



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 09:20 PM UTC

PDB ID : 2MZJ / pdb\_00002mzj  
BMRB ID : 19098  
Title : NMR-structure of the Nop6-RBD from *S. cerevisiae*  
Authors : Wurm, J.; Lioutikov, A.; Koetter, P.; Entian, K.; Woehnert, J.  
Deposited on : 2015-02-14

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

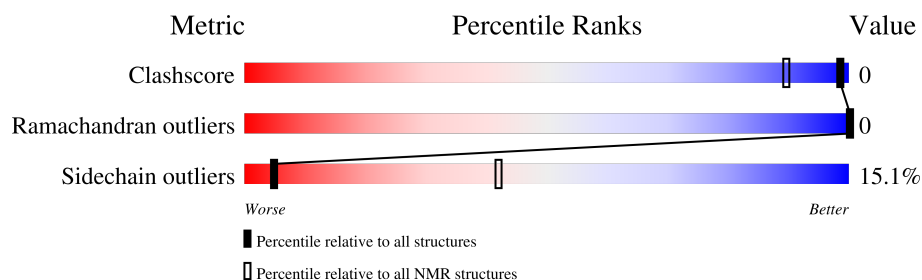
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 90%.

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     | 82     | <br>88% 6% 6%    |

## 2 Ensemble composition and analysis

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

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

| Well-defined (core) protein residues |                       |                   |              |
|--------------------------------------|-----------------------|-------------------|--------------|
| Well-defined core                    | Residue range (total) | Backbone RMSD (Å) | Medoid model |
| 1                                    | A:3-A:79 (77)         | 0.42              | 9            |

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

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

The models can be grouped into 3 clusters and 1 single-model cluster was found.

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

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

There is only 1 type of molecule in this entry. The entry contains 1319 atoms, of which 669 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Nucleolar protein 6.

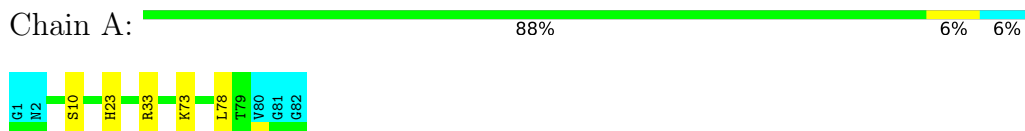
| Mol | Chain | Residues | Atoms |     |     |     |     |   | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|-------|
| 1   | A     | 82       | Total | C   | H   | N   | O   | S | 0     |
|     |       |          | 1319  | 409 | 669 | 121 | 119 | 1 |       |

## 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: Nucleolar protein 6

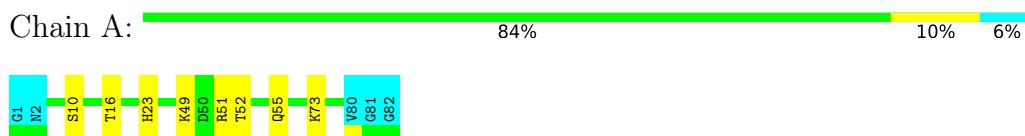


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section [4.1](#) above.

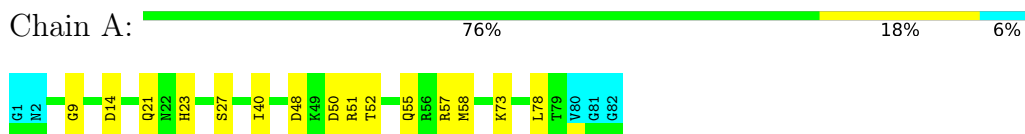
#### 4.2.1 Score per residue for model 1

- Molecule 1: Nucleolar protein 6



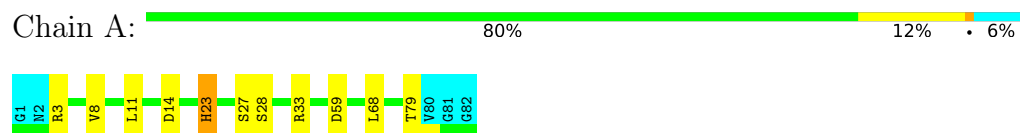
#### 4.2.2 Score per residue for model 2

- Molecule 1: Nucleolar protein 6



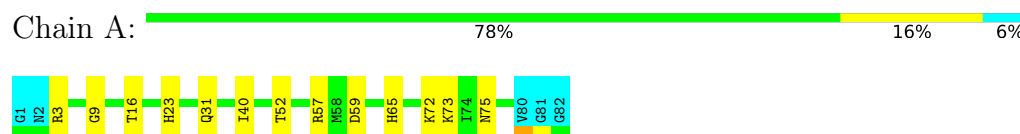
### 4.2.3 Score per residue for model 3

- Molecule 1: Nucleolar protein 6



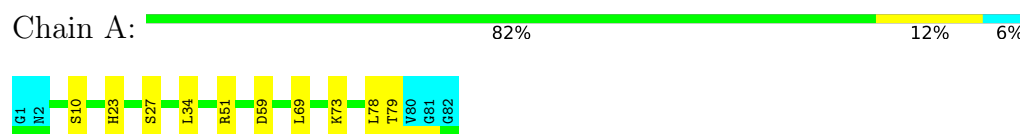
### 4.2.4 Score per residue for model 4

- Molecule 1: Nucleolar protein 6



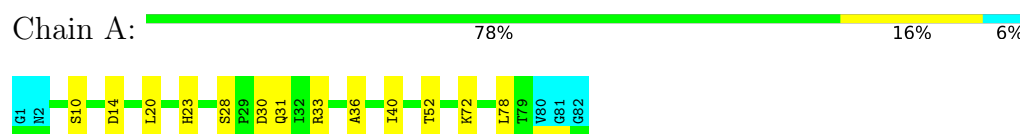
### 4.2.5 Score per residue for model 5

- Molecule 1: Nucleolar protein 6



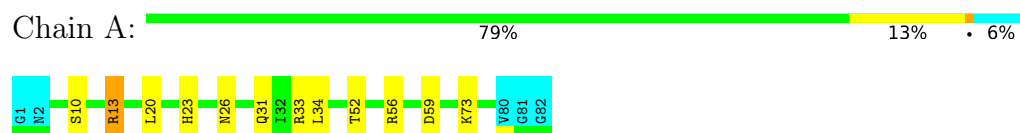
### 4.2.6 Score per residue for model 6

- Molecule 1: Nucleolar protein 6



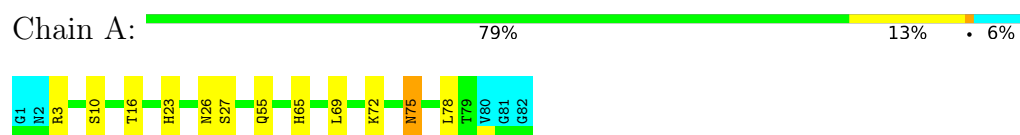
### 4.2.7 Score per residue for model 7

- Molecule 1: Nucleolar protein 6



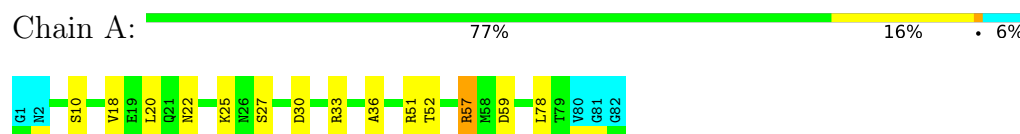
### 4.2.8 Score per residue for model 8

- Molecule 1: Nucleolar protein 6



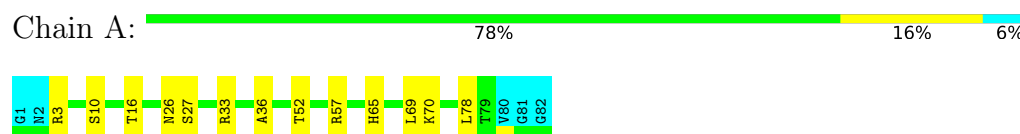
### 4.2.9 Score per residue for model 9 (medoid)

- Molecule 1: Nucleolar protein 6



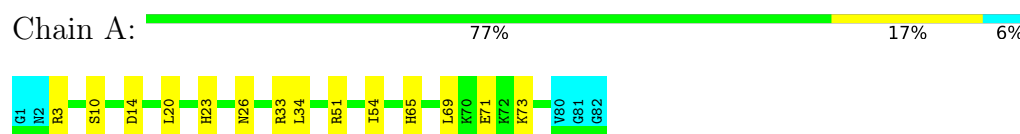
### 4.2.10 Score per residue for model 10

- Molecule 1: Nucleolar protein 6



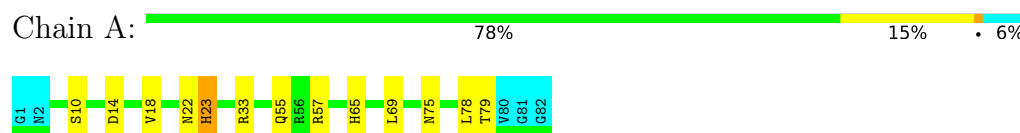
### 4.2.11 Score per residue for model 11

- Molecule 1: Nucleolar protein 6



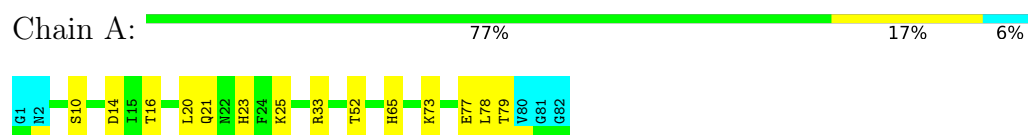
### 4.2.12 Score per residue for model 12

- Molecule 1: Nucleolar protein 6



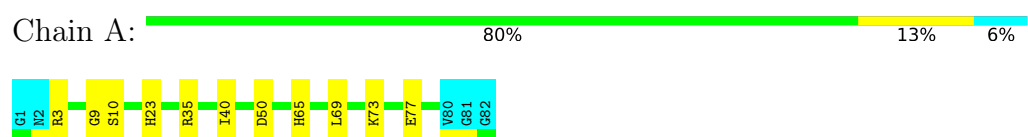
### 4.2.13 Score per residue for model 13

- Molecule 1: Nucleolar protein 6



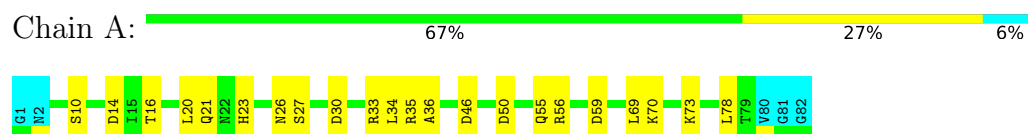
### 4.2.14 Score per residue for model 14

- Molecule 1: Nucleolar protein 6



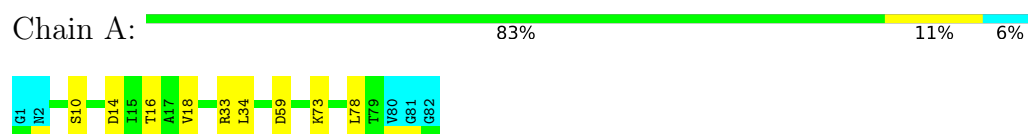
### 4.2.15 Score per residue for model 15

- Molecule 1: Nucleolar protein 6



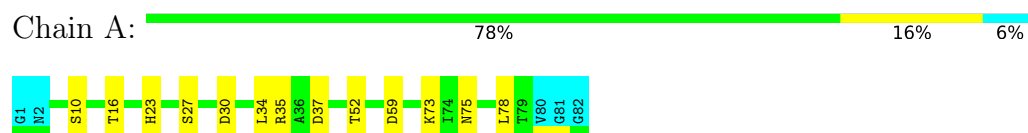
### 4.2.16 Score per residue for model 16

- Molecule 1: Nucleolar protein 6



### 4.2.17 Score per residue for model 17

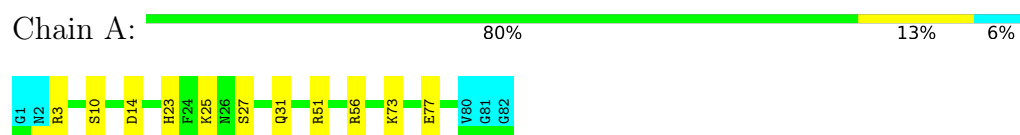
- Molecule 1: Nucleolar protein 6





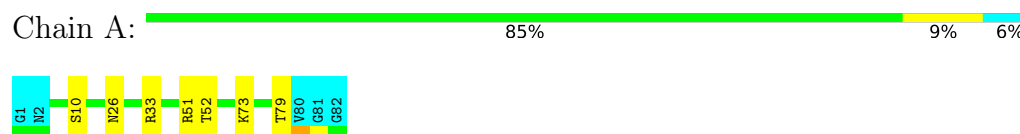
#### 4.2.18 Score per residue for model 18

- Molecule 1: Nucleolar protein 6



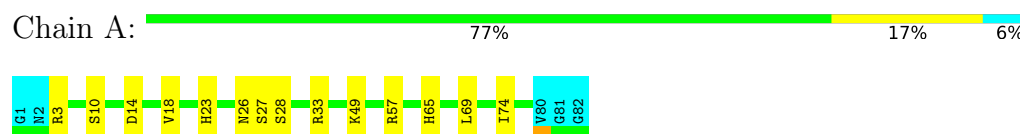
#### 4.2.19 Score per residue for model 19

- Molecule 1: Nucleolar protein 6



#### 4.2.20 Score per residue for model 20

- Molecule 1: Nucleolar protein 6



## 5 Refinement protocol and experimental data overview

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

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

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

| Software name | Classification     | Version |
|---------------|--------------------|---------|
| UNIO          | structure solution |         |
| OPAL          | refinement         |         |

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

|                                              |                |
|----------------------------------------------|----------------|
| Chemical shift file(s)                       | working_cs.cif |
| Number of chemical shift lists               | 2              |
| Total number of shifts                       | 2081           |
| Number of shifts mapped to atoms             | 2081           |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 90%            |

## 6 Model quality i

### 6.1 Standard geometry i

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

| Mol | Chain | Bond lengths |                      | Bond angles |                      |
|-----|-------|--------------|----------------------|-------------|----------------------|
|     |       | RMSZ         | #Z>5                 | RMSZ        | #Z>5                 |
| 1   | A     | 0.59±0.01    | 0±0/632 ( 0.0± 0.0%) | 1.38±0.03   | 2±1/849 ( 0.2± 0.2%) |
| All | All   | 0.59         | 0/12640 ( 0.0%)      | 1.38        | 32/16980 ( 0.2%)     |

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

| Mol | Chain | Chirality | Planarity |
|-----|-------|-----------|-----------|
| 1   | A     | 0.0±0.0   | 0.7±0.7   |
| All | All   | 0         | 13        |

There are no bond-length outliers.

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

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|-----------|-------|-------------|----------|--------|-------|
|     |       |     |      |           |       |             |          | Worst  | Total |
| 1   | A     | 23  | HIS  | CA-CB-CG  | -6.22 | 107.58      | 113.80   | 3      | 1     |
| 1   | A     | 65  | HIS  | CB-CG-CD2 | -6.15 | 123.21      | 131.20   | 8      | 8     |
| 1   | A     | 26  | ASN  | CA-CB-CG  | 5.99  | 118.59      | 112.60   | 7      | 1     |
| 1   | A     | 79  | THR  | CA-C-N    | 5.58  | 127.55      | 121.97   | 3      | 1     |
| 1   | A     | 79  | THR  | C-N-CA    | 5.58  | 127.55      | 121.97   | 3      | 1     |
| 1   | A     | 30  | ASP  | CA-CB-CG  | -5.58 | 107.02      | 112.60   | 6      | 4     |
| 1   | A     | 54  | ILE  | CA-C-N    | 5.55  | 127.98      | 120.65   | 11     | 1     |
| 1   | A     | 54  | ILE  | C-N-CA    | 5.55  | 127.98      | 120.65   | 11     | 1     |
| 1   | A     | 46  | ASP  | CA-CB-CG  | -5.48 | 107.12      | 112.60   | 15     | 1     |
| 1   | A     | 59  | ASP  | CA-CB-CG  | 5.43  | 118.03      | 112.60   | 15     | 1     |
| 1   | A     | 36  | ALA  | CA-C-N    | 5.41  | 128.28      | 120.38   | 9      | 4     |
| 1   | A     | 36  | ALA  | C-N-CA    | 5.41  | 128.28      | 120.38   | 9      | 4     |
| 1   | A     | 75  | ASN  | CA-CB-CG  | 5.34  | 117.94      | 112.60   | 8      | 1     |
| 1   | A     | 37  | ASP  | CA-CB-CG  | 5.15  | 117.75      | 112.60   | 17     | 1     |
| 1   | A     | 58  | MET  | CA-C-N    | 5.15  | 127.13      | 120.44   | 2      | 1     |

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| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|--------|------|-------------|----------|--------|-------|
|     |       |     |      |        |      |             |          | Worst  | Total |
| 1   | A     | 58  | MET  | C-N-CA | 5.15 | 127.13      | 120.44   | 2      | 1     |

There are no chirality outliers.

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

| Mol | Chain | Res | Type | Group     | Models (Total) |
|-----|-------|-----|------|-----------|----------------|
| 1   | A     | 57  | ARG  | Sidechain | 5              |
| 1   | A     | 51  | ARG  | Sidechain | 3              |
| 1   | A     | 3   | ARG  | Sidechain | 2              |
| 1   | A     | 13  | ARG  | Sidechain | 1              |
| 1   | A     | 33  | ARG  | Sidechain | 1              |
| 1   | A     | 56  | ARG  | Sidechain | 1              |

## 6.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1   | A     | 623   | 645      | 645      | 0±0     |
| All | All   | 12460 | 12900    | 12900    | 5       |

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 0.

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

| Atom-1         | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|----------------|-----------------|----------|-------------|--------|-------|
|                |                 |          |             | Worst  | Total |
| 1:A:8:VAL:HG12 | 1:A:11:LEU:HD11 | 0.51     | 1.82        | 3      | 1     |
| 1:A:9:GLY:CA   | 1:A:40:ILE:HG22 | 0.47     | 2.38        | 4      | 3     |
| 1:A:23:HIS:ND1 | 1:A:69:LEU:HD21 | 0.44     | 2.27        | 12     | 1     |

## 6.3 Torsion angles [i](#)

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

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

| Mol | Chain | Analysed        | Favoured     | Allowed    | Outliers   | Percentiles |     |
|-----|-------|-----------------|--------------|------------|------------|-------------|-----|
| 1   | A     | 77/82 (94%)     | 73±2 (95±2%) | 4±2 (5±2%) | 0±0 (0±0%) | 100         | 100 |
| All | All   | 1540/1640 (94%) | 1456 (95%)   | 84 (5%)    | 0 (0%)     | 100         | 100 |

There are no Ramachandran outliers.

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

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

| Mol | Chain | Analysed        | Rotameric    | Outliers     | Percentiles |    |
|-----|-------|-----------------|--------------|--------------|-------------|----|
| 1   | A     | 68/70 (97%)     | 58±3 (85±4%) | 10±3 (15±4%) | 5           | 42 |
| All | All   | 1360/1400 (97%) | 1154 (85%)   | 206 (15%)    | 5           | 42 |

All 39 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     | 10  | SER  | 17             |
| 1   | A     | 23  | HIS  | 16             |
| 1   | A     | 73  | LYS  | 13             |
| 1   | A     | 78  | LEU  | 11             |
| 1   | A     | 33  | ARG  | 11             |
| 1   | A     | 52  | THR  | 10             |
| 1   | A     | 14  | ASP  | 10             |
| 1   | A     | 27  | SER  | 10             |
| 1   | A     | 16  | THR  | 8              |
| 1   | A     | 59  | ASP  | 7              |
| 1   | A     | 69  | LEU  | 7              |
| 1   | A     | 3   | ARG  | 6              |
| 1   | A     | 34  | LEU  | 6              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 20  | LEU  | 6              |
| 1   | A     | 26  | ASN  | 6              |
| 1   | A     | 55  | GLN  | 5              |
| 1   | A     | 51  | ARG  | 4              |
| 1   | A     | 31  | GLN  | 4              |
| 1   | A     | 75  | ASN  | 4              |
| 1   | A     | 79  | THR  | 4              |
| 1   | A     | 18  | VAL  | 4              |
| 1   | A     | 21  | GLN  | 3              |
| 1   | A     | 50  | ASP  | 3              |
| 1   | A     | 28  | SER  | 3              |
| 1   | A     | 72  | LYS  | 3              |
| 1   | A     | 25  | LYS  | 3              |
| 1   | A     | 77  | GLU  | 3              |
| 1   | A     | 35  | ARG  | 3              |
| 1   | A     | 49  | LYS  | 2              |
| 1   | A     | 57  | ARG  | 2              |
| 1   | A     | 56  | ARG  | 2              |
| 1   | A     | 22  | ASN  | 2              |
| 1   | A     | 70  | LYS  | 2              |
| 1   | A     | 48  | ASP  | 1              |
| 1   | A     | 68  | LEU  | 1              |
| 1   | A     | 40  | ILE  | 1              |
| 1   | A     | 13  | ARG  | 1              |
| 1   | A     | 71  | GLU  | 1              |
| 1   | A     | 74  | ILE  | 1              |

### 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 ⓘ

There are no oligosaccharides in this entry.

## 6.6 Ligand geometry

There are no ligands in this entry.

## 6.7 Other polymers

There are no such molecules in this entry.

