |
| (1,408) | 1:12:A:LEU:HA  | 1:12:A:LEU:HD11 | 7        | 0.13          |
| (1,408) | 1:12:A:LEU:HA  | 1:12:A:LEU:HD12 | 7        | 0.13          |
| (1,408) | 1:12:A:LEU:HA  | 1:12:A:LEU:HD13 | 7        | 0.13          |
| (1,394) | 1:10:A:GLN:HA  | 1:10:A:GLN:HB2  | 5        | 0.13          |
| (1,394) | 1:10:A:GLN:HA  | 1:10:A:GLN:HB2  | 6        | 0.13          |
| (1,390) | 1:9:A:ILE:HG12 | 1:9:A:ILE:HG21  | 6        | 0.13          |
| (1,390) | 1:9:A:ILE:HG12 | 1:9:A:ILE:HG22  | 6        | 0.13          |
| (1,390) | 1:9:A:ILE:HG12 | 1:9:A:ILE:HG23  | 6        | 0.13          |
| (1,344) | 1:5:A:VAL:HB   | 1:5:A:VAL:HG11  | 3        | 0.13          |
| (1,344) | 1:5:A:VAL:HB   | 1:5:A:VAL:HG12  | 3        | 0.13          |
| (1,344) | 1:5:A:VAL:HB   | 1:5:A:VAL:HG13  | 3        | 0.13          |
| (1,344) | 1:5:A:VAL:HB   | 1:5:A:VAL:HG11  | 5        | 0.13          |
| (1,344) | 1:5:A:VAL:HB   | 1:5:A:VAL:HG12  | 5        | 0.13          |
| (1,344) | 1:5:A:VAL:HB   | 1:5:A:VAL:HG13  | 5        | 0.13          |
| (1,341) | 1:5:A:VAL:HA   | 1:5:A:VAL:HG21  | 2        | 0.13          |
| (1,341) | 1:5:A:VAL:HA   | 1:5:A:VAL:HG22  | 2        | 0.13          |
| (1,341) | 1:5:A:VAL:HA   | 1:5:A:VAL:HG23  | 2        | 0.13          |
| (1,341) | 1:5:A:VAL:HA   | 1:5:A:VAL:HG21  | 6        | 0.13          |
| (1,341) | 1:5:A:VAL:HA   | 1:5:A:VAL:HG22  | 6        | 0.13          |
| (1,341) | 1:5:A:VAL:HA   | 1:5:A:VAL:HG23  | 6        | 0.13          |
| (1,284) | 1:2:A:GLU:HA   | 1:3:A:GLU:H     | 6        | 0.13          |
| (1,255) | 1:11:A:TRP:HH2 | 1:17:A:PRO:HB2  | 10       | 0.13          |
| (1,200) | 1:11:A:TRP:HE3 | 1:23:A:PRO:HB3  | 10       | 0.13          |
| (1,199) | 1:8:A:TYR:HD1  | 1:23:A:PRO:HB3  | 2        | 0.13          |
| (1,199) | 1:8:A:TYR:HD2  | 1:23:A:PRO:HB3  | 2        | 0.13          |
| (1,152) | 1:8:A:TYR:HB2  | 1:9:A:ILE:H     | 10       | 0.13          |
| (1,152) | 1:8:A:TYR:HB3  | 1:9:A:ILE:H     | 10       | 0.13          |
| (1,123) | 1:24:A:PRO:HG2 | 1:25:A:CYS:H    | 5        | 0.13          |
| (1,75)  | 1:25:A:CYS:H   | 1:25:A:CYS:HB2  | 8        | 0.13          |
| (1,44)  | 1:14:A:ASP:H   | 1:14:A:ASP:HB3  | 7        | 0.13          |
| (1,16)  | 1:5:A:VAL:H    | 1:5:A:VAL:HG21  | 8        | 0.13          |
| (1,16)  | 1:5:A:VAL:H    | 1:5:A:VAL:HG22  | 8        | 0.13          |
| (1,16)  | 1:5:A:VAL:H    | 1:5:A:VAL:HG23  | 8        | 0.13          |
| (1,8)   | 1:5:A:VAL:H    | 1:5:A:VAL:HG21  | 8        | 0.13          |