## 6.8 Polymer linkage issues

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 90% for the well-defined parts and 89% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

Chemical shift list name: *assigned\_chem\_shift\_list\_2*

#### 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                  | 1040 |
| Number of shifts mapped to atoms        | 1040 |
| Number of unparsed shifts               | 0    |
| Number of shifts with mapping errors    | 0    |
| Number of shifts with mapping warnings  | 0    |
| Number of shift outliers (ShiftChecker) | 1    |

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 81       | $-0.21 \pm 0.16$                | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}_\beta$  | 75       | $0.06 \pm 0.21$                 | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}'$       | 78       | $-0.06 \pm 0.23$                | None needed ( $< 0.5$ ppm) |
| $^{15}\text{N}$        | 78       | $0.30 \pm 0.36$                 | None needed ( $< 0.5$ ppm) |

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 90%, i.e. 1006 atoms were assigned a chemical shift out of a possible 1120. 0 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total          | $^1\text{H}$   | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|----------------|----------------|-----------------|-----------------|
| Backbone  | 384/385 (100%) | 156/156 (100%) | 153/154 (99%)   | 75/75 (100%)    |
| Sidechain | 572/671 (85%)  | 395/433 (91%)  | 170/204 (83%)   | 7/34 (21%)      |

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|          | <b>Total</b>    | <b><sup>1</sup>H</b> | <b><sup>13</sup>C</b> | <b><sup>15</sup>N</b> |
|----------|-----------------|----------------------|-----------------------|-----------------------|
| Aromatic | 50/64 (78%)     | 25/33 (76%)          | 25/29 (86%)           | 0/2 (0%)              |
| Overall  | 1006/1120 (90%) | 576/622 (93%)        | 348/387 (90%)         | 82/111 (74%)          |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 89%, i.e. 1040 atoms were assigned a chemical shift out of a possible 1165. 0 out of 14 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | <b>Total</b>    | <b><sup>1</sup>H</b> | <b><sup>13</sup>C</b> | <b><sup>15</sup>N</b> |
|-----------|-----------------|----------------------|-----------------------|-----------------------|
| Backbone  | 402/413 (97%)   | 165/169 (98%)        | 159/164 (97%)         | 78/80 (98%)           |
| Sidechain | 588/688 (85%)   | 406/444 (91%)        | 174/209 (83%)         | 8/35 (23%)            |
| Aromatic  | 50/64 (78%)     | 25/33 (76%)          | 25/29 (86%)           | 0/2 (0%)              |
| Overall   | 1040/1165 (89%) | 596/646 (92%)        | 358/402 (89%)         | 86/117 (74%)          |

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

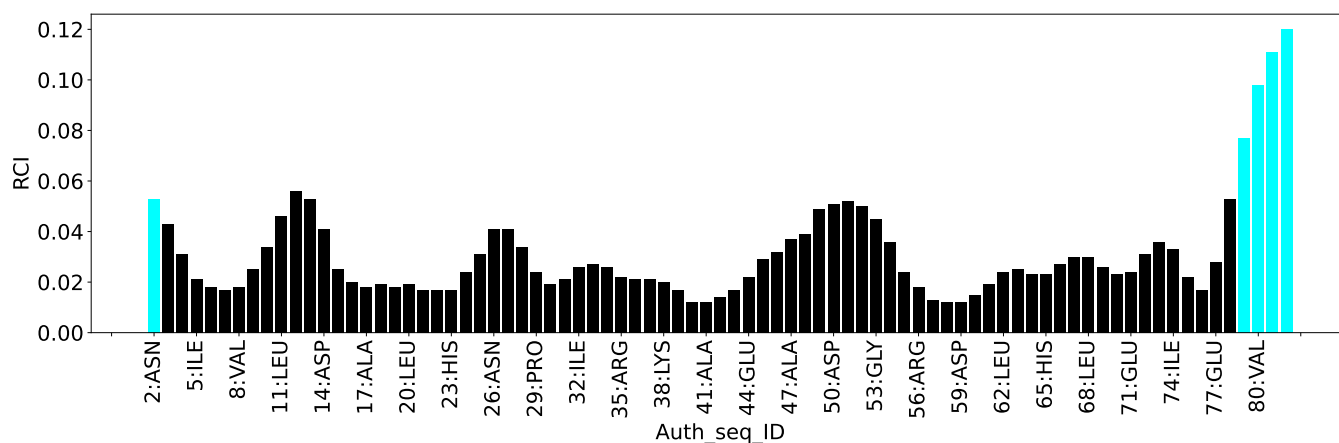
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

| List Id | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|---------|-------|-----|------|------|------------|---------------------|---------|
| 1       | A     | 52  | THR  | CG2  | 15.11      | 16.06 – 27.03       | -5.9    |

#### 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:



## 7.2 Chemical shift list 2

File name: working\_cs.cif

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

### 7.2.1 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                  | 1041 |
| Number of shifts mapped to atoms        | 1041 |
| Number of unparsed shifts               | 0    |
| Number of shifts with mapping errors    | 0    |
| Number of shifts with mapping warnings  | 0    |
| Number of shift outliers (ShiftChecker) | 0    |

### 7.2.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 81       | $-0.21 \pm 0.16$                | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}_\beta$  | 75       | $0.06 \pm 0.21$                 | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}'$       | 78       | $-0.06 \pm 0.23$                | None needed ( $< 0.5$ ppm) |
| $^{15}\text{N}$        | 78       | $0.30 \pm 0.36$                 | None needed ( $< 0.5$ ppm) |

### 7.2.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 90%, i.e. 1007 atoms were assigned a chemical shift out of a possible 1120. 0 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total           | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|-----------|-----------------|----------------|-----------------|-----------------|
| Backbone  | 384/385 (100%)  | 156/156 (100%) | 153/154 (99%)   | 75/75 (100%)    |
| Sidechain | 573/671 (85%)   | 395/433 (91%)  | 171/204 (84%)   | 7/34 (21%)      |
| Aromatic  | 50/64 (78%)     | 25/33 (76%)    | 25/29 (86%)     | 0/2 (0%)        |
| Overall   | 1007/1120 (90%) | 576/622 (93%)  | 349/387 (90%)   | 82/111 (74%)    |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 89%, i.e. 1041 atoms were assigned a chemical shift out of a possible 1165. 0 out of 14 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total           | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|-----------|-----------------|----------------|-----------------|-----------------|
| Backbone  | 402/413 (97%)   | 165/169 (98%)  | 159/164 (97%)   | 78/80 (98%)     |
| Sidechain | 589/688 (86%)   | 406/444 (91%)  | 175/209 (84%)   | 8/35 (23%)      |
| Aromatic  | 50/64 (78%)     | 25/33 (76%)    | 25/29 (86%)     | 0/2 (0%)        |
| Overall   | 1041/1165 (89%) | 596/646 (92%)  | 359/402 (89%)   | 86/117 (74%)    |

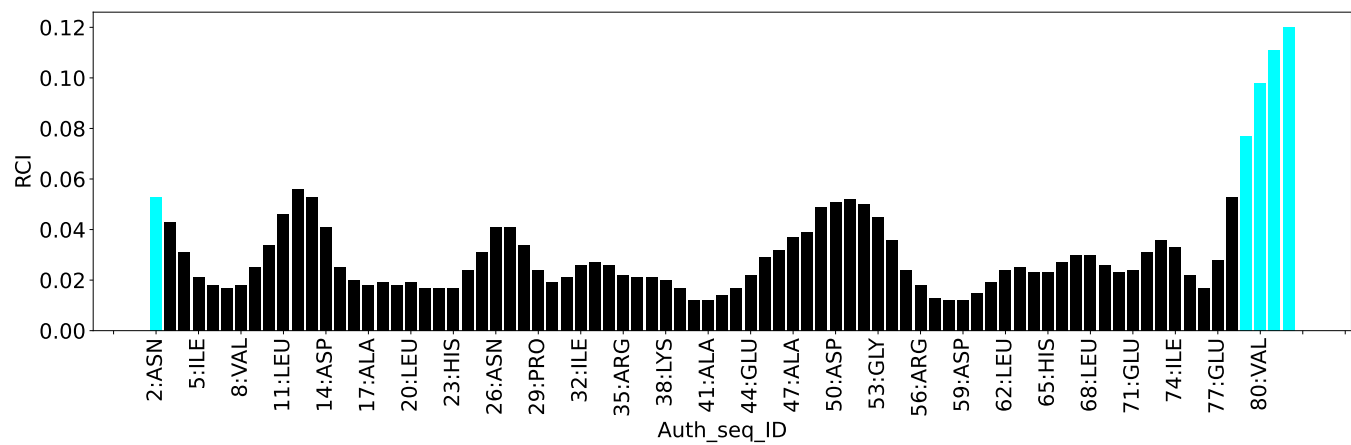
### 7.2.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

### 7.2.5 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                                | 1382  |
| Intra-residue ( $ i-j =0$ )                              | 363   |
| Sequential ( $ i-j =1$ )                                 | 365   |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 235   |
| Long range ( $ i-j \geq 5$ )                             | 417   |
| Inter-chain                                              | 0     |
| Hydrogen bond restraints                                 | 2     |
| Disulfide bond restraints                                | 0     |
| Total dihedral-angle restraints                          | 134   |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 18.5  |
| Number of long range restraints per residue <sup>1</sup> | 5.1   |

<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)  | 15.8                                   | 0.2     |
| 0.2-0.5 (Medium) | 29.8                                   | 0.5     |
| >0.5 (Large)     | 47.5                                   | 2.66    |

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

Dihedral-angle violations less than 1° are not included in the calculation.

| Bins (°)           | Average number of violations per model | Max (°) |
|--------------------|----------------------------------------|---------|
| 1.0-10.0 (Small)   | 1.8                                    | 3.3     |
| 10.0-20.0 (Medium) | None                                   | None    |
| >20.0 (Large)      | None                                   | None    |

## 9 Distance violation analysis ⓘ

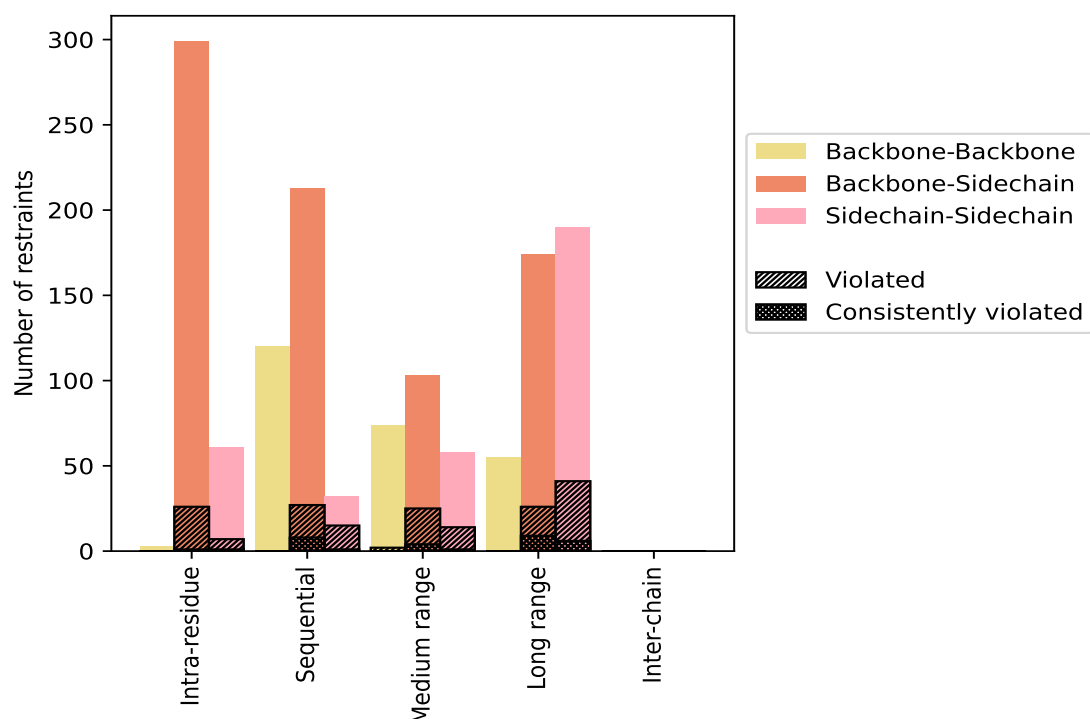
### 9.1 Summary of distance violations ⓘ

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

| Restrains type                                                              | Count       | % <sup>1</sup> | Violated <sup>3</sup> |                |                | Consistently Violated <sup>4</sup> |                |                |
|-----------------------------------------------------------------------------|-------------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
|                                                                             |             |                | Count                 | % <sup>2</sup> | % <sup>1</sup> | Count                              | % <sup>2</sup> | % <sup>1</sup> |
| <b>Intra-residue (<math> i-j =0</math>)</b>                                 | <b>363</b>  | <b>26.3</b>    | <b>33</b>             | <b>9.1</b>     | <b>2.4</b>     | <b>2</b>                           | <b>0.6</b>     | <b>0.1</b>     |
| Backbone-Backbone                                                           | 3           | 0.2            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 299         | 21.6           | 26                    | 8.7            | 1.9            | 1                                  | 0.3            | 0.1            |
| Sidechain-Sidechain                                                         | 61          | 4.4            | 7                     | 11.5           | 0.5            | 1                                  | 1.6            | 0.1            |
| <b>Sequential (<math> i-j =1</math>)</b>                                    | <b>365</b>  | <b>26.4</b>    | <b>42</b>             | <b>11.5</b>    | <b>3.0</b>     | <b>9</b>                           | <b>2.5</b>     | <b>0.7</b>     |
| Backbone-Backbone                                                           | 120         | 8.7            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 213         | 15.4           | 27                    | 12.7           | 2.0            | 8                                  | 3.8            | 0.6            |
| Sidechain-Sidechain                                                         | 32          | 2.3            | 15                    | 46.9           | 1.1            | 1                                  | 3.1            | 0.1            |
| <b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b> | <b>235</b>  | <b>17.0</b>    | <b>41</b>             | <b>17.4</b>    | <b>3.0</b>     | <b>5</b>                           | <b>2.1</b>     | <b>0.4</b>     |
| Backbone-Backbone                                                           | 74          | 5.4            | 2                     | 2.7            | 0.1            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 103         | 7.5            | 25                    | 24.3           | 1.8            | 4                                  | 3.9            | 0.3            |
| Sidechain-Sidechain                                                         | 58          | 4.2            | 14                    | 24.1           | 1.0            | 1                                  | 1.7            | 0.1            |
| <b>Long range (<math> i-j \geq 5</math>)</b>                                | <b>417</b>  | <b>30.2</b>    | <b>67</b>             | <b>16.1</b>    | <b>4.8</b>     | <b>15</b>                          | <b>3.6</b>     | <b>1.1</b>     |
| Backbone-Backbone                                                           | 55          | 4.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 172         | 12.4           | 26                    | 15.1           | 1.9            | 9                                  | 5.2            | 0.7            |
| Sidechain-Sidechain                                                         | 190         | 13.7           | 41                    | 21.6           | 3.0            | 6                                  | 3.2            | 0.4            |
| <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>2</b>    | <b>0.1</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>1382</b> | <b>100.0</b>   | <b>183</b>            | <b>13.2</b>    | <b>13.2</b>    | <b>31</b>                          | <b>2.2</b>     | <b>2.2</b>     |
| Backbone-Backbone                                                           | 252         | 18.2           | 2                     | 0.8            | 0.1            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 789         | 57.1           | 104                   | 13.2           | 7.5            | 22                                 | 2.8            | 1.6            |
| Sidechain-Sidechain                                                         | 341         | 24.7           | 77                    | 22.6           | 5.6            | 9                                  | 2.6            | 0.7            |

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

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



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and 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        | 16                   | 23              | 19              | 31              | 0               | 89    | 0.64     | 2.05    | 0.47                | 0.51       |
| 2        | 16                   | 23              | 20              | 34              | 0               | 93    | 0.62     | 1.99    | 0.47                | 0.45       |
| 3        | 14                   | 22              | 18              | 29              | 0               | 83    | 0.62     | 2.11    | 0.47                | 0.49       |
| 4        | 17                   | 20              | 21              | 36              | 0               | 94    | 0.63     | 2.25    | 0.48                | 0.51       |
| 5        | 14                   | 23              | 14              | 32              | 0               | 83    | 0.69     | 2.08    | 0.5                 | 0.54       |
| 6        | 21                   | 25              | 25              | 36              | 0               | 107   | 0.65     | 2.15    | 0.49                | 0.52       |
| 7        | 16                   | 23              | 24              | 38              | 0               | 101   | 0.65     | 2.3     | 0.5                 | 0.53       |
| 8        | 14                   | 27              | 16              | 30              | 0               | 87    | 0.59     | 2.08    | 0.45                | 0.46       |
| 9        | 17                   | 20              | 18              | 39              | 0               | 94    | 0.67     | 2.14    | 0.47                | 0.6        |
| 10       | 15                   | 17              | 16              | 36              | 0               | 84    | 0.59     | 2.24    | 0.45                | 0.44       |

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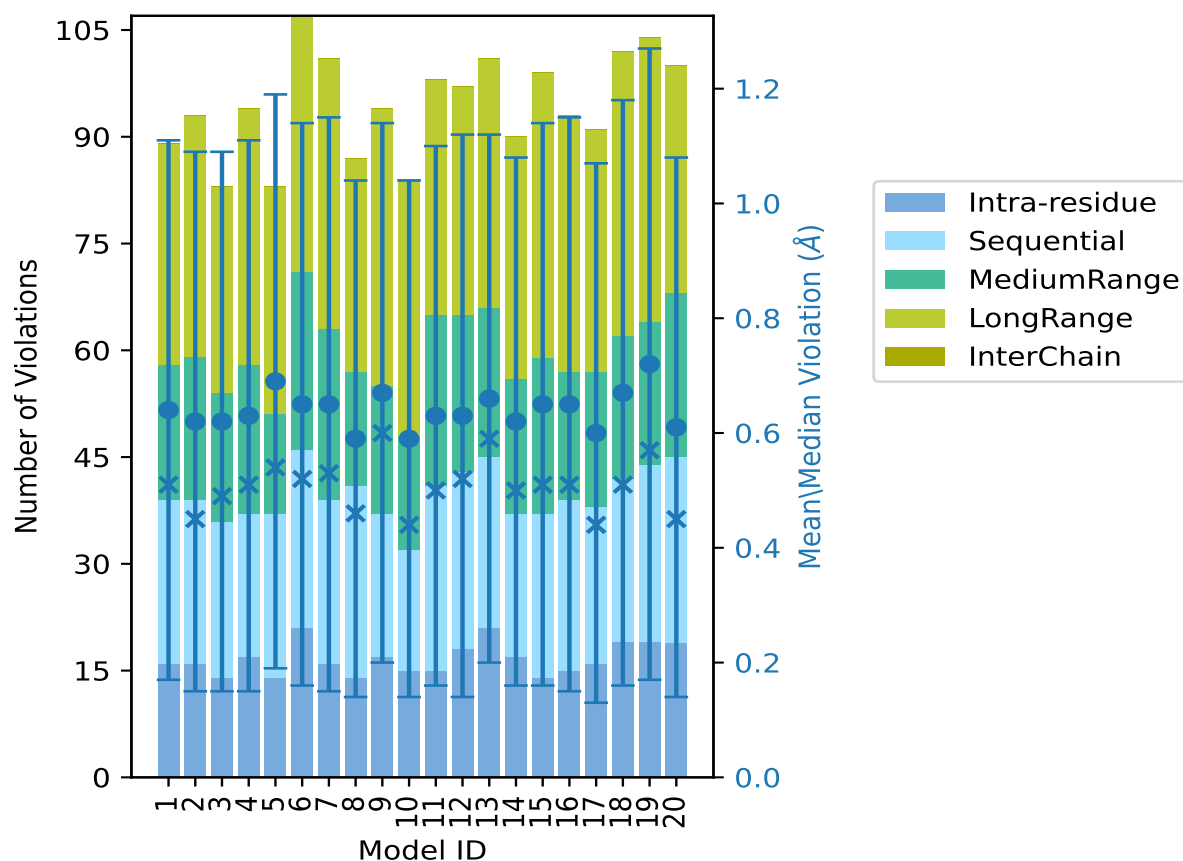
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| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 11       | 15                   | 26              | 24              | 33              | 0               | 98    | 0.63     | 2.41    | 0.47                | 0.5        |
| 12       | 18                   | 25              | 22              | 32              | 0               | 97    | 0.63     | 2.45    | 0.49                | 0.52       |
| 13       | 21                   | 24              | 21              | 35              | 0               | 101   | 0.66     | 2.05    | 0.46                | 0.59       |
| 14       | 17                   | 20              | 19              | 34              | 0               | 90    | 0.62     | 1.99    | 0.46                | 0.5        |
| 15       | 14                   | 23              | 22              | 40              | 0               | 99    | 0.65     | 2.66    | 0.49                | 0.51       |
| 16       | 15                   | 24              | 18              | 36              | 0               | 93    | 0.65     | 2.25    | 0.5                 | 0.51       |
| 17       | 16                   | 22              | 19              | 34              | 0               | 91    | 0.6      | 2.08    | 0.47                | 0.44       |
| 18       | 19                   | 23              | 20              | 40              | 0               | 102   | 0.67     | 2.25    | 0.51                | 0.51       |
| 19       | 19                   | 25              | 20              | 40              | 0               | 104   | 0.72     | 2.29    | 0.55                | 0.57       |
| 20       | 19                   | 26              | 23              | 32              | 0               | 100   | 0.61     | 2.14    | 0.47                | 0.45       |

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

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

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



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

### 9.3 Distance violation statistics for the ensemble

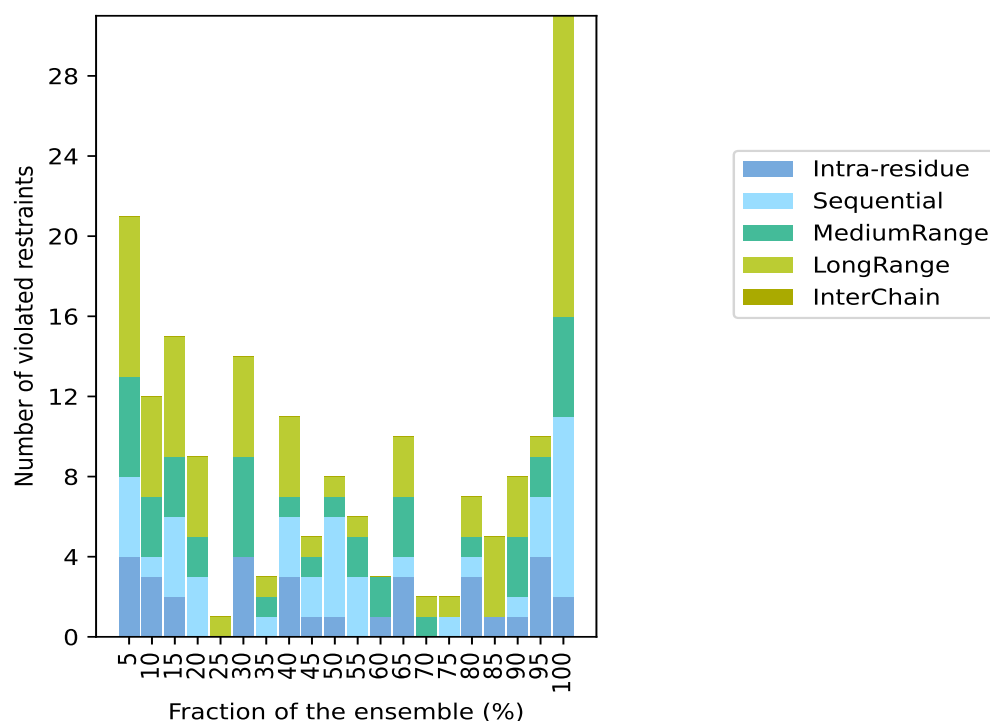
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1197(IR:330, SQ:323, MR:194, LR:350, IC:0) restraints are 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>       | %     |
| 4                             | 4               | 5               | 8               | 0               | 21    | 1                        | 5.0   |
| 3                             | 1               | 3               | 5               | 0               | 12    | 2                        | 10.0  |
| 2                             | 4               | 3               | 6               | 0               | 15    | 3                        | 15.0  |
| 0                             | 3               | 2               | 4               | 0               | 9     | 4                        | 20.0  |
| 0                             | 0               | 0               | 1               | 0               | 1     | 5                        | 25.0  |
| 4                             | 0               | 5               | 5               | 0               | 14    | 6                        | 30.0  |
| 0                             | 1               | 1               | 1               | 0               | 3     | 7                        | 35.0  |
| 3                             | 3               | 1               | 4               | 0               | 11    | 8                        | 40.0  |
| 1                             | 2               | 1               | 1               | 0               | 5     | 9                        | 45.0  |
| 1                             | 5               | 1               | 1               | 0               | 8     | 10                       | 50.0  |
| 0                             | 3               | 2               | 1               | 0               | 6     | 11                       | 55.0  |
| 1                             | 0               | 2               | 0               | 0               | 3     | 12                       | 60.0  |
| 3                             | 1               | 3               | 3               | 0               | 10    | 13                       | 65.0  |
| 0                             | 0               | 1               | 1               | 0               | 2     | 14                       | 70.0  |
| 0                             | 1               | 0               | 1               | 0               | 2     | 15                       | 75.0  |
| 3                             | 1               | 1               | 2               | 0               | 7     | 16                       | 80.0  |
| 1                             | 0               | 0               | 4               | 0               | 5     | 17                       | 85.0  |
| 1                             | 1               | 3               | 3               | 0               | 8     | 18                       | 90.0  |
| 4                             | 3               | 2               | 1               | 0               | 10    | 19                       | 95.0  |
| 2                             | 9               | 5               | 15              | 0               | 31    | 20                       | 100.0 |