| (1,8)   | 1:5:A:VAL:H    | 1:5:A:VAL:HG22  | 8        | 0.13          |
| (1,8)   | 1:5:A:VAL:H    | 1:5:A:VAL:HG23  | 8        | 0.13          |
| (1,706) | 1:6:A:ARG:HG3  | 1:7:A:LEU:HD11  | 3        | 0.12          |
| (1,706) | 1:6:A:ARG:HG3  | 1:7:A:LEU:HD12  | 3        | 0.12          |
| (1,706) | 1:6:A:ARG:HG3  | 1:7:A:LEU:HD13  | 3        | 0.12          |
| (1,706) | 1:6:A:ARG:HG3  | 1:7:A:LEU:HD21  | 3        | 0.12          |
| (1,706) | 1:6:A:ARG:HG3  | 1:7:A:LEU:HD22  | 3        | 0.12          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,706) | 1:6:A:ARG:HG3  | 1:7:A:LEU:HD23 | 3        | 0.12          |
| (1,682) | 1:4:A:CYS:HB2  | 1:5:A:VAL:HG11 | 10       | 0.12          |
| (1,682) | 1:4:A:CYS:HB2  | 1:5:A:VAL:HG12 | 10       | 0.12          |
| (1,682) | 1:4:A:CYS:HB2  | 1:5:A:VAL:HG13 | 10       | 0.12          |
| (1,664) | 1:21:A:ARG:HB3 | 1:22:A:PRO:HD2 | 6        | 0.12          |
| (1,641) | 1:8:A:TYR:HD1  | 1:25:A:CYS:HB3 | 7        | 0.12          |
| (1,641) | 1:8:A:TYR:HD2  | 1:25:A:CYS:HB3 | 7        | 0.12          |
| (1,633) | 1:11:A:TRP:HZ3 | 1:23:A:PRO:HB2 | 5        | 0.12          |
| (1,554) | 1:22:A:PRO:HB3 | 1:23:A:PRO:HD2 | 10       | 0.12          |
| (1,537) | 1:23:A:PRO:HB2 | 1:24:A:PRO:HD2 | 8        | 0.12          |
| (1,532) | 1:24:A:PRO:HB3 | 1:24:A:PRO:HG2 | 3        | 0.12          |
| (1,520) | 1:24:A:PRO:HA  | 1:24:A:PRO:HB3 | 3        | 0.12          |
| (1,469) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HB3 | 2        | 0.12          |
| (1,469) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HB3 | 3        | 0.12          |
| (1,469) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HB3 | 5        | 0.12          |
| (1,469) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HB3 | 6        | 0.12          |
| (1,469) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HB3 | 8        | 0.12          |
| (1,469) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HB3 | 9        | 0.12          |
| (1,469) | 1:21:A:ARG:HB2 | 1:21:A:ARG:HB3 | 10       | 0.12          |
| (1,453) | 1:19:A:SER:HA  | 1:19:A:SER:HB2 | 9        | 0.12          |
| (1,435) | 1:17:A:PRO:HA  | 1:17:A:PRO:HD2 | 5        | 0.12          |
| (1,435) | 1:17:A:PRO:HA  | 1:17:A:PRO:HD2 | 9        | 0.12          |
| (1,390) | 1:9:A:ILE:HG12 | 1:9:A:ILE:HG21 | 1        | 0.12          |
| (1,390) | 1:9:A:ILE:HG12 | 1:9:A:ILE:HG22 | 1        | 0.12          |
| (1,390) | 1:9:A:ILE:HG12 | 1:9:A:ILE:HG23 | 1        | 0.12          |
| (1,390) | 1:9:A:ILE:HG12 | 1:9:A:ILE:HG21 | 4        | 0.12          |
| (1,390) | 1:9:A:ILE:HG12 | 1:9:A:ILE:HG22 | 4        | 0.12          |
| (1,390) | 1:9:A:ILE:HG12 | 1:9:A:ILE:HG23 | 4        | 0.12          |
| (1,390) | 1:9:A:ILE:HG12 | 1:9:A:ILE:HG21 | 9        | 0.12          |
| (1,390) | 1:9:A:ILE:HG12 | 1:9:A:ILE:HG22 | 9        | 0.12          |
| (1,390) | 1:9:A:ILE:HG12 | 1:9:A:ILE:HG23 | 9        | 0.12          |
| (1,377) | 1:9:A:ILE:HA   | 1:9:A:ILE:HG13 | 1        | 0.12          |
| (1,377) | 1:9:A:ILE:HA   | 1:9:A:ILE:HG13 | 4        | 0.12          |
| (1,377) | 1:9:A:ILE:HA   | 1:9:A:ILE:HG13 | 9        | 0.12          |
| (1,344) | 1:5:A:VAL:HB   | 1:5:A:VAL:HG11 | 2        | 0.12          |
| (1,344) | 1:5:A:VAL:HB   | 1:5:A:VAL:HG12 | 2        | 0.12          |
| (1,344) | 1:5:A:VAL:HB   | 1:5:A:VAL:HG13 | 2        | 0.12          |
| (1,344) | 1:5:A:VAL:HB   | 1:5:A:VAL:HG11 | 4        | 0.12          |
| (1,344) | 1:5:A:VAL:HB   | 1:5:A:VAL:HG12 | 4        | 0.12          |
| (1,344) | 1:5:A:VAL:HB   | 1:5:A:VAL:HG13 | 4        | 0.12          |
| (1,344) | 1:5:A:VAL:HB   | 1:5:A:VAL:HG11 | 6        | 0.12          |
| (1,344) | 1:5:A:VAL:HB   | 1:5:A:VAL:HG12 | 6        | 0.12          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,344) | 1:5:A:VAL:HB   | 1:5:A:VAL:HG13 | 6        | 0.12          |
| (1,344) | 1:5:A:VAL:HB   | 1:5:A:VAL:HG11 | 7        | 0.12          |
| (1,344) | 1:5:A:VAL:HB   | 1:5:A:VAL:HG12 | 7        | 0.12          |
| (1,344) | 1:5:A:VAL:HB   | 1:5:A:VAL:HG13 | 7        | 0.12          |
| (1,344) | 1:5:A:VAL:HB   | 1:5:A:VAL:HG11 | 10       | 0.12          |
| (1,344) | 1:5:A:VAL:HB   | 1:5:A:VAL:HG12 | 10       | 0.12          |
| (1,344) | 1:5:A:VAL:HB   | 1:5:A:VAL:HG13 | 10       | 0.12          |
| (1,335) | 1:3:A:GLU:HA   | 1:3:A:GLU:HB2  | 3        | 0.12          |
| (1,335) | 1:3:A:GLU:HA   | 1:3:A:GLU:HB3  | 3        | 0.12          |
| (1,334) | 1:3:A:GLU:HA   | 1:3:A:GLU:HG2  | 8        | 0.12          |
| (1,334) | 1:3:A:GLU:HA   | 1:3:A:GLU:HG3  | 8        | 0.12          |
| (1,280) | 1:4:A:CYS:H    | 1:5:A:VAL:H    | 9        | 0.12          |
| (1,263) | 1:18:A:SER:HA  | 1:20:A:GLY:H   | 1        | 0.12          |
| (1,255) | 1:11:A:TRP:HH2 | 1:17:A:PRO:HB2 | 2        | 0.12          |
| (1,254) | 1:11:A:TRP:HZ2 | 1:17:A:PRO:HB2 | 5        | 0.12          |
| (1,254) | 1:11:A:TRP:HZ2 | 1:17:A:PRO:HB2 | 8        | 0.12          |
| (1,227) | 1:11:A:TRP:HZ2 | 1:23:A:PRO:HG2 | 10       | 0.12          |
| (1,220) | 1:8:A:TYR:HD1  | 1:9:A:ILE:HG12 | 6        | 0.12          |