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

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

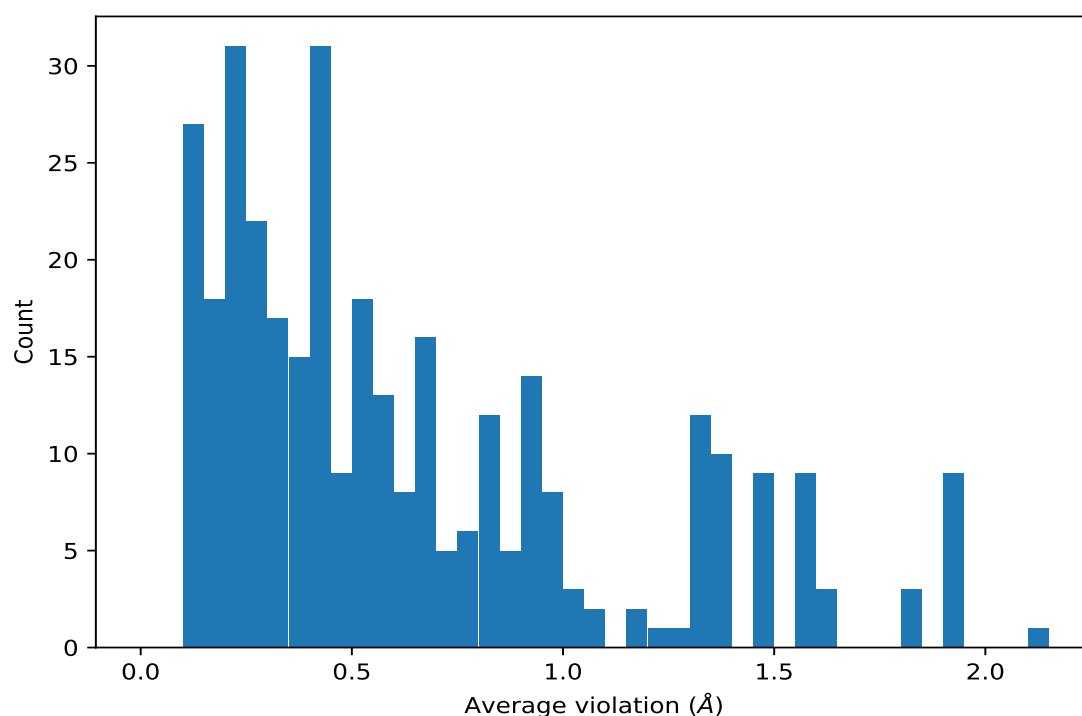
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,835)  | 1:29:A:PRO:HG2  | 1:43:A:LEU:HB2  | 20                  | 2.1      | 0.2                 | 2.12       |
| (1,1187) | 1:34:A:LEU:HD11 | 1:41:A:ALA:HA   | 20                  | 1.82     | 0.06                | 1.83       |
| (1,1187) | 1:34:A:LEU:HD12 | 1:41:A:ALA:HA   | 20                  | 1.82     | 0.06                | 1.83       |
| (1,1187) | 1:34:A:LEU:HD13 | 1:41:A:ALA:HA   | 20                  | 1.82     | 0.06                | 1.83       |
| (1,89)   | 1:8:A:VAL:HG11  | 1:43:A:LEU:H    | 20                  | 1.63     | 0.31                | 1.68       |
| (1,89)   | 1:8:A:VAL:HG12  | 1:43:A:LEU:H    | 20                  | 1.63     | 0.31                | 1.68       |
| (1,89)   | 1:8:A:VAL:HG13  | 1:43:A:LEU:H    | 20                  | 1.63     | 0.31                | 1.68       |
| (1,1189) | 1:20:A:LEU:HD21 | 1:34:A:LEU:HD11 | 20                  | 1.48     | 0.58                | 1.79       |
| (1,1189) | 1:20:A:LEU:HD21 | 1:34:A:LEU:HD12 | 20                  | 1.48     | 0.58                | 1.79       |
| (1,1189) | 1:20:A:LEU:HD21 | 1:34:A:LEU:HD13 | 20                  | 1.48     | 0.58                | 1.79       |
| (1,1189) | 1:20:A:LEU:HD22 | 1:34:A:LEU:HD11 | 20                  | 1.48     | 0.58                | 1.79       |
| (1,1189) | 1:20:A:LEU:HD22 | 1:34:A:LEU:HD12 | 20                  | 1.48     | 0.58                | 1.79       |
| (1,1189) | 1:20:A:LEU:HD22 | 1:34:A:LEU:HD13 | 20                  | 1.48     | 0.58                | 1.79       |
| (1,1189) | 1:20:A:LEU:HD23 | 1:34:A:LEU:HD11 | 20                  | 1.48     | 0.58                | 1.79       |
| (1,1189) | 1:20:A:LEU:HD23 | 1:34:A:LEU:HD12 | 20                  | 1.48     | 0.58                | 1.79       |
| (1,1189) | 1:20:A:LEU:HD23 | 1:34:A:LEU:HD13 | 20                  | 1.48     | 0.58                | 1.79       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1322) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HD11 | 20                  | 1.33     | 0.08                | 1.36       |
| (1,1322) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HD12 | 20                  | 1.33     | 0.08                | 1.36       |
| (1,1322) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HD13 | 20                  | 1.33     | 0.08                | 1.36       |
| (1,708)  | 1:42:A:PHE:HA   | 1:43:A:LEU:HB3  | 20                  | 1.19     | 0.02                | 1.18       |
| (1,482)  | 1:10:A:SER:HB3  | 1:75:A:ASN:HD21 | 20                  | 1.18     | 0.38                | 1.26       |
| (1,819)  | 1:67:A:THR:HA   | 1:68:A:LEU:HB3  | 20                  | 1.09     | 0.07                | 1.1        |
| (1,590)  | 1:29:A:PRO:HA   | 1:43:A:LEU:HB2  | 20                  | 1.07     | 0.18                | 1.1        |
| (1,309)  | 1:58:A:MET:H    | 1:59:A:ASP:HB3  | 20                  | 0.99     | 0.38                | 1.18       |
| (1,792)  | 1:11:A:LEU:HB3  | 1:39:A:GLY:HA3  | 20                  | 0.93     | 0.19                | 0.91       |
| (1,674)  | 1:68:A:LEU:HB2  | 1:71:A:GLU:HA   | 20                  | 0.93     | 0.39                | 0.83       |
| (1,711)  | 1:68:A:LEU:HD11 | 1:73:A:LYS:HA   | 20                  | 0.85     | 0.21                | 0.88       |
| (1,711)  | 1:68:A:LEU:HD12 | 1:73:A:LYS:HA   | 20                  | 0.85     | 0.21                | 0.88       |
| (1,711)  | 1:68:A:LEU:HD13 | 1:73:A:LYS:HA   | 20                  | 0.85     | 0.21                | 0.88       |
| (1,874)  | 1:74:A:ILE:HA   | 1:75:A:ASN:HB2  | 20                  | 0.84     | 0.03                | 0.84       |
| (1,536)  | 1:11:A:LEU:HB3  | 1:39:A:GLY:H    | 20                  | 0.8      | 0.16                | 0.78       |
| (1,55)   | 1:68:A:LEU:HD11 | 1:69:A:LEU:H    | 20                  | 0.78     | 0.15                | 0.8        |
| (1,55)   | 1:68:A:LEU:HD12 | 1:69:A:LEU:H    | 20                  | 0.78     | 0.15                | 0.8        |
| (1,55)   | 1:68:A:LEU:HD13 | 1:69:A:LEU:H    | 20                  | 0.78     | 0.15                | 0.8        |
| (1,785)  | 1:11:A:LEU:HB2  | 1:12:A:PRO:HD3  | 20                  | 0.73     | 0.07                | 0.74       |
| (1,181)  | 1:68:A:LEU:HB2  | 1:72:A:LYS:H    | 20                  | 0.7      | 0.25                | 0.74       |
| (1,1246) | 1:7:A:PHE:HA    | 1:8:A:VAL:HG11  | 20                  | 0.69     | 0.05                | 0.68       |
| (1,1246) | 1:7:A:PHE:HA    | 1:8:A:VAL:HG12  | 20                  | 0.69     | 0.05                | 0.68       |
| (1,1246) | 1:7:A:PHE:HA    | 1:8:A:VAL:HG13  | 20                  | 0.69     | 0.05                | 0.68       |
| (1,212)  | 1:8:A:VAL:HG21  | 1:75:A:ASN:H    | 20                  | 0.68     | 0.15                | 0.6        |
| (1,212)  | 1:8:A:VAL:HG22  | 1:75:A:ASN:H    | 20                  | 0.68     | 0.15                | 0.6        |
| (1,212)  | 1:8:A:VAL:HG23  | 1:75:A:ASN:H    | 20                  | 0.68     | 0.15                | 0.6        |
| (1,773)  | 1:65:A:HIS:HB3  | 1:75:A:ASN:HA   | 20                  | 0.66     | 0.09                | 0.64       |
| (1,1224) | 1:8:A:VAL:HG21  | 1:9:A:GLY:H     | 20                  | 0.63     | 0.06                | 0.64       |
| (1,1224) | 1:8:A:VAL:HG22  | 1:9:A:GLY:H     | 20                  | 0.63     | 0.06                | 0.64       |
| (1,1224) | 1:8:A:VAL:HG23  | 1:9:A:GLY:H     | 20                  | 0.63     | 0.06                | 0.64       |
| (1,1248) | 1:8:A:VAL:HG11  | 1:43:A:LEU:HD21 | 20                  | 0.56     | 0.24                | 0.62       |
| (1,1248) | 1:8:A:VAL:HG11  | 1:43:A:LEU:HD22 | 20                  | 0.56     | 0.24                | 0.62       |
| (1,1248) | 1:8:A:VAL:HG11  | 1:43:A:LEU:HD23 | 20                  | 0.56     | 0.24                | 0.62       |
| (1,1248) | 1:8:A:VAL:HG12  | 1:43:A:LEU:HD21 | 20                  | 0.56     | 0.24                | 0.62       |
| (1,1248) | 1:8:A:VAL:HG12  | 1:43:A:LEU:HD22 | 20                  | 0.56     | 0.24                | 0.62       |
| (1,1248) | 1:8:A:VAL:HG12  | 1:43:A:LEU:HD23 | 20                  | 0.56     | 0.24                | 0.62       |
| (1,1248) | 1:8:A:VAL:HG13  | 1:43:A:LEU:HD21 | 20                  | 0.56     | 0.24                | 0.62       |
| (1,1248) | 1:8:A:VAL:HG13  | 1:43:A:LEU:HD22 | 20                  | 0.56     | 0.24                | 0.62       |
| (1,1248) | 1:8:A:VAL:HG13  | 1:43:A:LEU:HD23 | 20                  | 0.56     | 0.24                | 0.62       |
| (1,868)  | 1:9:A:GLY:H     | 1:75:A:ASN:HB3  | 20                  | 0.55     | 0.16                | 0.5        |
| (1,820)  | 1:68:A:LEU:HB2  | 1:71:A:GLU:H    | 20                  | 0.53     | 0.27                | 0.52       |
| (1,1378) | 1:23:A:HIS:HB3  | 1:23:A:HIS:HE1  | 20                  | 0.51     | 0.02                | 0.52       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,890)  | 1:59:A:ASP:HA   | 1:62:A:LEU:HB3  | 20                  | 0.5      | 0.15                | 0.5        |
| (1,1030) | 1:29:A:PRO:HB2  | 1:43:A:LEU:HB2  | 20                  | 0.48     | 0.17                | 0.5        |
| (1,53)   | 1:68:A:LEU:HB2  | 1:69:A:LEU:H    | 20                  | 0.42     | 0.05                | 0.44       |
| (1,328)  | 1:62:A:LEU:H    | 1:62:A:LEU:HB3  | 20                  | 0.35     | 0.03                | 0.35       |
| (1,1011) | 1:65:A:HIS:HB3  | 1:76:A:VAL:HB   | 20                  | 0.34     | 0.05                | 0.34       |
| (1,670)  | 1:20:A:LEU:HA   | 1:23:A:HIS:HB3  | 19                  | 0.82     | 0.39                | 0.91       |
| (1,958)  | 1:77:A:GLU:HB2  | 1:78:A:LEU:HD11 | 19                  | 0.82     | 0.11                | 0.82       |
| (1,958)  | 1:77:A:GLU:HB2  | 1:78:A:LEU:HD12 | 19                  | 0.82     | 0.11                | 0.82       |
| (1,958)  | 1:77:A:GLU:HB2  | 1:78:A:LEU:HD13 | 19                  | 0.82     | 0.11                | 0.82       |
| (1,1040) | 1:12:A:PRO:HG2  | 1:70:A:LYS:HB3  | 19                  | 0.78     | 0.31                | 0.84       |
| (1,304)  | 1:56:A:ARG:H    | 1:59:A:ASP:HB3  | 19                  | 0.71     | 0.42                | 0.99       |
| (1,1280) | 1:36:A:ALA:HB1  | 1:37:A:ASP:HB3  | 19                  | 0.68     | 0.09                | 0.7        |
| (1,1280) | 1:36:A:ALA:HB2  | 1:37:A:ASP:HB3  | 19                  | 0.68     | 0.09                | 0.7        |
| (1,1280) | 1:36:A:ALA:HB3  | 1:37:A:ASP:HB3  | 19                  | 0.68     | 0.09                | 0.7        |
| (1,727)  | 1:37:A:ASP:HA   | 1:37:A:ASP:HB2  | 19                  | 0.43     | 0.01                | 0.43       |
| (1,343)  | 1:68:A:LEU:H    | 1:68:A:LEU:HB3  | 19                  | 0.37     | 0.05                | 0.37       |
| (1,592)  | 1:10:A:SER:H    | 1:10:A:SER:HB3  | 19                  | 0.24     | 0.06                | 0.26       |
| (1,787)  | 1:11:A:LEU:HB2  | 1:12:A:PRO:HD2  | 19                  | 0.19     | 0.05                | 0.18       |
| (1,673)  | 1:71:A:GLU:HA   | 1:71:A:GLU:HB2  | 19                  | 0.15     | 0.01                | 0.15       |
| (1,809)  | 1:7:A:PHE:HZ    | 1:9:A:GLY:HA2   | 18                  | 0.98     | 0.34                | 1.03       |
| (1,252)  | 1:63:A:LEU:H    | 1:64:A:GLN:HG3  | 18                  | 0.86     | 0.12                | 0.88       |
| (1,489)  | 1:10:A:SER:HB3  | 1:75:A:ASN:HD22 | 18                  | 0.84     | 0.31                | 0.82       |
| (1,76)   | 1:68:A:LEU:HD11 | 1:73:A:LYS:H    | 18                  | 0.65     | 0.24                | 0.66       |
| (1,76)   | 1:68:A:LEU:HD12 | 1:73:A:LYS:H    | 18                  | 0.65     | 0.24                | 0.66       |
| (1,76)   | 1:68:A:LEU:HD13 | 1:73:A:LYS:H    | 18                  | 0.65     | 0.24                | 0.66       |
| (1,811)  | 1:7:A:PHE:HE1   | 1:9:A:GLY:HA2   | 18                  | 0.51     | 0.3                 | 0.5        |
| (1,811)  | 1:7:A:PHE:HE2   | 1:9:A:GLY:HA2   | 18                  | 0.51     | 0.3                 | 0.5        |
| (1,88)   | 1:78:A:LEU:H    | 1:78:A:LEU:HD11 | 18                  | 0.33     | 0.09                | 0.33       |
| (1,88)   | 1:78:A:LEU:H    | 1:78:A:LEU:HD12 | 18                  | 0.33     | 0.09                | 0.33       |
| (1,88)   | 1:78:A:LEU:H    | 1:78:A:LEU:HD13 | 18                  | 0.33     | 0.09                | 0.33       |
| (1,15)   | 1:6:A:VAL:H     | 1:43:A:LEU:HB3  | 18                  | 0.26     | 0.06                | 0.27       |
| (1,182)  | 1:68:A:LEU:HD11 | 1:72:A:LYS:H    | 18                  | 0.13     | 0.01                | 0.13       |
| (1,182)  | 1:68:A:LEU:HD12 | 1:72:A:LYS:H    | 18                  | 0.13     | 0.01                | 0.13       |
| (1,182)  | 1:68:A:LEU:HD13 | 1:72:A:LYS:H    | 18                  | 0.13     | 0.01                | 0.13       |
| (1,1201) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD21 | 17                  | 0.91     | 0.33                | 1.0        |
| (1,1201) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD22 | 17                  | 0.91     | 0.33                | 1.0        |
| (1,1201) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD23 | 17                  | 0.91     | 0.33                | 1.0        |
| (1,1012) | 1:65:A:HIS:HB3  | 1:76:A:VAL:HG21 | 17                  | 0.3      | 0.18                | 0.26       |
| (1,1012) | 1:65:A:HIS:HB3  | 1:76:A:VAL:HG22 | 17                  | 0.3      | 0.18                | 0.26       |
| (1,1012) | 1:65:A:HIS:HB3  | 1:76:A:VAL:HG23 | 17                  | 0.3      | 0.18                | 0.26       |
| (1,1024) | 1:29:A:PRO:HB3  | 1:44:A:GLU:H    | 17                  | 0.29     | 0.06                | 0.31       |
| (1,789)  | 1:11:A:LEU:HB3  | 1:39:A:GLY:HA2  | 17                  | 0.27     | 0.16                | 0.23       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,312)  | 1:58:A:MET:H    | 1:58:A:MET:HB3  | 17                  | 0.21     | 0.06                | 0.22       |
| (1,1163) | 1:4:A:PHE:HB2   | 1:78:A:LEU:HD21 | 16                  | 0.93     | 0.64                | 0.91       |
| (1,1163) | 1:4:A:PHE:HB2   | 1:78:A:LEU:HD22 | 16                  | 0.93     | 0.64                | 0.91       |
| (1,1163) | 1:4:A:PHE:HB2   | 1:78:A:LEU:HD23 | 16                  | 0.93     | 0.64                | 0.91       |
| (1,1163) | 1:4:A:PHE:HB3   | 1:78:A:LEU:HD21 | 16                  | 0.93     | 0.64                | 0.91       |
| (1,1163) | 1:4:A:PHE:HB3   | 1:78:A:LEU:HD22 | 16                  | 0.93     | 0.64                | 0.91       |
| (1,1163) | 1:4:A:PHE:HB3   | 1:78:A:LEU:HD23 | 16                  | 0.93     | 0.64                | 0.91       |
| (1,1313) | 1:58:A:MET:HB3  | 1:58:A:MET:HE1  | 16                  | 0.53     | 0.25                | 0.5        |
| (1,1313) | 1:58:A:MET:HB3  | 1:58:A:MET:HE2  | 16                  | 0.53     | 0.25                | 0.5        |
| (1,1313) | 1:58:A:MET:HB3  | 1:58:A:MET:HE3  | 16                  | 0.53     | 0.25                | 0.5        |
| (1,180)  | 1:72:A:LYS:H    | 1:72:A:LYS:HG3  | 16                  | 0.36     | 0.16                | 0.3        |
| (1,197)  | 1:23:A:HIS:H    | 1:23:A:HIS:HB3  | 16                  | 0.32     | 0.11                | 0.32       |
| (1,1226) | 1:8:A:VAL:HG21  | 1:11:A:LEU:HD21 | 16                  | 0.24     | 0.08                | 0.22       |
| (1,1226) | 1:8:A:VAL:HG21  | 1:11:A:LEU:HD22 | 16                  | 0.24     | 0.08                | 0.22       |
| (1,1226) | 1:8:A:VAL:HG21  | 1:11:A:LEU:HD23 | 16                  | 0.24     | 0.08                | 0.22       |
| (1,1226) | 1:8:A:VAL:HG22  | 1:11:A:LEU:HD21 | 16                  | 0.24     | 0.08                | 0.22       |
| (1,1226) | 1:8:A:VAL:HG22  | 1:11:A:LEU:HD22 | 16                  | 0.24     | 0.08                | 0.22       |
| (1,1226) | 1:8:A:VAL:HG22  | 1:11:A:LEU:HD23 | 16                  | 0.24     | 0.08                | 0.22       |
| (1,1226) | 1:8:A:VAL:HG23  | 1:11:A:LEU:HD21 | 16                  | 0.24     | 0.08                | 0.22       |
| (1,1226) | 1:8:A:VAL:HG23  | 1:11:A:LEU:HD22 | 16                  | 0.24     | 0.08                | 0.22       |
| (1,1226) | 1:8:A:VAL:HG23  | 1:11:A:LEU:HD23 | 16                  | 0.24     | 0.08                | 0.22       |
| (1,808)  | 1:9:A:GLY:HA2   | 1:40:A:ILE:HG13 | 16                  | 0.21     | 0.05                | 0.22       |
| (1,892)  | 1:62:A:LEU:HB2  | 1:63:A:LEU:HA   | 16                  | 0.18     | 0.07                | 0.16       |
| (1,1258) | 1:79:A:THR:HG21 | 1:80:A:VAL:HG11 | 15                  | 1.38     | 0.73                | 1.89       |
| (1,1258) | 1:79:A:THR:HG21 | 1:80:A:VAL:HG12 | 15                  | 1.38     | 0.73                | 1.89       |
| (1,1258) | 1:79:A:THR:HG21 | 1:80:A:VAL:HG13 | 15                  | 1.38     | 0.73                | 1.89       |
| (1,1258) | 1:79:A:THR:HG22 | 1:80:A:VAL:HG11 | 15                  | 1.38     | 0.73                | 1.89       |
| (1,1258) | 1:79:A:THR:HG22 | 1:80:A:VAL:HG12 | 15                  | 1.38     | 0.73                | 1.89       |
| (1,1258) | 1:79:A:THR:HG22 | 1:80:A:VAL:HG13 | 15                  | 1.38     | 0.73                | 1.89       |
| (1,1258) | 1:79:A:THR:HG23 | 1:80:A:VAL:HG11 | 15                  | 1.38     | 0.73                | 1.89       |
| (1,1258) | 1:79:A:THR:HG23 | 1:80:A:VAL:HG12 | 15                  | 1.38     | 0.73                | 1.89       |
| (1,1258) | 1:79:A:THR:HG23 | 1:80:A:VAL:HG13 | 15                  | 1.38     | 0.73                | 1.89       |
| (1,1161) | 1:4:A:PHE:HD1   | 1:78:A:LEU:HD21 | 15                  | 0.99     | 0.63                | 0.85       |
| (1,1161) | 1:4:A:PHE:HD1   | 1:78:A:LEU:HD22 | 15                  | 0.99     | 0.63                | 0.85       |
| (1,1161) | 1:4:A:PHE:HD1   | 1:78:A:LEU:HD23 | 15                  | 0.99     | 0.63                | 0.85       |
| (1,1161) | 1:4:A:PHE:HD2   | 1:78:A:LEU:HD21 | 15                  | 0.99     | 0.63                | 0.85       |
| (1,1161) | 1:4:A:PHE:HD2   | 1:78:A:LEU:HD22 | 15                  | 0.99     | 0.63                | 0.85       |
| (1,1161) | 1:4:A:PHE:HD2   | 1:78:A:LEU:HD23 | 15                  | 0.99     | 0.63                | 0.85       |
| (1,1222) | 1:16:A:THR:HG21 | 1:18:A:VAL:HG21 | 14                  | 1.93     | 0.54                | 2.09       |
| (1,1222) | 1:16:A:THR:HG21 | 1:18:A:VAL:HG22 | 14                  | 1.93     | 0.54                | 2.09       |
| (1,1222) | 1:16:A:THR:HG21 | 1:18:A:VAL:HG23 | 14                  | 1.93     | 0.54                | 2.09       |
| (1,1222) | 1:16:A:THR:HG22 | 1:18:A:VAL:HG21 | 14                  | 1.93     | 0.54                | 2.09       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1222) | 1:16:A:THR:HG22 | 1:18:A:VAL:HG22 | 14                  | 1.93     | 0.54                | 2.09       |
| (1,1222) | 1:16:A:THR:HG22 | 1:18:A:VAL:HG23 | 14                  | 1.93     | 0.54                | 2.09       |
| (1,1222) | 1:16:A:THR:HG23 | 1:18:A:VAL:HG21 | 14                  | 1.93     | 0.54                | 2.09       |
| (1,1222) | 1:16:A:THR:HG23 | 1:18:A:VAL:HG22 | 14                  | 1.93     | 0.54                | 2.09       |
| (1,1222) | 1:16:A:THR:HG23 | 1:18:A:VAL:HG23 | 14                  | 1.93     | 0.54                | 2.09       |
| (1,961)  | 1:7:A:PHE:HB2   | 1:77:A:GLU:HB2  | 14                  | 0.81     | 0.0                 | 0.81       |
| (1,803)  | 1:80:A:VAL:HG21 | 1:81:A:GLY:HA3  | 13                  | 1.58     | 0.1                 | 1.64       |
| (1,803)  | 1:80:A:VAL:HG22 | 1:81:A:GLY:HA3  | 13                  | 1.58     | 0.1                 | 1.64       |
| (1,803)  | 1:80:A:VAL:HG23 | 1:81:A:GLY:HA3  | 13                  | 1.58     | 0.1                 | 1.64       |
| (1,803)  | 1:80:A:VAL:HG21 | 1:81:A:GLY:HA2  | 13                  | 1.58     | 0.1                 | 1.64       |
| (1,803)  | 1:80:A:VAL:HG22 | 1:81:A:GLY:HA2  | 13                  | 1.58     | 0.1                 | 1.64       |
| (1,803)  | 1:80:A:VAL:HG23 | 1:81:A:GLY:HA2  | 13                  | 1.58     | 0.1                 | 1.64       |
| (1,692)  | 1:4:A:PHE:HA    | 1:80:A:VAL:HG21 | 13                  | 1.3      | 0.4                 | 1.34       |
| (1,692)  | 1:4:A:PHE:HA    | 1:80:A:VAL:HG22 | 13                  | 1.3      | 0.4                 | 1.34       |
| (1,692)  | 1:4:A:PHE:HA    | 1:80:A:VAL:HG23 | 13                  | 1.3      | 0.4                 | 1.34       |
| (1,481)  | 1:18:A:VAL:HG11 | 1:22:A:ASN:HD21 | 13                  | 1.0      | 0.19                | 1.03       |
| (1,481)  | 1:18:A:VAL:HG12 | 1:22:A:ASN:HD21 | 13                  | 1.0      | 0.19                | 1.03       |
| (1,481)  | 1:18:A:VAL:HG13 | 1:22:A:ASN:HD21 | 13                  | 1.0      | 0.19                | 1.03       |
| (1,644)  | 1:56:A:ARG:HA   | 1:59:A:ASP:HB3  | 13                  | 0.81     | 0.22                | 0.91       |
| (1,418)  | 1:80:A:VAL:HG21 | 1:82:A:GLY:H    | 13                  | 0.8      | 0.51                | 0.58       |
| (1,418)  | 1:80:A:VAL:HG22 | 1:82:A:GLY:H    | 13                  | 0.8      | 0.51                | 0.58       |
| (1,418)  | 1:80:A:VAL:HG23 | 1:82:A:GLY:H    | 13                  | 0.8      | 0.51                | 0.58       |
| (1,378)  | 1:38:A:LYS:H    | 1:38:A:LYS:HG3  | 13                  | 0.67     | 0.14                | 0.74       |
| (1,744)  | 1:38:A:LYS:HA   | 1:38:A:LYS:HG3  | 13                  | 0.41     | 0.06                | 0.4        |
| (1,580)  | 1:10:A:SER:HB2  | 1:74:A:ILE:HB   | 13                  | 0.39     | 0.07                | 0.41       |
| (1,957)  | 1:6:A:VAL:HB    | 1:43:A:LEU:HB3  | 13                  | 0.21     | 0.07                | 0.2        |
| (1,1241) | 1:18:A:VAL:H    | 1:18:A:VAL:HG21 | 13                  | 0.21     | 0.03                | 0.21       |
| (1,1241) | 1:18:A:VAL:H    | 1:18:A:VAL:HG22 | 13                  | 0.21     | 0.03                | 0.21       |
| (1,1241) | 1:18:A:VAL:H    | 1:18:A:VAL:HG23 | 13                  | 0.21     | 0.03                | 0.21       |
| (1,1004) | 1:54:A:ILE:HD11 | 1:58:A:MET:HB3  | 12                  | 0.44     | 0.23                | 0.43       |
| (1,1004) | 1:54:A:ILE:HD12 | 1:58:A:MET:HB3  | 12                  | 0.44     | 0.23                | 0.43       |
| (1,1004) | 1:54:A:ILE:HD13 | 1:58:A:MET:HB3  | 12                  | 0.44     | 0.23                | 0.43       |
| (1,149)  | 1:23:A:HIS:HB2  | 1:25:A:LYS:H    | 12                  | 0.21     | 0.07                | 0.2        |
| (1,685)  | 1:13:A:ARG:HA   | 1:13:A:ARG:HB2  | 12                  | 0.2      | 0.01                | 0.2        |
| (1,877)  | 1:7:A:PHE:HB3   | 1:79:A:THR:HB   | 11                  | 0.69     | 0.17                | 0.7        |
| (1,1336) | 1:59:A:ASP:HB3  | 1:60:A:ILE:HD11 | 11                  | 0.5      | 0.19                | 0.52       |
| (1,1336) | 1:59:A:ASP:HB3  | 1:60:A:ILE:HD12 | 11                  | 0.5      | 0.19                | 0.52       |
| (1,1336) | 1:59:A:ASP:HB3  | 1:60:A:ILE:HD13 | 11                  | 0.5      | 0.19                | 0.52       |
| (1,1003) | 1:55:A:GLN:HA   | 1:58:A:MET:HB3  | 11                  | 0.38     | 0.08                | 0.42       |
| (1,468)  | 1:64:A:GLN:H    | 1:65:A:HIS:HB3  | 11                  | 0.22     | 0.07                | 0.21       |
| (1,440)  | 1:25:A:LYS:HB2  | 1:27:A:SER:H    | 11                  | 0.21     | 0.06                | 0.21       |
| (1,1041) | 1:70:A:LYS:HB3  | 1:71:A:GLU:H    | 11                  | 0.17     | 0.05                | 0.17       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,397)  | 1:55:A:GLN:HE22 | 1:56:A:ARG:H    | 10                  | 1.39     | 0.2                 | 1.47       |
| (1,1200) | 1:69:A:LEU:HD21 | 1:70:A:LYS:HA   | 10                  | 1.31     | 0.14                | 1.27       |
| (1,1200) | 1:69:A:LEU:HD22 | 1:70:A:LYS:HA   | 10                  | 1.31     | 0.14                | 1.27       |
| (1,1200) | 1:69:A:LEU:HD23 | 1:70:A:LYS:HA   | 10                  | 1.31     | 0.14                | 1.27       |
| (1,1198) | 1:69:A:LEU:HD21 | 1:70:A:LYS:H    | 10                  | 0.91     | 0.09                | 0.88       |
| (1,1198) | 1:69:A:LEU:HD22 | 1:70:A:LYS:H    | 10                  | 0.91     | 0.09                | 0.88       |
| (1,1198) | 1:69:A:LEU:HD23 | 1:70:A:LYS:H    | 10                  | 0.91     | 0.09                | 0.88       |
| (1,1359) | 1:23:A:HIS:HD2  | 1:64:A:GLN:HB2  | 10                  | 0.88     | 0.32                | 0.84       |
| (1,806)  | 1:68:A:LEU:HA   | 1:69:A:LEU:HB3  | 10                  | 0.61     | 0.17                | 0.66       |
| (1,1199) | 1:69:A:LEU:HA   | 1:69:A:LEU:HD21 | 10                  | 0.5      | 0.04                | 0.5        |
| (1,1199) | 1:69:A:LEU:HA   | 1:69:A:LEU:HD22 | 10                  | 0.5      | 0.04                | 0.5        |
| (1,1199) | 1:69:A:LEU:HA   | 1:69:A:LEU:HD23 | 10                  | 0.5      | 0.04                | 0.5        |
| (1,1148) | 1:68:A:LEU:HD21 | 1:71:A:GLU:HA   | 10                  | 0.47     | 0.13                | 0.52       |
| (1,1148) | 1:68:A:LEU:HD22 | 1:71:A:GLU:HA   | 10                  | 0.47     | 0.13                | 0.52       |
| (1,1148) | 1:68:A:LEU:HD23 | 1:71:A:GLU:HA   | 10                  | 0.47     | 0.13                | 0.52       |
| (1,69)   | 1:69:A:LEU:HB2  | 1:70:A:LYS:H    | 10                  | 0.21     | 0.04                | 0.2        |
| (1,598)  | 1:12:A:PRO:HA   | 1:72:A:LYS:HG2  | 9                   | 0.54     | 0.28                | 0.57       |
| (1,1160) | 1:78:A:LEU:HD21 | 1:79:A:THR:H    | 9                   | 0.43     | 0.19                | 0.41       |
| (1,1160) | 1:78:A:LEU:HD22 | 1:79:A:THR:H    | 9                   | 0.43     | 0.19                | 0.41       |
| (1,1160) | 1:78:A:LEU:HD23 | 1:79:A:THR:H    | 9                   | 0.43     | 0.19                | 0.41       |
| (1,1145) | 1:68:A:LEU:HD21 | 1:71:A:GLU:H    | 9                   | 0.39     | 0.08                | 0.36       |
| (1,1145) | 1:68:A:LEU:HD22 | 1:71:A:GLU:H    | 9                   | 0.39     | 0.08                | 0.36       |
| (1,1145) | 1:68:A:LEU:HD23 | 1:71:A:GLU:H    | 9                   | 0.39     | 0.08                | 0.36       |
| (1,566)  | 1:59:A:ASP:HB2  | 1:60:A:ILE:HA   | 9                   | 0.34     | 0.1                 | 0.35       |
| (1,1084) | 1:33:A:ARG:H    | 1:33:A:ARG:HG2  | 9                   | 0.33     | 0.08                | 0.32       |
| (1,396)  | 1:55:A:GLN:HE22 | 1:56:A:ARG:HG2  | 8                   | 1.25     | 0.69                | 1.25       |
| (1,595)  | 1:28:A:SER:HB2  | 1:45:A:PHE:HE1  | 8                   | 0.75     | 0.32                | 0.71       |
| (1,595)  | 1:28:A:SER:HB2  | 1:45:A:PHE:HE2  | 8                   | 0.75     | 0.32                | 0.71       |
| (1,1134) | 1:69:A:LEU:HD11 | 1:74:A:ILE:HD11 | 8                   | 0.44     | 0.17                | 0.44       |
| (1,1134) | 1:69:A:LEU:HD11 | 1:74:A:ILE:HD12 | 8                   | 0.44     | 0.17                | 0.44       |
| (1,1134) | 1:69:A:LEU:HD11 | 1:74:A:ILE:HD13 | 8                   | 0.44     | 0.17                | 0.44       |
| (1,1134) | 1:69:A:LEU:HD12 | 1:74:A:ILE:HD11 | 8                   | 0.44     | 0.17                | 0.44       |
| (1,1134) | 1:69:A:LEU:HD12 | 1:74:A:ILE:HD12 | 8                   | 0.44     | 0.17                | 0.44       |
| (1,1134) | 1:69:A:LEU:HD12 | 1:74:A:ILE:HD13 | 8                   | 0.44     | 0.17                | 0.44       |
| (1,1134) | 1:69:A:LEU:HD13 | 1:74:A:ILE:HD11 | 8                   | 0.44     | 0.17                | 0.44       |
| (1,1134) | 1:69:A:LEU:HD13 | 1:74:A:ILE:HD12 | 8                   | 0.44     | 0.17                | 0.44       |
| (1,1134) | 1:69:A:LEU:HD13 | 1:74:A:ILE:HD13 | 8                   | 0.44     | 0.17                | 0.44       |
| (1,325)  | 1:49:A:LYS:H    | 1:49:A:LYS:HG3  | 8                   | 0.4      | 0.05                | 0.42       |
| (1,1132) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD11 | 8                   | 0.27     | 0.12                | 0.28       |
| (1,1132) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD12 | 8                   | 0.27     | 0.12                | 0.28       |
| (1,1132) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD13 | 8                   | 0.27     | 0.12                | 0.28       |
| (1,1121) | 1:40:A:ILE:HG12 | 1:42:A:PHE:HE1  | 8                   | 0.27     | 0.15                | 0.26       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1121) | 1:40:A:ILE:HG12 | 1:42:A:PHE:HE2  | 8                   | 0.27     | 0.15                | 0.26       |
| (1,732)  | 1:31:A:GLN:HA   | 1:31:A:GLN:HG2  | 8                   | 0.25     | 0.08                | 0.22       |
| (1,1353) | 1:23:A:HIS:HB2  | 1:24:A:PHE:HD1  | 8                   | 0.22     | 0.07                | 0.2        |
| (1,1353) | 1:23:A:HIS:HB2  | 1:24:A:PHE:HD2  | 8                   | 0.22     | 0.07                | 0.2        |
| (1,1232) | 1:6:A:VAL:HG11  | 1:7:A:PHE:HB2   | 8                   | 0.22     | 0.08                | 0.2        |
| (1,1232) | 1:6:A:VAL:HG12  | 1:7:A:PHE:HB2   | 8                   | 0.22     | 0.08                | 0.2        |
| (1,1232) | 1:6:A:VAL:HG13  | 1:7:A:PHE:HB2   | 8                   | 0.22     | 0.08                | 0.2        |
| (1,621)  | 1:25:A:LYS:HA   | 1:25:A:LYS:HB3  | 8                   | 0.14     | 0.02                | 0.13       |
| (1,1013) | 1:65:A:HIS:HB3  | 1:76:A:VAL:H    | 8                   | 0.14     | 0.03                | 0.14       |
| (1,1080) | 1:33:A:ARG:HG3  | 1:42:A:PHE:HD1  | 7                   | 0.72     | 0.28                | 0.81       |
| (1,1080) | 1:33:A:ARG:HG3  | 1:42:A:PHE:HD2  | 7                   | 0.72     | 0.28                | 0.81       |
| (1,1309) | 1:55:A:GLN:HE21 | 1:58:A:MET:HE1  | 7                   | 0.31     | 0.08                | 0.32       |
| (1,1309) | 1:55:A:GLN:HE21 | 1:58:A:MET:HE2  | 7                   | 0.31     | 0.08                | 0.32       |
| (1,1309) | 1:55:A:GLN:HE21 | 1:58:A:MET:HE3  | 7                   | 0.31     | 0.08                | 0.32       |
| (1,222)  | 1:19:A:GLU:HB3  | 1:20:A:LEU:H    | 7                   | 0.22     | 0.14                | 0.17       |
| (1,1125) | 1:20:A:LEU:HD11 | 1:34:A:LEU:HB3  | 6                   | 1.58     | 0.16                | 1.6        |
| (1,1125) | 1:20:A:LEU:HD12 | 1:34:A:LEU:HB3  | 6                   | 1.58     | 0.16                | 1.6        |
| (1,1125) | 1:20:A:LEU:HD13 | 1:34:A:LEU:HB3  | 6                   | 1.58     | 0.16                | 1.6        |
| (1,47)   | 1:20:A:LEU:HD11 | 1:34:A:LEU:H    | 6                   | 1.32     | 0.14                | 1.3        |
| (1,47)   | 1:20:A:LEU:HD12 | 1:34:A:LEU:H    | 6                   | 1.32     | 0.14                | 1.3        |
| (1,47)   | 1:20:A:LEU:HD13 | 1:34:A:LEU:H    | 6                   | 1.32     | 0.14                | 1.3        |
| (1,846)  | 1:20:A:LEU:HB2  | 1:20:A:LEU:HG   | 6                   | 0.65     | 0.0                 | 0.65       |
| (1,101)  | 1:17:A:ALA:H    | 1:20:A:LEU:HD11 | 6                   | 0.64     | 0.16                | 0.66       |
| (1,101)  | 1:17:A:ALA:H    | 1:20:A:LEU:HD12 | 6                   | 0.64     | 0.16                | 0.66       |
| (1,101)  | 1:17:A:ALA:H    | 1:20:A:LEU:HD13 | 6                   | 0.64     | 0.16                | 0.66       |
| (1,1128) | 1:20:A:LEU:HD11 | 1:34:A:LEU:HB2  | 6                   | 0.51     | 0.14                | 0.5        |
| (1,1128) | 1:20:A:LEU:HD12 | 1:34:A:LEU:HB2  | 6                   | 0.51     | 0.14                | 0.5        |
| (1,1128) | 1:20:A:LEU:HD13 | 1:34:A:LEU:HB2  | 6                   | 0.51     | 0.14                | 0.5        |
| (1,672)  | 1:20:A:LEU:HA   | 1:20:A:LEU:HD21 | 6                   | 0.47     | 0.02                | 0.46       |
| (1,672)  | 1:20:A:LEU:HA   | 1:20:A:LEU:HD22 | 6                   | 0.47     | 0.02                | 0.46       |
| (1,672)  | 1:20:A:LEU:HA   | 1:20:A:LEU:HD23 | 6                   | 0.47     | 0.02                | 0.46       |
| (1,721)  | 1:17:A:ALA:HA   | 1:20:A:LEU:HD11 | 6                   | 0.43     | 0.15                | 0.48       |
| (1,721)  | 1:17:A:ALA:HA   | 1:20:A:LEU:HD12 | 6                   | 0.43     | 0.15                | 0.48       |
| (1,721)  | 1:17:A:ALA:HA   | 1:20:A:LEU:HD13 | 6                   | 0.43     | 0.15                | 0.48       |
| (1,1356) | 1:20:A:LEU:HD21 | 1:24:A:PHE:HD1  | 6                   | 0.41     | 0.05                | 0.41       |
| (1,1356) | 1:20:A:LEU:HD21 | 1:24:A:PHE:HD2  | 6                   | 0.41     | 0.05                | 0.41       |
| (1,1356) | 1:20:A:LEU:HD22 | 1:24:A:PHE:HD1  | 6                   | 0.41     | 0.05                | 0.41       |
| (1,1356) | 1:20:A:LEU:HD22 | 1:24:A:PHE:HD2  | 6                   | 0.41     | 0.05                | 0.41       |
| (1,1356) | 1:20:A:LEU:HD23 | 1:24:A:PHE:HD1  | 6                   | 0.41     | 0.05                | 0.41       |
| (1,1356) | 1:20:A:LEU:HD23 | 1:24:A:PHE:HD2  | 6                   | 0.41     | 0.05                | 0.41       |
| (1,290)  | 1:27:A:SER:HB2  | 1:60:A:ILE:H    | 6                   | 0.23     | 0.1                 | 0.2        |
| (1,461)  | 1:29:A:PRO:HB3  | 1:31:A:GLN:H    | 6                   | 0.19     | 0.07                | 0.19       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1001) | 1:22:A:ASN:HA   | 1:25:A:LYS:HB2  | 6                   | 0.15     | 0.01                | 0.15       |
| (1,282)  | 1:59:A:ASP:H    | 1:59:A:ASP:HB3  | 6                   | 0.14     | 0.02                | 0.14       |
| (1,581)  | 1:10:A:SER:HB3  | 1:75:A:ASN:H    | 6                   | 0.13     | 0.01                | 0.13       |
| (1,873)  | 1:75:A:ASN:H    | 1:75:A:ASN:HB2  | 6                   | 0.11     | 0.0                 | 0.11       |
| (2,2)    | 1:76:A:VAL:N    | 1:65:A:HIS:HD2  | 5                   | 0.26     | 0.04                | 0.25       |
| (1,1215) | 1:23:A:HIS:H    | 1:69:A:LEU:HD21 | 4                   | 0.58     | 0.26                | 0.52       |
| (1,1215) | 1:23:A:HIS:H    | 1:69:A:LEU:HD22 | 4                   | 0.58     | 0.26                | 0.52       |
| (1,1215) | 1:23:A:HIS:H    | 1:69:A:LEU:HD23 | 4                   | 0.58     | 0.26                | 0.52       |
| (1,901)  | 1:49:A:LYS:HG2  | 1:50:A:ASP:HB2  | 4                   | 0.46     | 0.09                | 0.44       |
| (1,901)  | 1:49:A:LYS:HG2  | 1:50:A:ASP:HB3  | 4                   | 0.46     | 0.09                | 0.44       |
| (1,1255) | 1:18:A:VAL:HG11 | 1:22:A:ASN:HB2  | 4                   | 0.35     | 0.17                | 0.28       |
| (1,1255) | 1:18:A:VAL:HG11 | 1:22:A:ASN:HB3  | 4                   | 0.35     | 0.17                | 0.28       |
| (1,1255) | 1:18:A:VAL:HG12 | 1:22:A:ASN:HB2  | 4                   | 0.35     | 0.17                | 0.28       |
| (1,1255) | 1:18:A:VAL:HG12 | 1:22:A:ASN:HB3  | 4                   | 0.35     | 0.17                | 0.28       |
| (1,1255) | 1:18:A:VAL:HG13 | 1:22:A:ASN:HB2  | 4                   | 0.35     | 0.17                | 0.28       |
| (1,1255) | 1:18:A:VAL:HG13 | 1:22:A:ASN:HB3  | 4                   | 0.35     | 0.17                | 0.28       |
| (1,423)  | 1:55:A:GLN:HE22 | 1:59:A:ASP:HB3  | 4                   | 0.32     | 0.21                | 0.22       |
| (1,1127) | 1:20:A:LEU:HD11 | 1:34:A:LEU:HG   | 4                   | 0.26     | 0.09                | 0.25       |
| (1,1127) | 1:20:A:LEU:HD12 | 1:34:A:LEU:HG   | 4                   | 0.26     | 0.09                | 0.25       |
| (1,1127) | 1:20:A:LEU:HD13 | 1:34:A:LEU:HG   | 4                   | 0.26     | 0.09                | 0.25       |
| (1,1071) | 1:24:A:PHE:HE1  | 1:64:A:GLN:HB3  | 4                   | 0.26     | 0.06                | 0.26       |
| (1,1071) | 1:24:A:PHE:HE2  | 1:64:A:GLN:HB3  | 4                   | 0.26     | 0.06                | 0.26       |
| (2,1)    | 1:76:A:VAL:N    | 1:65:A:HIS:HE2  | 4                   | 0.23     | 0.03                | 0.23       |
| (1,909)  | 1:59:A:ASP:HB3  | 1:60:A:ILE:HB   | 4                   | 0.21     | 0.05                | 0.22       |
| (1,204)  | 1:43:A:LEU:HB2  | 1:44:A:GLU:H    | 4                   | 0.13     | 0.02                | 0.13       |
| (1,946)  | 1:7:A:PHE:HB2   | 1:77:A:GLU:HG2  | 3                   | 1.21     | 0.04                | 1.23       |
| (1,30)   | 1:32:A:ILE:HG12 | 1:33:A:ARG:H    | 3                   | 0.61     | 0.15                | 0.52       |
| (1,987)  | 1:24:A:PHE:HD1  | 1:64:A:GLN:HG2  | 3                   | 0.31     | 0.14                | 0.4        |
| (1,987)  | 1:24:A:PHE:HD2  | 1:64:A:GLN:HG2  | 3                   | 0.31     | 0.14                | 0.4        |
| (1,1053) | 1:12:A:PRO:HG2  | 1:70:A:LYS:HD2  | 3                   | 0.27     | 0.03                | 0.29       |
| (1,1053) | 1:12:A:PRO:HG2  | 1:70:A:LYS:HD3  | 3                   | 0.27     | 0.03                | 0.29       |
| (1,924)  | 1:37:A:ASP:HB2  | 1:38:A:LYS:HA   | 3                   | 0.2      | 0.07                | 0.21       |
| (1,1120) | 1:40:A:ILE:HG12 | 1:41:A:ALA:H    | 3                   | 0.17     | 0.02                | 0.18       |
| (1,813)  | 1:33:A:ARG:HB2  | 1:33:A:ARG:HD2  | 3                   | 0.16     | 0.03                | 0.16       |
| (1,555)  | 1:27:A:SER:HB2  | 1:60:A:ILE:HB   | 3                   | 0.16     | 0.03                | 0.15       |
| (1,1196) | 1:34:A:LEU:HD21 | 1:36:A:ALA:H    | 3                   | 0.16     | 0.03                | 0.14       |
| (1,1196) | 1:34:A:LEU:HD22 | 1:36:A:ALA:H    | 3                   | 0.16     | 0.03                | 0.14       |
| (1,1196) | 1:34:A:LEU:HD23 | 1:36:A:ALA:H    | 3                   | 0.16     | 0.03                | 0.14       |
| (1,872)  | 1:30:A:ASP:HB3  | 1:46:A:ASP:H    | 3                   | 0.15     | 0.04                | 0.15       |
| (1,428)  | 1:9:A:GLY:HA3   | 1:11:A:LEU:H    | 3                   | 0.14     | 0.02                | 0.15       |
| (1,896)  | 1:62:A:LEU:HB2  | 1:64:A:GLN:H    | 3                   | 0.13     | 0.02                | 0.13       |
| (1,799)  | 1:57:A:ARG:H    | 1:57:A:ARG:HD3  | 3                   | 0.13     | 0.02                | 0.14       |