| (1,220) | 1:8:A:TYR:HD2  | 1:9:A:ILE:HG12 | 6        | 0.12          |
| (1,180) | 1:11:A:TRP:HB2 | 1:11:A:TRP:HE3 | 1        | 0.12          |
| (1,180) | 1:11:A:TRP:HB2 | 1:11:A:TRP:HE3 | 2        | 0.12          |
| (1,180) | 1:11:A:TRP:HB2 | 1:11:A:TRP:HE3 | 5        | 0.12          |
| (1,180) | 1:11:A:TRP:HB2 | 1:11:A:TRP:HE3 | 6        | 0.12          |
| (1,155) | 1:7:A:LEU:H    | 1:7:A:LEU:HD11 | 3        | 0.12          |
| (1,155) | 1:7:A:LEU:H    | 1:7:A:LEU:HD12 | 3        | 0.12          |
| (1,155) | 1:7:A:LEU:H    | 1:7:A:LEU:HD13 | 3        | 0.12          |
| (1,155) | 1:7:A:LEU:H    | 1:7:A:LEU:HD21 | 3        | 0.12          |
| (1,155) | 1:7:A:LEU:H    | 1:7:A:LEU:HD22 | 3        | 0.12          |
| (1,155) | 1:7:A:LEU:H    | 1:7:A:LEU:HD23 | 3        | 0.12          |
| (1,152) | 1:8:A:TYR:HB2  | 1:9:A:ILE:H    | 7        | 0.12          |
| (1,152) | 1:8:A:TYR:HB3  | 1:9:A:ILE:H    | 7        | 0.12          |
| (1,152) | 1:8:A:TYR:HB2  | 1:9:A:ILE:H    | 8        | 0.12          |
| (1,152) | 1:8:A:TYR:HB3  | 1:9:A:ILE:H    | 8        | 0.12          |
| (1,119) | 1:7:A:LEU:H    | 1:10:A:GLN:HB2 | 9        | 0.12          |
| (1,117) | 1:12:A:LEU:H   | 1:12:A:LEU:HB3 | 4        | 0.12          |
| (1,117) | 1:12:A:LEU:H   | 1:12:A:LEU:HB3 | 9        | 0.12          |
| (1,108) | 1:14:A:ASP:H   | 1:15:A:GLY:H   | 4        | 0.12          |
| (1,94)  | 1:20:A:GLY:HA3 | 1:21:A:ARG:H   | 5        | 0.12          |
| (1,93)  | 1:19:A:SER:HG  | 1:21:A:ARG:H   | 9        | 0.12          |
| (1,75)  | 1:25:A:CYS:H   | 1:25:A:CYS:HB2 | 9        | 0.12          |
| (1,65)  | 1:20:A:GLY:H   | 1:20:A:GLY:HA2 | 3        | 0.12          |
| (1,65)  | 1:20:A:GLY:H   | 1:20:A:GLY:HA2 | 8        | 0.12          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,35)  | 1:10:A:GLN:H    | 1:10:A:GLN:HB2  | 2        | 0.12          |
| (1,723) | 1:12:A:LEU:HB3  | 1:13:A:LYS:HG2  | 2        | 0.11          |
| (1,723) | 1:12:A:LEU:HB3  | 1:13:A:LYS:HG3  | 2        | 0.11          |
| (1,694) | 1:9:A:ILE:HG21  | 1:12:A:LEU:HB3  | 6        | 0.11          |
| (1,694) | 1:9:A:ILE:HG22  | 1:12:A:LEU:HB3  | 6        | 0.11          |
| (1,694) | 1:9:A:ILE:HG23  | 1:12:A:LEU:HB3  | 6        | 0.11          |
| (1,622) | 1:2:A:GLU:HB3   | 1:5:A:VAL:H     | 10       | 0.11          |
| (1,565) | 1:4:A:CYS:HA    | 1:7:A:LEU:HG    | 7        | 0.11          |
| (1,554) | 1:22:A:PRO:HB3  | 1:23:A:PRO:HD2  | 3        | 0.11          |
| (1,552) | 1:11:A:TRP:HB2  | 1:24:A:PRO:HD2  | 1        | 0.11          |
| (1,551) | 1:16:A:GLY:HA3  | 1:17:A:PRO:HD3  | 7        | 0.11          |
| (1,471) | 1:21:A:ARG:HB3  | 1:21:A:ARG:HG2  | 2        | 0.11          |
| (1,471) | 1:21:A:ARG:HB3  | 1:21:A:ARG:HG3  | 2        | 0.11          |
| (1,413) | 1:12:A:LEU:HD11 | 1:12:A:LEU:HG   | 1        | 0.11          |
| (1,413) | 1:12:A:LEU:HD12 | 1:12:A:LEU:HG   | 1        | 0.11          |
| (1,413) | 1:12:A:LEU:HD13 | 1:12:A:LEU:HG   | 1        | 0.11          |
| (1,413) | 1:12:A:LEU:HD11 | 1:12:A:LEU:HG   | 2        | 0.11          |
| (1,413) | 1:12:A:LEU:HD12 | 1:12:A:LEU:HG   | 2        | 0.11          |
| (1,413) | 1:12:A:LEU:HD13 | 1:12:A:LEU:HG   | 2        | 0.11          |
| (1,413) | 1:12:A:LEU:HD11 | 1:12:A:LEU:HG   | 5        | 0.11          |
| (1,413) | 1:12:A:LEU:HD12 | 1:12:A:LEU:HG   | 5        | 0.11          |
| (1,413) | 1:12:A:LEU:HD13 | 1:12:A:LEU:HG   | 5        | 0.11          |
| (1,413) | 1:12:A:LEU:HD11 | 1:12:A:LEU:HG   | 6        | 0.11          |
| (1,413) | 1:12:A:LEU:HD12 | 1:12:A:LEU:HG   | 6        | 0.11          |
| (1,413) | 1:12:A:LEU:HD13 | 1:12:A:LEU:HG   | 6        | 0.11          |
| (1,408) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD11 | 2        | 0.11          |
| (1,408) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD12 | 2        | 0.11          |
| (1,408) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD13 | 2        | 0.11          |
| (1,397) | 1:10:A:GLN:HB2  | 1:10:A:GLN:HG2  | 1        | 0.11          |
| (1,397) | 1:10:A:GLN:HB2  | 1:10:A:GLN:HG2  | 3        | 0.11          |
| (1,394) | 1:10:A:GLN:HA   | 1:10:A:GLN:HB2  | 1        | 0.11          |
| (1,394) | 1:10:A:GLN:HA   | 1:10:A:GLN:HB2  | 7        | 0.11          |
| (1,390) | 1:9:A:ILE:HG12  | 1:9:A:ILE:HG21  | 7        | 0.11          |
| (1,390) | 1:9:A:ILE:HG12  | 1:9:A:ILE:HG22  | 7        | 0.11          |
| (1,390) | 1:9:A:ILE:HG12  | 1:9:A:ILE:HG23  | 7        | 0.11          |
| (1,384) | 1:9:A:ILE:HB    | 1:9:A:ILE:HG12  | 3        | 0.11          |
| (1,377) | 1:9:A:ILE:HA    | 1:9:A:ILE:HG13  | 2        | 0.11          |
| (1,377) | 1:9:A:ILE:HA    | 1:9:A:ILE:HG13  | 7        | 0.11          |
| (1,377) | 1:9:A:ILE:HA    | 1:9:A:ILE:HG13  | 10       | 0.11          |
| (1,352) | 1:6:A:ARG:HB3   | 1:6:A:ARG:HD2   | 8        | 0.11          |
| (1,344) | 1:5:A:VAL:HB    | 1:5:A:VAL:HG11  | 1        | 0.11          |
| (1,344) | 1:5:A:VAL:HB    | 1:5:A:VAL:HG12  | 1        | 0.11          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,344) | 1:5:A:VAL:HB    | 1:5:A:VAL:HG13  | 1        | 0.11          |