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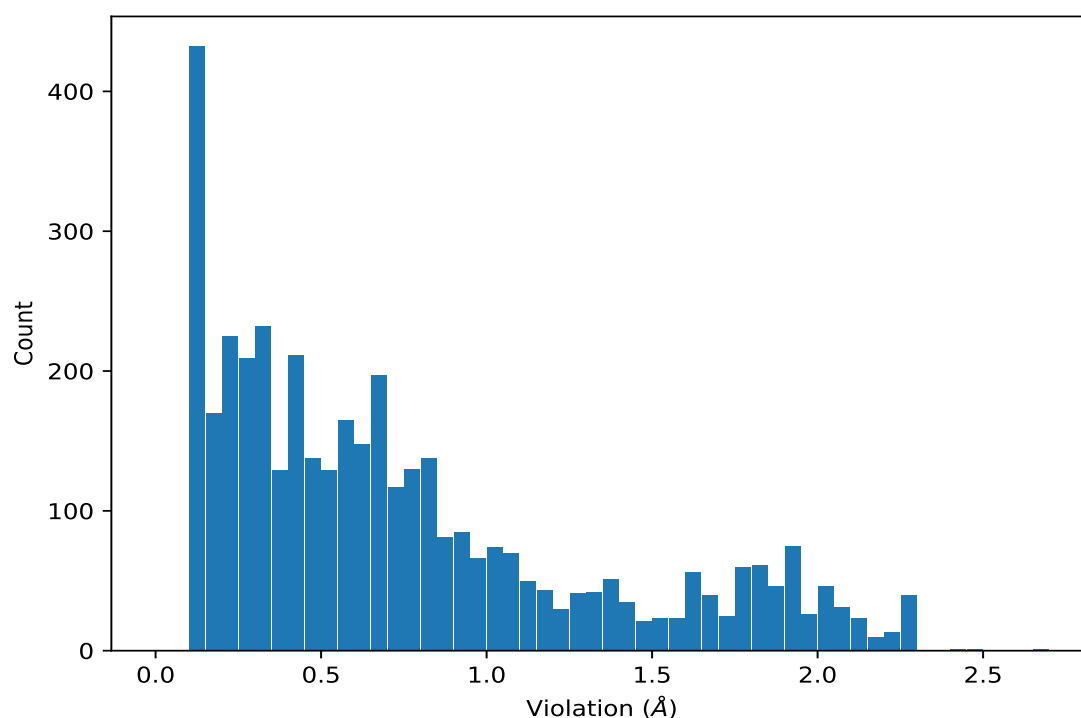
| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1049) | 1:15:A:ILE:HG13 | 1:70:A:LYS:HE2  | 3                   | 0.1      | 0.0                 | 0.1        |
| (1,1049) | 1:15:A:ILE:HG13 | 1:70:A:LYS:HE3  | 3                   | 0.1      | 0.0                 | 0.1        |
| (1,979)  | 1:54:A:ILE:HG21 | 1:55:A:GLN:HG2  | 3                   | 0.1      | 0.0                 | 0.1        |
| (1,979)  | 1:54:A:ILE:HG21 | 1:55:A:GLN:HG3  | 3                   | 0.1      | 0.0                 | 0.1        |
| (1,979)  | 1:54:A:ILE:HG22 | 1:55:A:GLN:HG2  | 3                   | 0.1      | 0.0                 | 0.1        |
| (1,979)  | 1:54:A:ILE:HG22 | 1:55:A:GLN:HG3  | 3                   | 0.1      | 0.0                 | 0.1        |
| (1,979)  | 1:54:A:ILE:HG23 | 1:55:A:GLN:HG2  | 3                   | 0.1      | 0.0                 | 0.1        |
| (1,979)  | 1:54:A:ILE:HG23 | 1:55:A:GLN:HG3  | 3                   | 0.1      | 0.0                 | 0.1        |
| (1,988)  | 1:23:A:HIS:HD2  | 1:64:A:GLN:HG2  | 2                   | 0.44     | 0.01                | 0.44       |
| (1,867)  | 1:70:A:LYS:HB2  | 1:70:A:LYS:HE2  | 2                   | 0.44     | 0.01                | 0.44       |
| (1,867)  | 1:70:A:LYS:HB2  | 1:70:A:LYS:HE3  | 2                   | 0.44     | 0.01                | 0.44       |
| (1,135)  | 1:32:A:ILE:H    | 1:32:A:ILE:HG12 | 2                   | 0.35     | 0.11                | 0.35       |
| (1,949)  | 1:7:A:PHE:HB2   | 1:77:A:GLU:HG3  | 2                   | 0.3      | 0.12                | 0.3        |
| (1,1026) | 1:29:A:PRO:HB3  | 1:32:A:ILE:HD11 | 2                   | 0.28     | 0.15                | 0.28       |
| (1,1026) | 1:29:A:PRO:HB3  | 1:32:A:ILE:HD12 | 2                   | 0.28     | 0.15                | 0.28       |
| (1,1026) | 1:29:A:PRO:HB3  | 1:32:A:ILE:HD13 | 2                   | 0.28     | 0.15                | 0.28       |
| (1,824)  | 1:56:A:ARG:HB2  | 1:56:A:ARG:HD2  | 2                   | 0.26     | 0.06                | 0.26       |
| (1,824)  | 1:56:A:ARG:HB3  | 1:56:A:ARG:HD2  | 2                   | 0.26     | 0.06                | 0.26       |
| (1,1113) | 1:11:A:LEU:HD11 | 1:39:A:GLY:HA3  | 2                   | 0.18     | 0.0                 | 0.18       |
| (1,1113) | 1:11:A:LEU:HD12 | 1:39:A:GLY:HA3  | 2                   | 0.18     | 0.0                 | 0.18       |
| (1,1113) | 1:11:A:LEU:HD13 | 1:39:A:GLY:HA3  | 2                   | 0.18     | 0.0                 | 0.18       |
| (1,1140) | 1:12:A:PRO:HG2  | 1:70:A:LYS:HG2  | 2                   | 0.16     | 0.04                | 0.16       |
| (1,1140) | 1:12:A:PRO:HG2  | 1:70:A:LYS:HG3  | 2                   | 0.16     | 0.04                | 0.16       |
| (1,1069) | 1:61:A:ALA:HA   | 1:64:A:GLN:HB3  | 2                   | 0.12     | 0.02                | 0.12       |
| (1,78)   | 1:59:A:ASP:HB3  | 1:61:A:ALA:H    | 2                   | 0.12     | 0.01                | 0.12       |
| (1,989)  | 1:24:A:PHE:HE1  | 1:64:A:GLN:HG2  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,989)  | 1:24:A:PHE:HE2  | 1:64:A:GLN:HG2  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,650)  | 1:51:A:ARG:HA   | 1:52:A:THR:HG21 | 2                   | 0.1      | 0.0                 | 0.1        |
| (1,650)  | 1:51:A:ARG:HA   | 1:52:A:THR:HG22 | 2                   | 0.1      | 0.0                 | 0.1        |
| (1,650)  | 1:51:A:ARG:HA   | 1:52:A:THR:HG23 | 2                   | 0.1      | 0.0                 | 0.1        |