| (1,344) | 1:5:A:VAL:HB    | 1:5:A:VAL:HG11  | 8        | 0.11          |
| (1,344) | 1:5:A:VAL:HB    | 1:5:A:VAL:HG12  | 8        | 0.11          |
| (1,344) | 1:5:A:VAL:HB    | 1:5:A:VAL:HG13  | 8        | 0.11          |
| (1,344) | 1:5:A:VAL:HB    | 1:5:A:VAL:HG11  | 9        | 0.11          |
| (1,344) | 1:5:A:VAL:HB    | 1:5:A:VAL:HG12  | 9        | 0.11          |
| (1,344) | 1:5:A:VAL:HB    | 1:5:A:VAL:HG13  | 9        | 0.11          |
| (1,334) | 1:3:A:GLU:HA    | 1:3:A:GLU:HG2   | 4        | 0.11          |
| (1,334) | 1:3:A:GLU:HA    | 1:3:A:GLU:HG3   | 4        | 0.11          |
| (1,262) | 1:10:A:GLN:HA   | 1:10:A:GLN:HE22 | 7        | 0.11          |
| (1,262) | 1:10:A:GLN:HA   | 1:10:A:GLN:HE22 | 8        | 0.11          |
| (1,255) | 1:11:A:TRP:HH2  | 1:17:A:PRO:HB2  | 7        | 0.11          |
| (1,254) | 1:11:A:TRP:HZ2  | 1:17:A:PRO:HB2  | 2        | 0.11          |
| (1,220) | 1:8:A:TYR:HD1   | 1:9:A:ILE:HG12  | 5        | 0.11          |
| (1,220) | 1:8:A:TYR:HD2   | 1:9:A:ILE:HG12  | 5        | 0.11          |
| (1,208) | 1:11:A:TRP:HZ3  | 1:12:A:LEU:HD11 | 8        | 0.11          |
| (1,208) | 1:11:A:TRP:HZ3  | 1:12:A:LEU:HD12 | 8        | 0.11          |
| (1,208) | 1:11:A:TRP:HZ3  | 1:12:A:LEU:HD13 | 8        | 0.11          |
| (1,199) | 1:8:A:TYR:HD1   | 1:23:A:PRO:HB3  | 3        | 0.11          |
| (1,199) | 1:8:A:TYR:HD2   | 1:23:A:PRO:HB3  | 3        | 0.11          |
| (1,155) | 1:7:A:LEU:H     | 1:7:A:LEU:HD11  | 6        | 0.11          |
| (1,155) | 1:7:A:LEU:H     | 1:7:A:LEU:HD12  | 6        | 0.11          |
| (1,155) | 1:7:A:LEU:H     | 1:7:A:LEU:HD13  | 6        | 0.11          |
| (1,155) | 1:7:A:LEU:H     | 1:7:A:LEU:HD21  | 6        | 0.11          |
| (1,155) | 1:7:A:LEU:H     | 1:7:A:LEU:HD22  | 6        | 0.11          |
| (1,155) | 1:7:A:LEU:H     | 1:7:A:LEU:HD23  | 6        | 0.11          |
| (1,123) | 1:24:A:PRO:HG2  | 1:25:A:CYS:H    | 2        | 0.11          |
| (1,117) | 1:12:A:LEU:H    | 1:12:A:LEU:HB3  | 2        | 0.11          |
| (1,117) | 1:12:A:LEU:H    | 1:12:A:LEU:HB3  | 7        | 0.11          |
| (1,117) | 1:12:A:LEU:H    | 1:12:A:LEU:HB3  | 8        | 0.11          |
| (1,117) | 1:12:A:LEU:H    | 1:12:A:LEU:HB3  | 10       | 0.11          |
| (1,115) | 1:9:A:ILE:H     | 1:9:A:ILE:HG13  | 7        | 0.11          |
| (1,115) | 1:9:A:ILE:H     | 1:9:A:ILE:HG13  | 10       | 0.11          |
| (1,112) | 1:7:A:LEU:H     | 1:7:A:LEU:HB3   | 1        | 0.11          |