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

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

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

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



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

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

| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,396)  | 1:55:A:GLN:HE22 | 1:56:A:ARG:HG2  | 15       | 2.66          |
| (1,835)  | 1:29:A:PRO:HG2  | 1:43:A:LEU:HB2  | 12       | 2.45          |
| (1,835)  | 1:29:A:PRO:HG2  | 1:43:A:LEU:HB2  | 11       | 2.41          |
| (1,1222) | 1:16:A:THR:HG21 | 1:18:A:VAL:HG21 | 7        | 2.3           |
| (1,1222) | 1:16:A:THR:HG21 | 1:18:A:VAL:HG22 | 7        | 2.3           |
| (1,1222) | 1:16:A:THR:HG21 | 1:18:A:VAL:HG23 | 7        | 2.3           |
| (1,1222) | 1:16:A:THR:HG22 | 1:18:A:VAL:HG21 | 7        | 2.3           |
| (1,1222) | 1:16:A:THR:HG22 | 1:18:A:VAL:HG22 | 7        | 2.3           |
| (1,1222) | 1:16:A:THR:HG22 | 1:18:A:VAL:HG23 | 7        | 2.3           |
| (1,1222) | 1:16:A:THR:HG23 | 1:18:A:VAL:HG21 | 7        | 2.3           |
| (1,1222) | 1:16:A:THR:HG23 | 1:18:A:VAL:HG22 | 7        | 2.3           |
| (1,1222) | 1:16:A:THR:HG23 | 1:18:A:VAL:HG23 | 7        | 2.3           |
| (1,1222) | 1:16:A:THR:HG21 | 1:18:A:VAL:HG21 | 19       | 2.29          |
| (1,1222) | 1:16:A:THR:HG21 | 1:18:A:VAL:HG22 | 19       | 2.29          |
| (1,1222) | 1:16:A:THR:HG21 | 1:18:A:VAL:HG23 | 19       | 2.29          |
| (1,1222) | 1:16:A:THR:HG22 | 1:18:A:VAL:HG21 | 19       | 2.29          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1222) | 1:16:A:THR:HG22 | 1:18:A:VAL:HG22 | 19       | 2.29          |
| (1,1222) | 1:16:A:THR:HG22 | 1:18:A:VAL:HG23 | 19       | 2.29          |
| (1,1222) | 1:16:A:THR:HG23 | 1:18:A:VAL:HG21 | 19       | 2.29          |
| (1,1222) | 1:16:A:THR:HG23 | 1:18:A:VAL:HG22 | 19       | 2.29          |
| (1,1222) | 1:16:A:THR:HG23 | 1:18:A:VAL:HG23 | 19       | 2.29          |
| (1,835)  | 1:29:A:PRO:HG2  | 1:43:A:LEU:HB2  | 19       | 2.27          |
| (1,1222) | 1:16:A:THR:HG21 | 1:18:A:VAL:HG21 | 16       | 2.25          |
| (1,1222) | 1:16:A:THR:HG21 | 1:18:A:VAL:HG22 | 16       | 2.25          |
| (1,1222) | 1:16:A:THR:HG21 | 1:18:A:VAL:HG23 | 16       | 2.25          |
| (1,1222) | 1:16:A:THR:HG22 | 1:18:A:VAL:HG21 | 16       | 2.25          |
| (1,1222) | 1:16:A:THR:HG22 | 1:18:A:VAL:HG22 | 16       | 2.25          |
| (1,1222) | 1:16:A:THR:HG22 | 1:18:A:VAL:HG23 | 16       | 2.25          |
| (1,1222) | 1:16:A:THR:HG23 | 1:18:A:VAL:HG21 | 16       | 2.25          |
| (1,1222) | 1:16:A:THR:HG23 | 1:18:A:VAL:HG22 | 16       | 2.25          |
| (1,1222) | 1:16:A:THR:HG23 | 1:18:A:VAL:HG23 | 16       | 2.25          |
| (1,1222) | 1:16:A:THR:HG21 | 1:18:A:VAL:HG21 | 18       | 2.25          |
| (1,1222) | 1:16:A:THR:HG21 | 1:18:A:VAL:HG22 | 18       | 2.25          |
| (1,1222) | 1:16:A:THR:HG21 | 1:18:A:VAL:HG23 | 18       | 2.25          |
| (1,1222) | 1:16:A:THR:HG22 | 1:18:A:VAL:HG21 | 18       | 2.25          |
| (1,1222) | 1:16:A:THR:HG22 | 1:18:A:VAL:HG22 | 18       | 2.25          |
| (1,1222) | 1:16:A:THR:HG22 | 1:18:A:VAL:HG23 | 18       | 2.25          |
| (1,1222) | 1:16:A:THR:HG23 | 1:18:A:VAL:HG21 | 18       | 2.25          |
| (1,1222) | 1:16:A:THR:HG23 | 1:18:A:VAL:HG22 | 18       | 2.25          |
| (1,1222) | 1:16:A:THR:HG23 | 1:18:A:VAL:HG23 | 18       | 2.25          |
| (1,89)   | 1:8:A:VAL:HG11  | 1:43:A:LEU:H    | 4        | 2.25          |
| (1,89)   | 1:8:A:VAL:HG12  | 1:43:A:LEU:H    | 4        | 2.25          |
| (1,89)   | 1:8:A:VAL:HG13  | 1:43:A:LEU:H    | 4        | 2.25          |
| (1,835)  | 1:29:A:PRO:HG2  | 1:43:A:LEU:HB2  | 10       | 2.24          |
| (1,835)  | 1:29:A:PRO:HG2  | 1:43:A:LEU:HB2  | 15       | 2.22          |
| (1,1222) | 1:16:A:THR:HG21 | 1:18:A:VAL:HG21 | 4        | 2.21          |
| (1,1222) | 1:16:A:THR:HG21 | 1:18:A:VAL:HG22 | 4        | 2.21          |
| (1,1222) | 1:16:A:THR:HG21 | 1:18:A:VAL:HG23 | 4        | 2.21          |
| (1,1222) | 1:16:A:THR:HG22 | 1:18:A:VAL:HG21 | 4        | 2.21          |
| (1,1222) | 1:16:A:THR:HG22 | 1:18:A:VAL:HG22 | 4        | 2.21          |
| (1,1222) | 1:16:A:THR:HG22 | 1:18:A:VAL:HG23 | 4        | 2.21          |
| (1,1222) | 1:16:A:THR:HG23 | 1:18:A:VAL:HG21 | 4        | 2.21          |
| (1,1222) | 1:16:A:THR:HG23 | 1:18:A:VAL:HG22 | 4        | 2.21          |
| (1,1222) | 1:16:A:THR:HG23 | 1:18:A:VAL:HG23 | 4        | 2.21          |
| (1,835)  | 1:29:A:PRO:HG2  | 1:43:A:LEU:HB2  | 4        | 2.2           |
| (1,835)  | 1:29:A:PRO:HG2  | 1:43:A:LEU:HB2  | 16       | 2.2           |
| (1,835)  | 1:29:A:PRO:HG2  | 1:43:A:LEU:HB2  | 7        | 2.17          |
| (1,1222) | 1:16:A:THR:HG21 | 1:18:A:VAL:HG21 | 6        | 2.15          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1222) | 1:16:A:THR:HG21 | 1:18:A:VAL:HG22 | 6        | 2.15          |
| (1,1222) | 1:16:A:THR:HG21 | 1:18:A:VAL:HG23 | 6        | 2.15          |
| (1,1222) | 1:16:A:THR:HG22 | 1:18:A:VAL:HG21 | 6        | 2.15          |
| (1,1222) | 1:16:A:THR:HG22 | 1:18:A:VAL:HG22 | 6        | 2.15          |
| (1,1222) | 1:16:A:THR:HG22 | 1:18:A:VAL:HG23 | 6        | 2.15          |
| (1,1222) | 1:16:A:THR:HG23 | 1:18:A:VAL:HG21 | 6        | 2.15          |
| (1,1222) | 1:16:A:THR:HG23 | 1:18:A:VAL:HG22 | 6        | 2.15          |
| (1,1222) | 1:16:A:THR:HG23 | 1:18:A:VAL:HG23 | 6        | 2.15          |
| (1,835)  | 1:29:A:PRO:HG2  | 1:43:A:LEU:HB2  | 9        | 2.14          |
| (1,835)  | 1:29:A:PRO:HG2  | 1:43:A:LEU:HB2  | 20       | 2.14          |
| (1,1161) | 1:4:A:PHE:HD1   | 1:78:A:LEU:HD21 | 7        | 2.13          |
| (1,1161) | 1:4:A:PHE:HD1   | 1:78:A:LEU:HD22 | 7        | 2.13          |
| (1,1161) | 1:4:A:PHE:HD1   | 1:78:A:LEU:HD23 | 7        | 2.13          |
| (1,1161) | 1:4:A:PHE:HD2   | 1:78:A:LEU:HD21 | 7        | 2.13          |
| (1,1161) | 1:4:A:PHE:HD2   | 1:78:A:LEU:HD22 | 7        | 2.13          |
| (1,1161) | 1:4:A:PHE:HD2   | 1:78:A:LEU:HD23 | 7        | 2.13          |
| (1,1222) | 1:16:A:THR:HG21 | 1:18:A:VAL:HG21 | 3        | 2.11          |
| (1,1222) | 1:16:A:THR:HG21 | 1:18:A:VAL:HG22 | 3        | 2.11          |
| (1,1222) | 1:16:A:THR:HG21 | 1:18:A:VAL:HG23 | 3        | 2.11          |
| (1,1222) | 1:16:A:THR:HG22 | 1:18:A:VAL:HG21 | 3        | 2.11          |
| (1,1222) | 1:16:A:THR:HG22 | 1:18:A:VAL:HG22 | 3        | 2.11          |
| (1,1222) | 1:16:A:THR:HG22 | 1:18:A:VAL:HG23 | 3        | 2.11          |
| (1,1222) | 1:16:A:THR:HG23 | 1:18:A:VAL:HG21 | 3        | 2.11          |
| (1,1222) | 1:16:A:THR:HG23 | 1:18:A:VAL:HG22 | 3        | 2.11          |
| (1,1222) | 1:16:A:THR:HG23 | 1:18:A:VAL:HG23 | 3        | 2.11          |
| (1,1161) | 1:4:A:PHE:HD1   | 1:78:A:LEU:HD21 | 18       | 2.11          |
| (1,1161) | 1:4:A:PHE:HD1   | 1:78:A:LEU:HD22 | 18       | 2.11          |
| (1,1161) | 1:4:A:PHE:HD1   | 1:78:A:LEU:HD23 | 18       | 2.11          |
| (1,1161) | 1:4:A:PHE:HD2   | 1:78:A:LEU:HD21 | 18       | 2.11          |
| (1,1161) | 1:4:A:PHE:HD2   | 1:78:A:LEU:HD22 | 18       | 2.11          |
| (1,1161) | 1:4:A:PHE:HD2   | 1:78:A:LEU:HD23 | 18       | 2.11          |
| (1,1258) | 1:79:A:THR:HG21 | 1:80:A:VAL:HG11 | 9        | 2.09          |
| (1,1258) | 1:79:A:THR:HG21 | 1:80:A:VAL:HG12 | 9        | 2.09          |
| (1,1258) | 1:79:A:THR:HG21 | 1:80:A:VAL:HG13 | 9        | 2.09          |
| (1,1258) | 1:79:A:THR:HG22 | 1:80:A:VAL:HG11 | 9        | 2.09          |
| (1,1258) | 1:79:A:THR:HG22 | 1:80:A:VAL:HG12 | 9        | 2.09          |
| (1,1258) | 1:79:A:THR:HG22 | 1:80:A:VAL:HG13 | 9        | 2.09          |
| (1,1258) | 1:79:A:THR:HG23 | 1:80:A:VAL:HG11 | 9        | 2.09          |
| (1,1258) | 1:79:A:THR:HG23 | 1:80:A:VAL:HG12 | 9        | 2.09          |
| (1,1258) | 1:79:A:THR:HG23 | 1:80:A:VAL:HG13 | 9        | 2.09          |
| (1,835)  | 1:29:A:PRO:HG2  | 1:43:A:LEU:HB2  | 6        | 2.09          |
| (1,1222) | 1:16:A:THR:HG21 | 1:18:A:VAL:HG21 | 5        | 2.08          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1222) | 1:16:A:THR:HG21 | 1:18:A:VAL:HG22 | 5        | 2.08          |
| (1,1222) | 1:16:A:THR:HG21 | 1:18:A:VAL:HG23 | 5        | 2.08          |
| (1,1222) | 1:16:A:THR:HG22 | 1:18:A:VAL:HG21 | 5        | 2.08          |
| (1,1222) | 1:16:A:THR:HG22 | 1:18:A:VAL:HG22 | 5        | 2.08          |
| (1,1222) | 1:16:A:THR:HG22 | 1:18:A:VAL:HG23 | 5        | 2.08          |
| (1,1222) | 1:16:A:THR:HG23 | 1:18:A:VAL:HG21 | 5        | 2.08          |
| (1,1222) | 1:16:A:THR:HG23 | 1:18:A:VAL:HG22 | 5        | 2.08          |
| (1,1222) | 1:16:A:THR:HG23 | 1:18:A:VAL:HG23 | 5        | 2.08          |
| (1,835)  | 1:29:A:PRO:HG2  | 1:43:A:LEU:HB2  | 8        | 2.08          |
| (1,835)  | 1:29:A:PRO:HG2  | 1:43:A:LEU:HB2  | 17       | 2.08          |
| (1,1258) | 1:79:A:THR:HG21 | 1:80:A:VAL:HG11 | 16       | 2.07          |
| (1,1258) | 1:79:A:THR:HG21 | 1:80:A:VAL:HG12 | 16       | 2.07          |
| (1,1258) | 1:79:A:THR:HG21 | 1:80:A:VAL:HG13 | 16       | 2.07          |
| (1,1258) | 1:79:A:THR:HG22 | 1:80:A:VAL:HG11 | 16       | 2.07          |
| (1,1258) | 1:79:A:THR:HG22 | 1:80:A:VAL:HG12 | 16       | 2.07          |
| (1,1258) | 1:79:A:THR:HG22 | 1:80:A:VAL:HG13 | 16       | 2.07          |
| (1,1258) | 1:79:A:THR:HG23 | 1:80:A:VAL:HG11 | 16       | 2.07          |
| (1,1258) | 1:79:A:THR:HG23 | 1:80:A:VAL:HG12 | 16       | 2.07          |
| (1,1258) | 1:79:A:THR:HG23 | 1:80:A:VAL:HG13 | 16       | 2.07          |
| (1,835)  | 1:29:A:PRO:HG2  | 1:43:A:LEU:HB2  | 5        | 2.06          |
| (1,1258) | 1:79:A:THR:HG21 | 1:80:A:VAL:HG11 | 13       | 2.05          |
| (1,1258) | 1:79:A:THR:HG21 | 1:80:A:VAL:HG12 | 13       | 2.05          |
| (1,1258) | 1:79:A:THR:HG21 | 1:80:A:VAL:HG13 | 13       | 2.05          |
| (1,1258) | 1:79:A:THR:HG22 | 1:80:A:VAL:HG11 | 13       | 2.05          |
| (1,1258) | 1:79:A:THR:HG22 | 1:80:A:VAL:HG12 | 13       | 2.05          |
| (1,1258) | 1:79:A:THR:HG22 | 1:80:A:VAL:HG13 | 13       | 2.05          |
| (1,1258) | 1:79:A:THR:HG23 | 1:80:A:VAL:HG11 | 13       | 2.05          |
| (1,1258) | 1:79:A:THR:HG23 | 1:80:A:VAL:HG12 | 13       | 2.05          |
| (1,1258) | 1:79:A:THR:HG23 | 1:80:A:VAL:HG13 | 13       | 2.05          |
| (1,835)  | 1:29:A:PRO:HG2  | 1:43:A:LEU:HB2  | 1        | 2.05          |
| (1,692)  | 1:4:A:PHE:HA    | 1:80:A:VAL:HG21 | 6        | 2.03          |
| (1,692)  | 1:4:A:PHE:HA    | 1:80:A:VAL:HG22 | 6        | 2.03          |
| (1,692)  | 1:4:A:PHE:HA    | 1:80:A:VAL:HG23 | 6        | 2.03          |
| (1,1258) | 1:79:A:THR:HG21 | 1:80:A:VAL:HG11 | 15       | 2.02          |
| (1,1258) | 1:79:A:THR:HG21 | 1:80:A:VAL:HG12 | 15       | 2.02          |
| (1,1258) | 1:79:A:THR:HG21 | 1:80:A:VAL:HG13 | 15       | 2.02          |
| (1,1258) | 1:79:A:THR:HG22 | 1:80:A:VAL:HG11 | 15       | 2.02          |
| (1,1258) | 1:79:A:THR:HG22 | 1:80:A:VAL:HG12 | 15       | 2.02          |
| (1,1258) | 1:79:A:THR:HG22 | 1:80:A:VAL:HG13 | 15       | 2.02          |
| (1,1258) | 1:79:A:THR:HG23 | 1:80:A:VAL:HG11 | 15       | 2.02          |
| (1,1258) | 1:79:A:THR:HG23 | 1:80:A:VAL:HG12 | 15       | 2.02          |
| (1,1258) | 1:79:A:THR:HG23 | 1:80:A:VAL:HG13 | 15       | 2.02          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1189) | 1:20:A:LEU:HD21 | 1:34:A:LEU:HD11 | 12       | 2.02          |
| (1,1189) | 1:20:A:LEU:HD21 | 1:34:A:LEU:HD12 | 12       | 2.02          |
| (1,1189) | 1:20:A:LEU:HD21 | 1:34:A:LEU:HD13 | 12       | 2.02          |
| (1,1189) | 1:20:A:LEU:HD22 | 1:34:A:LEU:HD11 | 12       | 2.02          |
| (1,1189) | 1:20:A:LEU:HD22 | 1:34:A:LEU:HD12 | 12       | 2.02          |
| (1,1189) | 1:20:A:LEU:HD22 | 1:34:A:LEU:HD13 | 12       | 2.02          |
| (1,1189) | 1:20:A:LEU:HD23 | 1:34:A:LEU:HD11 | 12       | 2.02          |
| (1,1189) | 1:20:A:LEU:HD23 | 1:34:A:LEU:HD12 | 12       | 2.02          |
| (1,1189) | 1:20:A:LEU:HD23 | 1:34:A:LEU:HD13 | 12       | 2.02          |
| (1,1258) | 1:79:A:THR:HG21 | 1:80:A:VAL:HG11 | 6        | 2.01          |
| (1,1258) | 1:79:A:THR:HG21 | 1:80:A:VAL:HG12 | 6        | 2.01          |
| (1,1258) | 1:79:A:THR:HG21 | 1:80:A:VAL:HG13 | 6        | 2.01          |
| (1,1258) | 1:79:A:THR:HG22 | 1:80:A:VAL:HG11 | 6        | 2.01          |
| (1,1258) | 1:79:A:THR:HG22 | 1:80:A:VAL:HG12 | 6        | 2.01          |
| (1,1258) | 1:79:A:THR:HG22 | 1:80:A:VAL:HG13 | 6        | 2.01          |
| (1,1258) | 1:79:A:THR:HG23 | 1:80:A:VAL:HG11 | 6        | 2.01          |
| (1,1258) | 1:79:A:THR:HG23 | 1:80:A:VAL:HG12 | 6        | 2.01          |
| (1,1258) | 1:79:A:THR:HG23 | 1:80:A:VAL:HG13 | 6        | 2.01          |
| (1,1163) | 1:4:A:PHE:HB2   | 1:78:A:LEU:HD21 | 11       | 2.01          |
| (1,1163) | 1:4:A:PHE:HB2   | 1:78:A:LEU:HD22 | 11       | 2.01          |
| (1,1163) | 1:4:A:PHE:HB2   | 1:78:A:LEU:HD23 | 11       | 2.01          |
| (1,1163) | 1:4:A:PHE:HB3   | 1:78:A:LEU:HD21 | 11       | 2.01          |
| (1,1163) | 1:4:A:PHE:HB3   | 1:78:A:LEU:HD22 | 11       | 2.01          |
| (1,1163) | 1:4:A:PHE:HB3   | 1:78:A:LEU:HD23 | 11       | 2.01          |
| (1,1222) | 1:16:A:THR:HG21 | 1:18:A:VAL:HG21 | 2        | 1.99          |
| (1,1222) | 1:16:A:THR:HG21 | 1:18:A:VAL:HG22 | 2        | 1.99          |
| (1,1222) | 1:16:A:THR:HG21 | 1:18:A:VAL:HG23 | 2        | 1.99          |
| (1,1222) | 1:16:A:THR:HG22 | 1:18:A:VAL:HG21 | 2        | 1.99          |
| (1,1222) | 1:16:A:THR:HG22 | 1:18:A:VAL:HG22 | 2        | 1.99          |
| (1,1222) | 1:16:A:THR:HG22 | 1:18:A:VAL:HG23 | 2        | 1.99          |
| (1,1222) | 1:16:A:THR:HG23 | 1:18:A:VAL:HG21 | 2        | 1.99          |
| (1,1222) | 1:16:A:THR:HG23 | 1:18:A:VAL:HG22 | 2        | 1.99          |
| (1,1222) | 1:16:A:THR:HG23 | 1:18:A:VAL:HG23 | 2        | 1.99          |
| (1,835)  | 1:29:A:PRO:HG2  | 1:43:A:LEU:HB2  | 14       | 1.99          |
| (1,1189) | 1:20:A:LEU:HD21 | 1:34:A:LEU:HD11 | 8        | 1.97          |
| (1,1189) | 1:20:A:LEU:HD21 | 1:34:A:LEU:HD12 | 8        | 1.97          |
| (1,1189) | 1:20:A:LEU:HD21 | 1:34:A:LEU:HD13 | 8        | 1.97          |
| (1,1189) | 1:20:A:LEU:HD22 | 1:34:A:LEU:HD11 | 8        | 1.97          |
| (1,1189) | 1:20:A:LEU:HD22 | 1:34:A:LEU:HD12 | 8        | 1.97          |
| (1,1189) | 1:20:A:LEU:HD22 | 1:34:A:LEU:HD13 | 8        | 1.97          |
| (1,1189) | 1:20:A:LEU:HD23 | 1:34:A:LEU:HD11 | 8        | 1.97          |
| (1,1189) | 1:20:A:LEU:HD23 | 1:34:A:LEU:HD12 | 8        | 1.97          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1189) | 1:20:A:LEU:HD23 | 1:34:A:LEU:HD13 | 8        | 1.97          |
| (1,1163) | 1:4:A:PHE:HB2   | 1:78:A:LEU:HD21 | 19       | 1.97          |
| (1,1163) | 1:4:A:PHE:HB2   | 1:78:A:LEU:HD22 | 19       | 1.97          |
| (1,1163) | 1:4:A:PHE:HB2   | 1:78:A:LEU:HD23 | 19       | 1.97          |
| (1,1163) | 1:4:A:PHE:HB3   | 1:78:A:LEU:HD21 | 19       | 1.97          |
| (1,1163) | 1:4:A:PHE:HB3   | 1:78:A:LEU:HD22 | 19       | 1.97          |
| (1,1163) | 1:4:A:PHE:HB3   | 1:78:A:LEU:HD23 | 19       | 1.97          |
| (1,835)  | 1:29:A:PRO:HG2  | 1:43:A:LEU:HB2  | 18       | 1.96          |