| (1,112) | 1:7:A:LEU:H     | 1:7:A:LEU:HB3   | 5        | 0.11          |
| (1,108) | 1:14:A:ASP:H    | 1:15:A:GLY:H    | 9        | 0.11          |
| (1,65)  | 1:20:A:GLY:H    | 1:20:A:GLY:HA2  | 1        | 0.11          |
| (1,65)  | 1:20:A:GLY:H    | 1:20:A:GLY:HA2  | 5        | 0.11          |
| (1,48)  | 1:10:A:GLN:HE21 | 1:10:A:GLN:HG3  | 9        | 0.11          |
| (1,35)  | 1:10:A:GLN:H    | 1:10:A:GLN:HB2  | 3        | 0.11          |
| (1,27)  | 1:3:A:GLU:H     | 1:3:A:GLU:HB2   | 7        | 0.11          |
| (1,27)  | 1:3:A:GLU:H     | 1:3:A:GLU:HB3   | 7        | 0.11          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,717) | 1:12:A:LEU:HD11 | 1:16:A:GLY:HA2  | 9        | 0.1           |
| (1,717) | 1:12:A:LEU:HD12 | 1:16:A:GLY:HA2  | 9        | 0.1           |
| (1,717) | 1:12:A:LEU:HD13 | 1:16:A:GLY:HA2  | 9        | 0.1           |
| (1,706) | 1:6:A:ARG:HG3   | 1:7:A:LEU:HD11  | 2        | 0.1           |
| (1,706) | 1:6:A:ARG:HG3   | 1:7:A:LEU:HD12  | 2        | 0.1           |
| (1,706) | 1:6:A:ARG:HG3   | 1:7:A:LEU:HD13  | 2        | 0.1           |
| (1,706) | 1:6:A:ARG:HG3   | 1:7:A:LEU:HD21  | 2        | 0.1           |
| (1,706) | 1:6:A:ARG:HG3   | 1:7:A:LEU:HD22  | 2        | 0.1           |
| (1,706) | 1:6:A:ARG:HG3   | 1:7:A:LEU:HD23  | 2        | 0.1           |
| (1,705) | 1:9:A:ILE:HG21  | 1:13:A:LYS:HD2  | 9        | 0.1           |
| (1,705) | 1:9:A:ILE:HG22  | 1:13:A:LYS:HD2  | 9        | 0.1           |
| (1,705) | 1:9:A:ILE:HG23  | 1:13:A:LYS:HD2  | 9        | 0.1           |
| (1,695) | 1:5:A:VAL:HG11  | 1:9:A:ILE:HB    | 10       | 0.1           |
| (1,695) | 1:5:A:VAL:HG12  | 1:9:A:ILE:HB    | 10       | 0.1           |
| (1,695) | 1:5:A:VAL:HG13  | 1:9:A:ILE:HB    | 10       | 0.1           |
| (1,646) | 1:15:A:GLY:HA2  | 1:18:A:SER:HB3  | 9        | 0.1           |
| (1,613) | 1:18:A:SER:HB3  | 1:19:A:SER:H    | 5        | 0.1           |
| (1,545) | 1:13:A:LYS:HB2  | 1:13:A:LYS:HE2  | 3        | 0.1           |
| (1,545) | 1:13:A:LYS:HB2  | 1:13:A:LYS:HE3  | 3        | 0.1           |
| (1,545) | 1:13:A:LYS:HB3  | 1:13:A:LYS:HE2  | 3        | 0.1           |
| (1,545) | 1:13:A:LYS:HB3  | 1:13:A:LYS:HE3  | 3        | 0.1           |
| (1,413) | 1:12:A:LEU:HD11 | 1:12:A:LEU:HG   | 7        | 0.1           |
| (1,413) | 1:12:A:LEU:HD12 | 1:12:A:LEU:HG   | 7        | 0.1           |
| (1,413) | 1:12:A:LEU:HD13 | 1:12:A:LEU:HG   | 7        | 0.1           |
| (1,413) | 1:12:A:LEU:HD11 | 1:12:A:LEU:HG   | 8        | 0.1           |