| (1,1258) | 1:79:A:THR:HG21 | 1:80:A:VAL:HG11 | 18       | 1.95          |
| (1,1258) | 1:79:A:THR:HG21 | 1:80:A:VAL:HG12 | 18       | 1.95          |
| (1,1258) | 1:79:A:THR:HG21 | 1:80:A:VAL:HG13 | 18       | 1.95          |
| (1,1258) | 1:79:A:THR:HG22 | 1:80:A:VAL:HG11 | 18       | 1.95          |
| (1,1258) | 1:79:A:THR:HG22 | 1:80:A:VAL:HG12 | 18       | 1.95          |
| (1,1258) | 1:79:A:THR:HG22 | 1:80:A:VAL:HG13 | 18       | 1.95          |
| (1,1258) | 1:79:A:THR:HG23 | 1:80:A:VAL:HG11 | 18       | 1.95          |
| (1,1258) | 1:79:A:THR:HG23 | 1:80:A:VAL:HG12 | 18       | 1.95          |
| (1,1258) | 1:79:A:THR:HG23 | 1:80:A:VAL:HG13 | 18       | 1.95          |
| (1,1189) | 1:20:A:LEU:HD21 | 1:34:A:LEU:HD11 | 14       | 1.94          |
| (1,1189) | 1:20:A:LEU:HD21 | 1:34:A:LEU:HD12 | 14       | 1.94          |
| (1,1189) | 1:20:A:LEU:HD21 | 1:34:A:LEU:HD13 | 14       | 1.94          |
| (1,1189) | 1:20:A:LEU:HD22 | 1:34:A:LEU:HD11 | 14       | 1.94          |
| (1,1189) | 1:20:A:LEU:HD22 | 1:34:A:LEU:HD12 | 14       | 1.94          |
| (1,1189) | 1:20:A:LEU:HD22 | 1:34:A:LEU:HD13 | 14       | 1.94          |
| (1,1189) | 1:20:A:LEU:HD23 | 1:34:A:LEU:HD11 | 14       | 1.94          |
| (1,1189) | 1:20:A:LEU:HD23 | 1:34:A:LEU:HD12 | 14       | 1.94          |
| (1,1189) | 1:20:A:LEU:HD23 | 1:34:A:LEU:HD13 | 14       | 1.94          |
| (1,89)   | 1:8:A:VAL:HG11  | 1:43:A:LEU:H    | 1        | 1.94          |
| (1,89)   | 1:8:A:VAL:HG12  | 1:43:A:LEU:H    | 1        | 1.94          |
| (1,89)   | 1:8:A:VAL:HG13  | 1:43:A:LEU:H    | 1        | 1.94          |
| (1,1258) | 1:79:A:THR:HG21 | 1:80:A:VAL:HG11 | 2        | 1.93          |
| (1,1258) | 1:79:A:THR:HG21 | 1:80:A:VAL:HG12 | 2        | 1.93          |
| (1,1258) | 1:79:A:THR:HG21 | 1:80:A:VAL:HG13 | 2        | 1.93          |
| (1,1258) | 1:79:A:THR:HG22 | 1:80:A:VAL:HG11 | 2        | 1.93          |
| (1,1258) | 1:79:A:THR:HG22 | 1:80:A:VAL:HG12 | 2        | 1.93          |
| (1,1258) | 1:79:A:THR:HG22 | 1:80:A:VAL:HG13 | 2        | 1.93          |
| (1,1258) | 1:79:A:THR:HG23 | 1:80:A:VAL:HG11 | 2        | 1.93          |
| (1,1258) | 1:79:A:THR:HG23 | 1:80:A:VAL:HG12 | 2        | 1.93          |
| (1,1258) | 1:79:A:THR:HG23 | 1:80:A:VAL:HG13 | 2        | 1.93          |
| (1,1222) | 1:16:A:THR:HG21 | 1:18:A:VAL:HG21 | 14       | 1.93          |
| (1,1222) | 1:16:A:THR:HG21 | 1:18:A:VAL:HG22 | 14       | 1.93          |
| (1,1222) | 1:16:A:THR:HG21 | 1:18:A:VAL:HG23 | 14       | 1.93          |
| (1,1222) | 1:16:A:THR:HG22 | 1:18:A:VAL:HG21 | 14       | 1.93          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1222) | 1:16:A:THR:HG22 | 1:18:A:VAL:HG22 | 14       | 1.93          |
| (1,1222) | 1:16:A:THR:HG22 | 1:18:A:VAL:HG23 | 14       | 1.93          |
| (1,1222) | 1:16:A:THR:HG23 | 1:18:A:VAL:HG21 | 14       | 1.93          |
| (1,1222) | 1:16:A:THR:HG23 | 1:18:A:VAL:HG22 | 14       | 1.93          |
| (1,1222) | 1:16:A:THR:HG23 | 1:18:A:VAL:HG23 | 14       | 1.93          |
| (1,1189) | 1:20:A:LEU:HD21 | 1:34:A:LEU:HD11 | 17       | 1.93          |
| (1,1189) | 1:20:A:LEU:HD21 | 1:34:A:LEU:HD12 | 17       | 1.93          |
| (1,1189) | 1:20:A:LEU:HD21 | 1:34:A:LEU:HD13 | 17       | 1.93          |
| (1,1189) | 1:20:A:LEU:HD22 | 1:34:A:LEU:HD11 | 17       | 1.93          |
| (1,1189) | 1:20:A:LEU:HD22 | 1:34:A:LEU:HD12 | 17       | 1.93          |
| (1,1189) | 1:20:A:LEU:HD22 | 1:34:A:LEU:HD13 | 17       | 1.93          |
| (1,1189) | 1:20:A:LEU:HD23 | 1:34:A:LEU:HD11 | 17       | 1.93          |
| (1,1189) | 1:20:A:LEU:HD23 | 1:34:A:LEU:HD12 | 17       | 1.93          |
| (1,1189) | 1:20:A:LEU:HD23 | 1:34:A:LEU:HD13 | 17       | 1.93          |
| (1,1187) | 1:34:A:LEU:HD11 | 1:41:A:ALA:HA   | 18       | 1.92          |
| (1,1187) | 1:34:A:LEU:HD12 | 1:41:A:ALA:HA   | 18       | 1.92          |
| (1,1187) | 1:34:A:LEU:HD13 | 1:41:A:ALA:HA   | 18       | 1.92          |
| (1,1187) | 1:34:A:LEU:HD11 | 1:41:A:ALA:HA   | 20       | 1.92          |
| (1,1187) | 1:34:A:LEU:HD12 | 1:41:A:ALA:HA   | 20       | 1.92          |
| (1,1187) | 1:34:A:LEU:HD13 | 1:41:A:ALA:HA   | 20       | 1.92          |
| (1,89)   | 1:8:A:VAL:HG11  | 1:43:A:LEU:H    | 18       | 1.92          |
| (1,89)   | 1:8:A:VAL:HG12  | 1:43:A:LEU:H    | 18       | 1.92          |
| (1,89)   | 1:8:A:VAL:HG13  | 1:43:A:LEU:H    | 18       | 1.92          |
| (1,1189) | 1:20:A:LEU:HD21 | 1:34:A:LEU:HD11 | 4        | 1.91          |
| (1,1189) | 1:20:A:LEU:HD21 | 1:34:A:LEU:HD12 | 4        | 1.91          |
| (1,1189) | 1:20:A:LEU:HD21 | 1:34:A:LEU:HD13 | 4        | 1.91          |
| (1,1189) | 1:20:A:LEU:HD22 | 1:34:A:LEU:HD11 | 4        | 1.91          |
| (1,1189) | 1:20:A:LEU:HD22 | 1:34:A:LEU:HD12 | 4        | 1.91          |
| (1,1189) | 1:20:A:LEU:HD22 | 1:34:A:LEU:HD13 | 4        | 1.91          |
| (1,1189) | 1:20:A:LEU:HD23 | 1:34:A:LEU:HD11 | 4        | 1.91          |
| (1,1189) | 1:20:A:LEU:HD23 | 1:34:A:LEU:HD12 | 4        | 1.91          |
| (1,1189) | 1:20:A:LEU:HD23 | 1:34:A:LEU:HD13 | 4        | 1.91          |
| (1,1187) | 1:34:A:LEU:HD11 | 1:41:A:ALA:HA   | 5        | 1.91          |
| (1,1187) | 1:34:A:LEU:HD12 | 1:41:A:ALA:HA   | 5        | 1.91          |
| (1,1187) | 1:34:A:LEU:HD13 | 1:41:A:ALA:HA   | 5        | 1.91          |
| (1,1187) | 1:34:A:LEU:HD11 | 1:41:A:ALA:HA   | 10       | 1.91          |
| (1,1187) | 1:34:A:LEU:HD12 | 1:41:A:ALA:HA   | 10       | 1.91          |
| (1,1187) | 1:34:A:LEU:HD13 | 1:41:A:ALA:HA   | 10       | 1.91          |
| (1,89)   | 1:8:A:VAL:HG11  | 1:43:A:LEU:H    | 13       | 1.91          |
| (1,89)   | 1:8:A:VAL:HG12  | 1:43:A:LEU:H    | 13       | 1.91          |
| (1,89)   | 1:8:A:VAL:HG13  | 1:43:A:LEU:H    | 13       | 1.91          |
| (1,1258) | 1:79:A:THR:HG21 | 1:80:A:VAL:HG11 | 17       | 1.89          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1258) | 1:79:A:THR:HG21 | 1:80:A:VAL:HG12 | 17       | 1.89          |
| (1,1258) | 1:79:A:THR:HG21 | 1:80:A:VAL:HG13 | 17       | 1.89          |
| (1,1258) | 1:79:A:THR:HG22 | 1:80:A:VAL:HG11 | 17       | 1.89          |
| (1,1258) | 1:79:A:THR:HG22 | 1:80:A:VAL:HG12 | 17       | 1.89          |
| (1,1258) | 1:79:A:THR:HG22 | 1:80:A:VAL:HG13 | 17       | 1.89          |
| (1,1258) | 1:79:A:THR:HG23 | 1:80:A:VAL:HG11 | 17       | 1.89          |
| (1,1258) | 1:79:A:THR:HG23 | 1:80:A:VAL:HG12 | 17       | 1.89          |
| (1,1258) | 1:79:A:THR:HG23 | 1:80:A:VAL:HG13 | 17       | 1.89          |
| (1,1189) | 1:20:A:LEU:HD21 | 1:34:A:LEU:HD11 | 19       | 1.89          |
| (1,1189) | 1:20:A:LEU:HD21 | 1:34:A:LEU:HD12 | 19       | 1.89          |
| (1,1189) | 1:20:A:LEU:HD21 | 1:34:A:LEU:HD13 | 19       | 1.89          |
| (1,1189) | 1:20:A:LEU:HD22 | 1:34:A:LEU:HD11 | 19       | 1.89          |
| (1,1189) | 1:20:A:LEU:HD22 | 1:34:A:LEU:HD12 | 19       | 1.89          |
| (1,1189) | 1:20:A:LEU:HD22 | 1:34:A:LEU:HD13 | 19       | 1.89          |
| (1,1189) | 1:20:A:LEU:HD23 | 1:34:A:LEU:HD11 | 19       | 1.89          |
| (1,1189) | 1:20:A:LEU:HD23 | 1:34:A:LEU:HD12 | 19       | 1.89          |
| (1,1189) | 1:20:A:LEU:HD23 | 1:34:A:LEU:HD13 | 19       | 1.89          |
| (1,1187) | 1:34:A:LEU:HD11 | 1:41:A:ALA:HA   | 6        | 1.89          |
| (1,1187) | 1:34:A:LEU:HD12 | 1:41:A:ALA:HA   | 6        | 1.89          |
| (1,1187) | 1:34:A:LEU:HD13 | 1:41:A:ALA:HA   | 6        | 1.89          |
| (1,1163) | 1:4:A:PHE:HB2   | 1:78:A:LEU:HD21 | 7        | 1.89          |
| (1,1163) | 1:4:A:PHE:HB2   | 1:78:A:LEU:HD22 | 7        | 1.89          |
| (1,1163) | 1:4:A:PHE:HB2   | 1:78:A:LEU:HD23 | 7        | 1.89          |
| (1,1163) | 1:4:A:PHE:HB3   | 1:78:A:LEU:HD21 | 7        | 1.89          |
| (1,1163) | 1:4:A:PHE:HB3   | 1:78:A:LEU:HD22 | 7        | 1.89          |
| (1,1163) | 1:4:A:PHE:HB3   | 1:78:A:LEU:HD23 | 7        | 1.89          |
| (1,835)  | 1:29:A:PRO:HG2  | 1:43:A:LEU:HB2  | 3        | 1.89          |
| (1,1189) | 1:20:A:LEU:HD21 | 1:34:A:LEU:HD11 | 2        | 1.88          |
| (1,1189) | 1:20:A:LEU:HD21 | 1:34:A:LEU:HD12 | 2        | 1.88          |
| (1,1189) | 1:20:A:LEU:HD21 | 1:34:A:LEU:HD13 | 2        | 1.88          |
| (1,1189) | 1:20:A:LEU:HD22 | 1:34:A:LEU:HD11 | 2        | 1.88          |
| (1,1189) | 1:20:A:LEU:HD22 | 1:34:A:LEU:HD12 | 2        | 1.88          |
| (1,1189) | 1:20:A:LEU:HD22 | 1:34:A:LEU:HD13 | 2        | 1.88          |
| (1,1189) | 1:20:A:LEU:HD23 | 1:34:A:LEU:HD11 | 2        | 1.88          |
| (1,1189) | 1:20:A:LEU:HD23 | 1:34:A:LEU:HD12 | 2        | 1.88          |
| (1,1189) | 1:20:A:LEU:HD23 | 1:34:A:LEU:HD13 | 2        | 1.88          |
| (1,1187) | 1:34:A:LEU:HD11 | 1:41:A:ALA:HA   | 12       | 1.86          |
| (1,1187) | 1:34:A:LEU:HD12 | 1:41:A:ALA:HA   | 12       | 1.86          |
| (1,1187) | 1:34:A:LEU:HD13 | 1:41:A:ALA:HA   | 12       | 1.86          |
| (1,1187) | 1:34:A:LEU:HD11 | 1:41:A:ALA:HA   | 19       | 1.86          |
| (1,1187) | 1:34:A:LEU:HD12 | 1:41:A:ALA:HA   | 19       | 1.86          |
| (1,1187) | 1:34:A:LEU:HD13 | 1:41:A:ALA:HA   | 19       | 1.86          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,89)   | 1:8:A:VAL:HG11  | 1:43:A:LEU:H    | 17       | 1.86          |
| (1,89)   | 1:8:A:VAL:HG12  | 1:43:A:LEU:H    | 17       | 1.86          |
| (1,89)   | 1:8:A:VAL:HG13  | 1:43:A:LEU:H    | 17       | 1.86          |
| (1,1189) | 1:20:A:LEU:HD21 | 1:34:A:LEU:HD11 | 10       | 1.84          |
| (1,1189) | 1:20:A:LEU:HD21 | 1:34:A:LEU:HD12 | 10       | 1.84          |
| (1,1189) | 1:20:A:LEU:HD21 | 1:34:A:LEU:HD13 | 10       | 1.84          |
| (1,1189) | 1:20:A:LEU:HD22 | 1:34:A:LEU:HD11 | 10       | 1.84          |
| (1,1189) | 1:20:A:LEU:HD22 | 1:34:A:LEU:HD12 | 10       | 1.84          |
| (1,1189) | 1:20:A:LEU:HD22 | 1:34:A:LEU:HD13 | 10       | 1.84          |
| (1,1189) | 1:20:A:LEU:HD23 | 1:34:A:LEU:HD11 | 10       | 1.84          |
| (1,1189) | 1:20:A:LEU:HD23 | 1:34:A:LEU:HD12 | 10       | 1.84          |
| (1,1189) | 1:20:A:LEU:HD23 | 1:34:A:LEU:HD13 | 10       | 1.84          |
| (1,1187) | 1:34:A:LEU:HD11 | 1:41:A:ALA:HA   | 8        | 1.84          |
| (1,1187) | 1:34:A:LEU:HD12 | 1:41:A:ALA:HA   | 8        | 1.84          |
| (1,1187) | 1:34:A:LEU:HD13 | 1:41:A:ALA:HA   | 8        | 1.84          |
| (1,1187) | 1:34:A:LEU:HD11 | 1:41:A:ALA:HA   | 13       | 1.84          |
| (1,1187) | 1:34:A:LEU:HD12 | 1:41:A:ALA:HA   | 13       | 1.84          |
| (1,1187) | 1:34:A:LEU:HD13 | 1:41:A:ALA:HA   | 13       | 1.84          |
| (1,1222) | 1:16:A:THR:HG21 | 1:18:A:VAL:HG21 | 9        | 1.83          |
| (1,1222) | 1:16:A:THR:HG21 | 1:18:A:VAL:HG22 | 9        | 1.83          |
| (1,1222) | 1:16:A:THR:HG21 | 1:18:A:VAL:HG23 | 9        | 1.83          |
| (1,1222) | 1:16:A:THR:HG22 | 1:18:A:VAL:HG21 | 9        | 1.83          |
| (1,1222) | 1:16:A:THR:HG22 | 1:18:A:VAL:HG22 | 9        | 1.83          |
| (1,1222) | 1:16:A:THR:HG22 | 1:18:A:VAL:HG23 | 9        | 1.83          |
| (1,1222) | 1:16:A:THR:HG23 | 1:18:A:VAL:HG21 | 9        | 1.83          |
| (1,1222) | 1:16:A:THR:HG23 | 1:18:A:VAL:HG22 | 9        | 1.83          |
| (1,1222) | 1:16:A:THR:HG23 | 1:18:A:VAL:HG23 | 9        | 1.83          |
| (1,1189) | 1:20:A:LEU:HD21 | 1:34:A:LEU:HD11 | 18       | 1.83          |
| (1,1189) | 1:20:A:LEU:HD21 | 1:34:A:LEU:HD12 | 18       | 1.83          |
| (1,1189) | 1:20:A:LEU:HD21 | 1:34:A:LEU:HD13 | 18       | 1.83          |
| (1,1189) | 1:20:A:LEU:HD22 | 1:34:A:LEU:HD11 | 18       | 1.83          |
| (1,1189) | 1:20:A:LEU:HD22 | 1:34:A:LEU:HD12 | 18       | 1.83          |
| (1,1189) | 1:20:A:LEU:HD22 | 1:34:A:LEU:HD13 | 18       | 1.83          |
| (1,1189) | 1:20:A:LEU:HD23 | 1:34:A:LEU:HD11 | 18       | 1.83          |
| (1,1189) | 1:20:A:LEU:HD23 | 1:34:A:LEU:HD12 | 18       | 1.83          |
| (1,1189) | 1:20:A:LEU:HD23 | 1:34:A:LEU:HD13 | 18       | 1.83          |
| (1,1187) | 1:34:A:LEU:HD11 | 1:41:A:ALA:HA   | 2        | 1.83          |
| (1,1187) | 1:34:A:LEU:HD12 | 1:41:A:ALA:HA   | 2        | 1.83          |
| (1,1187) | 1:34:A:LEU:HD13 | 1:41:A:ALA:HA   | 2        | 1.83          |
| (1,1187) | 1:34:A:LEU:HD11 | 1:41:A:ALA:HA   | 7        | 1.83          |
| (1,1187) | 1:34:A:LEU:HD12 | 1:41:A:ALA:HA   | 7        | 1.83          |
| (1,1187) | 1:34:A:LEU:HD13 | 1:41:A:ALA:HA   | 7        | 1.83          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,835)  | 1:29:A:PRO:HG2  | 1:43:A:LEU:HB2  | 13       | 1.83          |
| (1,89)   | 1:8:A:VAL:HG11  | 1:43:A:LEU:H    | 16       | 1.83          |
| (1,89)   | 1:8:A:VAL:HG12  | 1:43:A:LEU:H    | 16       | 1.83          |
| (1,89)   | 1:8:A:VAL:HG13  | 1:43:A:LEU:H    | 16       | 1.83          |
| (1,1187) | 1:34:A:LEU:HD11 | 1:41:A:ALA:HA   | 11       | 1.82          |
| (1,1187) | 1:34:A:LEU:HD12 | 1:41:A:ALA:HA   | 11       | 1.82          |
| (1,1187) | 1:34:A:LEU:HD13 | 1:41:A:ALA:HA   | 11       | 1.82          |
| (1,1187) | 1:34:A:LEU:HD11 | 1:41:A:ALA:HA   | 3        | 1.81          |
| (1,1187) | 1:34:A:LEU:HD12 | 1:41:A:ALA:HA   | 3        | 1.81          |
| (1,1187) | 1:34:A:LEU:HD13 | 1:41:A:ALA:HA   | 3        | 1.81          |
| (1,1125) | 1:20:A:LEU:HD11 | 1:34:A:LEU:HB3  | 9        | 1.81          |
| (1,1125) | 1:20:A:LEU:HD12 | 1:34:A:LEU:HB3  | 9        | 1.81          |
| (1,1125) | 1:20:A:LEU:HD13 | 1:34:A:LEU:HB3  | 9        | 1.81          |
| (1,1189) | 1:20:A:LEU:HD21 | 1:34:A:LEU:HD11 | 3        | 1.8           |
| (1,1189) | 1:20:A:LEU:HD21 | 1:34:A:LEU:HD12 | 3        | 1.8           |
| (1,1189) | 1:20:A:LEU:HD21 | 1:34:A:LEU:HD13 | 3        | 1.8           |
| (1,1189) | 1:20:A:LEU:HD22 | 1:34:A:LEU:HD11 | 3        | 1.8           |
| (1,1189) | 1:20:A:LEU:HD22 | 1:34:A:LEU:HD12 | 3        | 1.8           |
| (1,1189) | 1:20:A:LEU:HD22 | 1:34:A:LEU:HD13 | 3        | 1.8           |
| (1,1189) | 1:20:A:LEU:HD23 | 1:34:A:LEU:HD11 | 3        | 1.8           |
| (1,1189) | 1:20:A:LEU:HD23 | 1:34:A:LEU:HD12 | 3        | 1.8           |
| (1,1189) | 1:20:A:LEU:HD23 | 1:34:A:LEU:HD13 | 3        | 1.8           |
| (1,1222) | 1:16:A:THR:HG21 | 1:18:A:VAL:HG21 | 12       | 1.78          |
| (1,1222) | 1:16:A:THR:HG21 | 1:18:A:VAL:HG22 | 12       | 1.78          |
| (1,1222) | 1:16:A:THR:HG21 | 1:18:A:VAL:HG23 | 12       | 1.78          |
| (1,1222) | 1:16:A:THR:HG22 | 1:18:A:VAL:HG21 | 12       | 1.78          |
| (1,1222) | 1:16:A:THR:HG22 | 1:18:A:VAL:HG22 | 12       | 1.78          |
| (1,1222) | 1:16:A:THR:HG22 | 1:18:A:VAL:HG23 | 12       | 1.78          |
| (1,1222) | 1:16:A:THR:HG23 | 1:18:A:VAL:HG21 | 12       | 1.78          |
| (1,1222) | 1:16:A:THR:HG23 | 1:18:A:VAL:HG22 | 12       | 1.78          |
| (1,1222) | 1:16:A:THR:HG23 | 1:18:A:VAL:HG23 | 12       | 1.78          |
| (1,1189) | 1:20:A:LEU:HD21 | 1:34:A:LEU:HD11 | 1        | 1.78          |
| (1,1189) | 1:20:A:LEU:HD21 | 1:34:A:LEU:HD12 | 1        | 1.78          |
| (1,1189) | 1:20:A:LEU:HD21 | 1:34:A:LEU:HD13 | 1        | 1.78          |
| (1,1189) | 1:20:A:LEU:HD22 | 1:34:A:LEU:HD11 | 1        | 1.78          |
| (1,1189) | 1:20:A:LEU:HD22 | 1:34:A:LEU:HD12 | 1        | 1.78          |
| (1,1189) | 1:20:A:LEU:HD22 | 1:34:A:LEU:HD13 | 1        | 1.78          |
| (1,1189) | 1:20:A:LEU:HD23 | 1:34:A:LEU:HD11 | 1        | 1.78          |