| (1,413) | 1:12:A:LEU:HD12 | 1:12:A:LEU:HG   | 8        | 0.1           |
| (1,413) | 1:12:A:LEU:HD13 | 1:12:A:LEU:HG   | 8        | 0.1           |
| (1,413) | 1:12:A:LEU:HD11 | 1:12:A:LEU:HG   | 9        | 0.1           |
| (1,413) | 1:12:A:LEU:HD12 | 1:12:A:LEU:HG   | 9        | 0.1           |
| (1,413) | 1:12:A:LEU:HD13 | 1:12:A:LEU:HG   | 9        | 0.1           |
| (1,413) | 1:12:A:LEU:HD11 | 1:12:A:LEU:HG   | 10       | 0.1           |
| (1,413) | 1:12:A:LEU:HD12 | 1:12:A:LEU:HG   | 10       | 0.1           |
| (1,413) | 1:12:A:LEU:HD13 | 1:12:A:LEU:HG   | 10       | 0.1           |
| (1,408) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD11 | 8        | 0.1           |
| (1,408) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD12 | 8        | 0.1           |
| (1,408) | 1:12:A:LEU:HA   | 1:12:A:LEU:HD13 | 8        | 0.1           |
| (1,390) | 1:9:A:ILE:HG12  | 1:9:A:ILE:HG21  | 2        | 0.1           |
| (1,390) | 1:9:A:ILE:HG12  | 1:9:A:ILE:HG22  | 2        | 0.1           |
| (1,390) | 1:9:A:ILE:HG12  | 1:9:A:ILE:HG23  | 2        | 0.1           |
| (1,384) | 1:9:A:ILE:HB    | 1:9:A:ILE:HG12  | 1        | 0.1           |
| (1,384) | 1:9:A:ILE:HB    | 1:9:A:ILE:HG12  | 2        | 0.1           |
| (1,384) | 1:9:A:ILE:HB    | 1:9:A:ILE:HG12  | 4        | 0.1           |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,384) | 1:9:A:ILE:HB   | 1:9:A:ILE:HG12 | 5        | 0.1           |
| (1,384) | 1:9:A:ILE:HB   | 1:9:A:ILE:HG12 | 6        | 0.1           |
| (1,384) | 1:9:A:ILE:HB   | 1:9:A:ILE:HG12 | 8        | 0.1           |
| (1,384) | 1:9:A:ILE:HB   | 1:9:A:ILE:HG12 | 9        | 0.1           |
| (1,384) | 1:9:A:ILE:HB   | 1:9:A:ILE:HG12 | 10       | 0.1           |
| (1,334) | 1:3:A:GLU:HA   | 1:3:A:GLU:HG2  | 9        | 0.1           |
| (1,334) | 1:3:A:GLU:HA   | 1:3:A:GLU:HG3  | 9        | 0.1           |
| (1,237) | 1:11:A:TRP:HZ2 | 1:22:A:PRO:HB2 | 2        | 0.1           |
| (1,226) | 1:11:A:TRP:HH2 | 1:23:A:PRO:HG2 | 10       | 0.1           |
| (1,127) | 1:19:A:SER:HA  | 1:20:A:GLY:H   | 6        | 0.1           |
| (1,117) | 1:12:A:LEU:H   | 1:12:A:LEU:HB3 | 1        | 0.1           |
| (1,112) | 1:7:A:LEU:H    | 1:7:A:LEU:HB3  | 6        | 0.1           |
| (1,112) | 1:7:A:LEU:H    | 1:7:A:LEU:HB3  | 7        | 0.1           |
| (1,112) | 1:7:A:LEU:H    | 1:7:A:LEU:HB3  | 9        | 0.1           |
| (1,65)  | 1:20:A:GLY:H   | 1:20:A:GLY:HA2 | 6        | 0.1           |

## 10 Dihedral-angle violation analysis

No dihedral-angle restraints found