| (1,1189) | 1:20:A:LEU:HD23 | 1:34:A:LEU:HD12 | 1        | 1.78          |
| (1,1189) | 1:20:A:LEU:HD23 | 1:34:A:LEU:HD13 | 1        | 1.78          |
| (1,1189) | 1:20:A:LEU:HD21 | 1:34:A:LEU:HD11 | 16       | 1.78          |
| (1,1189) | 1:20:A:LEU:HD21 | 1:34:A:LEU:HD12 | 16       | 1.78          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1189) | 1:20:A:LEU:HD21 | 1:34:A:LEU:HD13 | 16       | 1.78          |
| (1,1189) | 1:20:A:LEU:HD22 | 1:34:A:LEU:HD11 | 16       | 1.78          |
| (1,1189) | 1:20:A:LEU:HD22 | 1:34:A:LEU:HD12 | 16       | 1.78          |
| (1,1189) | 1:20:A:LEU:HD22 | 1:34:A:LEU:HD13 | 16       | 1.78          |
| (1,1189) | 1:20:A:LEU:HD23 | 1:34:A:LEU:HD11 | 16       | 1.78          |
| (1,1189) | 1:20:A:LEU:HD23 | 1:34:A:LEU:HD12 | 16       | 1.78          |
| (1,1189) | 1:20:A:LEU:HD23 | 1:34:A:LEU:HD13 | 16       | 1.78          |
| (1,1187) | 1:34:A:LEU:HD11 | 1:41:A:ALA:HA   | 15       | 1.78          |
| (1,1187) | 1:34:A:LEU:HD12 | 1:41:A:ALA:HA   | 15       | 1.78          |
| (1,1187) | 1:34:A:LEU:HD13 | 1:41:A:ALA:HA   | 15       | 1.78          |
| (1,1161) | 1:4:A:PHE:HD1   | 1:78:A:LEU:HD21 | 19       | 1.78          |
| (1,1161) | 1:4:A:PHE:HD1   | 1:78:A:LEU:HD22 | 19       | 1.78          |
| (1,1161) | 1:4:A:PHE:HD1   | 1:78:A:LEU:HD23 | 19       | 1.78          |
| (1,1161) | 1:4:A:PHE:HD2   | 1:78:A:LEU:HD21 | 19       | 1.78          |
| (1,1161) | 1:4:A:PHE:HD2   | 1:78:A:LEU:HD22 | 19       | 1.78          |
| (1,1161) | 1:4:A:PHE:HD2   | 1:78:A:LEU:HD23 | 19       | 1.78          |
| (1,89)   | 1:8:A:VAL:HG11  | 1:43:A:LEU:H    | 5        | 1.78          |
| (1,89)   | 1:8:A:VAL:HG12  | 1:43:A:LEU:H    | 5        | 1.78          |
| (1,89)   | 1:8:A:VAL:HG13  | 1:43:A:LEU:H    | 5        | 1.78          |
| (1,1189) | 1:20:A:LEU:HD21 | 1:34:A:LEU:HD11 | 5        | 1.77          |
| (1,1189) | 1:20:A:LEU:HD21 | 1:34:A:LEU:HD12 | 5        | 1.77          |
| (1,1189) | 1:20:A:LEU:HD21 | 1:34:A:LEU:HD13 | 5        | 1.77          |
| (1,1189) | 1:20:A:LEU:HD22 | 1:34:A:LEU:HD11 | 5        | 1.77          |
| (1,1189) | 1:20:A:LEU:HD22 | 1:34:A:LEU:HD12 | 5        | 1.77          |
| (1,1189) | 1:20:A:LEU:HD22 | 1:34:A:LEU:HD13 | 5        | 1.77          |
| (1,1189) | 1:20:A:LEU:HD23 | 1:34:A:LEU:HD11 | 5        | 1.77          |
| (1,1189) | 1:20:A:LEU:HD23 | 1:34:A:LEU:HD12 | 5        | 1.77          |
| (1,1189) | 1:20:A:LEU:HD23 | 1:34:A:LEU:HD13 | 5        | 1.77          |
| (1,1187) | 1:34:A:LEU:HD11 | 1:41:A:ALA:HA   | 14       | 1.77          |
| (1,1187) | 1:34:A:LEU:HD12 | 1:41:A:ALA:HA   | 14       | 1.77          |
| (1,1187) | 1:34:A:LEU:HD13 | 1:41:A:ALA:HA   | 14       | 1.77          |
| (1,1187) | 1:34:A:LEU:HD11 | 1:41:A:ALA:HA   | 1        | 1.75          |
| (1,1187) | 1:34:A:LEU:HD12 | 1:41:A:ALA:HA   | 1        | 1.75          |
| (1,1187) | 1:34:A:LEU:HD13 | 1:41:A:ALA:HA   | 1        | 1.75          |
| (1,1187) | 1:34:A:LEU:HD11 | 1:41:A:ALA:HA   | 16       | 1.75          |
| (1,1187) | 1:34:A:LEU:HD12 | 1:41:A:ALA:HA   | 16       | 1.75          |
| (1,1187) | 1:34:A:LEU:HD13 | 1:41:A:ALA:HA   | 16       | 1.75          |
| (1,89)   | 1:8:A:VAL:HG11  | 1:43:A:LEU:H    | 14       | 1.75          |
| (1,89)   | 1:8:A:VAL:HG12  | 1:43:A:LEU:H    | 14       | 1.75          |
| (1,89)   | 1:8:A:VAL:HG13  | 1:43:A:LEU:H    | 14       | 1.75          |
| (1,1187) | 1:34:A:LEU:HD11 | 1:41:A:ALA:HA   | 4        | 1.74          |
| (1,1187) | 1:34:A:LEU:HD12 | 1:41:A:ALA:HA   | 4        | 1.74          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1187) | 1:34:A:LEU:HD13 | 1:41:A:ALA:HA   | 4        | 1.74          |
| (1,89)   | 1:8:A:VAL:HG11  | 1:43:A:LEU:H    | 8        | 1.74          |
| (1,89)   | 1:8:A:VAL:HG12  | 1:43:A:LEU:H    | 8        | 1.74          |
| (1,89)   | 1:8:A:VAL:HG13  | 1:43:A:LEU:H    | 8        | 1.74          |
| (1,1222) | 1:16:A:THR:HG21 | 1:18:A:VAL:HG21 | 20       | 1.73          |
| (1,1222) | 1:16:A:THR:HG21 | 1:18:A:VAL:HG22 | 20       | 1.73          |
| (1,1222) | 1:16:A:THR:HG21 | 1:18:A:VAL:HG23 | 20       | 1.73          |
| (1,1222) | 1:16:A:THR:HG22 | 1:18:A:VAL:HG21 | 20       | 1.73          |
| (1,1222) | 1:16:A:THR:HG22 | 1:18:A:VAL:HG22 | 20       | 1.73          |
| (1,1222) | 1:16:A:THR:HG22 | 1:18:A:VAL:HG23 | 20       | 1.73          |
| (1,1222) | 1:16:A:THR:HG23 | 1:18:A:VAL:HG21 | 20       | 1.73          |
| (1,1222) | 1:16:A:THR:HG23 | 1:18:A:VAL:HG22 | 20       | 1.73          |
| (1,1222) | 1:16:A:THR:HG23 | 1:18:A:VAL:HG23 | 20       | 1.73          |
| (1,1187) | 1:34:A:LEU:HD11 | 1:41:A:ALA:HA   | 9        | 1.73          |
| (1,1187) | 1:34:A:LEU:HD12 | 1:41:A:ALA:HA   | 9        | 1.73          |
| (1,1187) | 1:34:A:LEU:HD13 | 1:41:A:ALA:HA   | 9        | 1.73          |
| (1,1187) | 1:34:A:LEU:HD11 | 1:41:A:ALA:HA   | 17       | 1.73          |
| (1,1187) | 1:34:A:LEU:HD12 | 1:41:A:ALA:HA   | 17       | 1.73          |
| (1,1187) | 1:34:A:LEU:HD13 | 1:41:A:ALA:HA   | 17       | 1.73          |
| (1,692)  | 1:4:A:PHE:HA    | 1:80:A:VAL:HG21 | 17       | 1.72          |
| (1,692)  | 1:4:A:PHE:HA    | 1:80:A:VAL:HG22 | 17       | 1.72          |
| (1,692)  | 1:4:A:PHE:HA    | 1:80:A:VAL:HG23 | 17       | 1.72          |
| (1,674)  | 1:68:A:LEU:HB2  | 1:71:A:GLU:HA   | 1        | 1.72          |
| (1,89)   | 1:8:A:VAL:HG11  | 1:43:A:LEU:H    | 6        | 1.7           |
| (1,89)   | 1:8:A:VAL:HG12  | 1:43:A:LEU:H    | 6        | 1.7           |
| (1,89)   | 1:8:A:VAL:HG13  | 1:43:A:LEU:H    | 6        | 1.7           |
| (1,1125) | 1:20:A:LEU:HD11 | 1:34:A:LEU:HB3  | 6        | 1.69          |
| (1,1125) | 1:20:A:LEU:HD12 | 1:34:A:LEU:HB3  | 6        | 1.69          |
| (1,1125) | 1:20:A:LEU:HD13 | 1:34:A:LEU:HB3  | 6        | 1.69          |
| (1,1189) | 1:20:A:LEU:HD21 | 1:34:A:LEU:HD11 | 20       | 1.68          |
| (1,1189) | 1:20:A:LEU:HD21 | 1:34:A:LEU:HD12 | 20       | 1.68          |
| (1,1189) | 1:20:A:LEU:HD21 | 1:34:A:LEU:HD13 | 20       | 1.68          |
| (1,1189) | 1:20:A:LEU:HD22 | 1:34:A:LEU:HD11 | 20       | 1.68          |
| (1,1189) | 1:20:A:LEU:HD22 | 1:34:A:LEU:HD12 | 20       | 1.68          |
| (1,1189) | 1:20:A:LEU:HD22 | 1:34:A:LEU:HD13 | 20       | 1.68          |
| (1,1189) | 1:20:A:LEU:HD23 | 1:34:A:LEU:HD11 | 20       | 1.68          |
| (1,1189) | 1:20:A:LEU:HD23 | 1:34:A:LEU:HD12 | 20       | 1.68          |
| (1,1189) | 1:20:A:LEU:HD23 | 1:34:A:LEU:HD13 | 20       | 1.68          |
| (1,803)  | 1:80:A:VAL:HG21 | 1:81:A:GLY:HA3  | 8        | 1.68          |
| (1,803)  | 1:80:A:VAL:HG22 | 1:81:A:GLY:HA3  | 8        | 1.68          |
| (1,803)  | 1:80:A:VAL:HG23 | 1:81:A:GLY:HA3  | 8        | 1.68          |
| (1,803)  | 1:80:A:VAL:HG21 | 1:81:A:GLY:HA2  | 8        | 1.68          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,803) | 1:80:A:VAL:HG22 | 1:81:A:GLY:HA2  | 8        | 1.68          |
| (1,803) | 1:80:A:VAL:HG23 | 1:81:A:GLY:HA2  | 8        | 1.68          |
| (1,418) | 1:80:A:VAL:HG21 | 1:82:A:GLY:H    | 5        | 1.67          |
| (1,418) | 1:80:A:VAL:HG22 | 1:82:A:GLY:H    | 5        | 1.67          |
| (1,418) | 1:80:A:VAL:HG23 | 1:82:A:GLY:H    | 5        | 1.67          |
| (1,396) | 1:55:A:GLN:HE22 | 1:56:A:ARG:HG2  | 19       | 1.67          |
| (1,803) | 1:80:A:VAL:HG21 | 1:81:A:GLY:HA3  | 2        | 1.66          |
| (1,803) | 1:80:A:VAL:HG22 | 1:81:A:GLY:HA3  | 2        | 1.66          |
| (1,803) | 1:80:A:VAL:HG23 | 1:81:A:GLY:HA3  | 2        | 1.66          |
| (1,803) | 1:80:A:VAL:HG21 | 1:81:A:GLY:HA2  | 2        | 1.66          |
| (1,803) | 1:80:A:VAL:HG22 | 1:81:A:GLY:HA2  | 2        | 1.66          |
| (1,803) | 1:80:A:VAL:HG23 | 1:81:A:GLY:HA2  | 2        | 1.66          |
| (1,803) | 1:80:A:VAL:HG21 | 1:81:A:GLY:HA3  | 7        | 1.66          |
| (1,803) | 1:80:A:VAL:HG22 | 1:81:A:GLY:HA3  | 7        | 1.66          |
| (1,803) | 1:80:A:VAL:HG23 | 1:81:A:GLY:HA3  | 7        | 1.66          |
| (1,803) | 1:80:A:VAL:HG21 | 1:81:A:GLY:HA2  | 7        | 1.66          |
| (1,803) | 1:80:A:VAL:HG22 | 1:81:A:GLY:HA2  | 7        | 1.66          |
| (1,803) | 1:80:A:VAL:HG23 | 1:81:A:GLY:HA2  | 7        | 1.66          |
| (1,89)  | 1:8:A:VAL:HG11  | 1:43:A:LEU:H    | 9        | 1.66          |
| (1,89)  | 1:8:A:VAL:HG12  | 1:43:A:LEU:H    | 9        | 1.66          |
| (1,89)  | 1:8:A:VAL:HG13  | 1:43:A:LEU:H    | 9        | 1.66          |
| (1,803) | 1:80:A:VAL:HG21 | 1:81:A:GLY:HA3  | 13       | 1.65          |
| (1,803) | 1:80:A:VAL:HG22 | 1:81:A:GLY:HA3  | 13       | 1.65          |
| (1,803) | 1:80:A:VAL:HG23 | 1:81:A:GLY:HA3  | 13       | 1.65          |
| (1,803) | 1:80:A:VAL:HG21 | 1:81:A:GLY:HA2  | 13       | 1.65          |
| (1,803) | 1:80:A:VAL:HG22 | 1:81:A:GLY:HA2  | 13       | 1.65          |
| (1,803) | 1:80:A:VAL:HG23 | 1:81:A:GLY:HA2  | 13       | 1.65          |
| (1,803) | 1:80:A:VAL:HG21 | 1:81:A:GLY:HA3  | 16       | 1.65          |
| (1,803) | 1:80:A:VAL:HG22 | 1:81:A:GLY:HA3  | 16       | 1.65          |
| (1,803) | 1:80:A:VAL:HG23 | 1:81:A:GLY:HA3  | 16       | 1.65          |
| (1,803) | 1:80:A:VAL:HG21 | 1:81:A:GLY:HA2  | 16       | 1.65          |
| (1,803) | 1:80:A:VAL:HG22 | 1:81:A:GLY:HA2  | 16       | 1.65          |
| (1,803) | 1:80:A:VAL:HG23 | 1:81:A:GLY:HA2  | 16       | 1.65          |
| (1,692) | 1:4:A:PHE:HA    | 1:80:A:VAL:HG21 | 8        | 1.65          |
| (1,692) | 1:4:A:PHE:HA    | 1:80:A:VAL:HG22 | 8        | 1.65          |
| (1,692) | 1:4:A:PHE:HA    | 1:80:A:VAL:HG23 | 8        | 1.65          |
| (1,482) | 1:10:A:SER:HB3  | 1:75:A:ASN:HD21 | 2        | 1.65          |
| (1,89)  | 1:8:A:VAL:HG11  | 1:43:A:LEU:H    | 10       | 1.65          |
| (1,89)  | 1:8:A:VAL:HG12  | 1:43:A:LEU:H    | 10       | 1.65          |
| (1,89)  | 1:8:A:VAL:HG13  | 1:43:A:LEU:H    | 10       | 1.65          |
| (1,803) | 1:80:A:VAL:HG21 | 1:81:A:GLY:HA3  | 5        | 1.64          |
| (1,803) | 1:80:A:VAL:HG22 | 1:81:A:GLY:HA3  | 5        | 1.64          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,803)  | 1:80:A:VAL:HG23 | 1:81:A:GLY:HA3  | 5        | 1.64          |
| (1,803)  | 1:80:A:VAL:HG21 | 1:81:A:GLY:HA2  | 5        | 1.64          |
| (1,803)  | 1:80:A:VAL:HG22 | 1:81:A:GLY:HA2  | 5        | 1.64          |
| (1,803)  | 1:80:A:VAL:HG23 | 1:81:A:GLY:HA2  | 5        | 1.64          |
| (1,803)  | 1:80:A:VAL:HG21 | 1:81:A:GLY:HA3  | 15       | 1.64          |
| (1,803)  | 1:80:A:VAL:HG22 | 1:81:A:GLY:HA3  | 15       | 1.64          |
| (1,803)  | 1:80:A:VAL:HG23 | 1:81:A:GLY:HA3  | 15       | 1.64          |
| (1,803)  | 1:80:A:VAL:HG21 | 1:81:A:GLY:HA2  | 15       | 1.64          |
| (1,803)  | 1:80:A:VAL:HG22 | 1:81:A:GLY:HA2  | 15       | 1.64          |
| (1,803)  | 1:80:A:VAL:HG23 | 1:81:A:GLY:HA2  | 15       | 1.64          |
| (1,1125) | 1:20:A:LEU:HD11 | 1:34:A:LEU:HB3  | 15       | 1.63          |
| (1,1125) | 1:20:A:LEU:HD12 | 1:34:A:LEU:HB3  | 15       | 1.63          |
| (1,1125) | 1:20:A:LEU:HD13 | 1:34:A:LEU:HB3  | 15       | 1.63          |
| (1,674)  | 1:68:A:LEU:HB2  | 1:71:A:GLU:HA   | 3        | 1.62          |
| (1,89)   | 1:8:A:VAL:HG11  | 1:43:A:LEU:H    | 15       | 1.62          |
| (1,89)   | 1:8:A:VAL:HG12  | 1:43:A:LEU:H    | 15       | 1.62          |
| (1,89)   | 1:8:A:VAL:HG13  | 1:43:A:LEU:H    | 15       | 1.62          |
| (1,1359) | 1:23:A:HIS:HD2  | 1:64:A:GLN:HB2  | 19       | 1.61          |
| (1,1163) | 1:4:A:PHE:HB2   | 1:78:A:LEU:HD21 | 20       | 1.61          |
| (1,1163) | 1:4:A:PHE:HB2   | 1:78:A:LEU:HD22 | 20       | 1.61          |
| (1,1163) | 1:4:A:PHE:HB2   | 1:78:A:LEU:HD23 | 20       | 1.61          |
| (1,1163) | 1:4:A:PHE:HB3   | 1:78:A:LEU:HD21 | 20       | 1.61          |
| (1,1163) | 1:4:A:PHE:HB3   | 1:78:A:LEU:HD22 | 20       | 1.61          |
| (1,1163) | 1:4:A:PHE:HB3   | 1:78:A:LEU:HD23 | 20       | 1.61          |
| (1,482)  | 1:10:A:SER:HB3  | 1:75:A:ASN:HD21 | 5        | 1.61          |
| (1,803)  | 1:80:A:VAL:HG21 | 1:81:A:GLY:HA3  | 6        | 1.6           |
| (1,803)  | 1:80:A:VAL:HG22 | 1:81:A:GLY:HA3  | 6        | 1.6           |
| (1,803)  | 1:80:A:VAL:HG23 | 1:81:A:GLY:HA3  | 6        | 1.6           |
| (1,803)  | 1:80:A:VAL:HG21 | 1:81:A:GLY:HA2  | 6        | 1.6           |
| (1,803)  | 1:80:A:VAL:HG22 | 1:81:A:GLY:HA2  | 6        | 1.6           |
| (1,803)  | 1:80:A:VAL:HG23 | 1:81:A:GLY:HA2  | 6        | 1.6           |
| (1,670)  | 1:20:A:LEU:HA   | 1:23:A:HIS:HB3  | 19       | 1.6           |
| (1,418)  | 1:80:A:VAL:HG21 | 1:82:A:GLY:H    | 16       | 1.6           |
| (1,418)  | 1:80:A:VAL:HG22 | 1:82:A:GLY:H    | 16       | 1.6           |
| (1,418)  | 1:80:A:VAL:HG23 | 1:82:A:GLY:H    | 16       | 1.6           |
| (1,692)  | 1:4:A:PHE:HA    | 1:80:A:VAL:HG21 | 9        | 1.59          |
| (1,692)  | 1:4:A:PHE:HA    | 1:80:A:VAL:HG22 | 9        | 1.59          |
| (1,692)  | 1:4:A:PHE:HA    | 1:80:A:VAL:HG23 | 9        | 1.59          |
| (1,397)  | 1:55:A:GLN:HE22 | 1:56:A:ARG:H    | 14       | 1.59          |
| (1,1161) | 1:4:A:PHE:HD1   | 1:78:A:LEU:HD21 | 12       | 1.58          |
| (1,1161) | 1:4:A:PHE:HD1   | 1:78:A:LEU:HD22 | 12       | 1.58          |
| (1,1161) | 1:4:A:PHE:HD1   | 1:78:A:LEU:HD23 | 12       | 1.58          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1161) | 1:4:A:PHE:HD2   | 1:78:A:LEU:HD21 | 12       | 1.58          |
| (1,1161) | 1:4:A:PHE:HD2   | 1:78:A:LEU:HD22 | 12       | 1.58          |
| (1,1161) | 1:4:A:PHE:HD2   | 1:78:A:LEU:HD23 | 12       | 1.58          |
| (1,803)  | 1:80:A:VAL:HG21 | 1:81:A:GLY:HA3  | 17       | 1.58          |
| (1,803)  | 1:80:A:VAL:HG22 | 1:81:A:GLY:HA3  | 17       | 1.58          |
| (1,803)  | 1:80:A:VAL:HG23 | 1:81:A:GLY:HA3  | 17       | 1.58          |
| (1,803)  | 1:80:A:VAL:HG21 | 1:81:A:GLY:HA2  | 17       | 1.58          |
| (1,803)  | 1:80:A:VAL:HG22 | 1:81:A:GLY:HA2  | 17       | 1.58          |
| (1,803)  | 1:80:A:VAL:HG23 | 1:81:A:GLY:HA2  | 17       | 1.58          |
| (1,482)  | 1:10:A:SER:HB3  | 1:75:A:ASN:HD21 | 7        | 1.58          |
| (1,397)  | 1:55:A:GLN:HE22 | 1:56:A:ARG:H    | 20       | 1.58          |
| (1,1125) | 1:20:A:LEU:HD11 | 1:34:A:LEU:HB3  | 13       | 1.56          |
| (1,1125) | 1:20:A:LEU:HD12 | 1:34:A:LEU:HB3  | 13       | 1.56          |
| (1,1125) | 1:20:A:LEU:HD13 | 1:34:A:LEU:HB3  | 13       | 1.56          |
| (1,397)  | 1:55:A:GLN:HE22 | 1:56:A:ARG:H    | 11       | 1.56          |
| (1,397)  | 1:55:A:GLN:HE22 | 1:56:A:ARG:H    | 6        | 1.55          |
| (1,692)  | 1:4:A:PHE:HA    | 1:80:A:VAL:HG21 | 18       | 1.54          |
| (1,692)  | 1:4:A:PHE:HA    | 1:80:A:VAL:HG22 | 18       | 1.54          |
| (1,692)  | 1:4:A:PHE:HA    | 1:80:A:VAL:HG23 | 18       | 1.54          |
| (1,1200) | 1:69:A:LEU:HD21 | 1:70:A:LYS:HA   | 19       | 1.53          |
| (1,1200) | 1:69:A:LEU:HD22 | 1:70:A:LYS:HA   | 19       | 1.53          |
| (1,1200) | 1:69:A:LEU:HD23 | 1:70:A:LYS:HA   | 19       | 1.53          |
| (1,1125) | 1:20:A:LEU:HD11 | 1:34:A:LEU:HB3  | 7        | 1.53          |
| (1,1125) | 1:20:A:LEU:HD12 | 1:34:A:LEU:HB3  | 7        | 1.53          |
| (1,1125) | 1:20:A:LEU:HD13 | 1:34:A:LEU:HB3  | 7        | 1.53          |
| (1,835)  | 1:29:A:PRO:HG2  | 1:43:A:LEU:HB2  | 2        | 1.53          |
| (1,809)  | 1:7:A:PHE:HZ    | 1:9:A:GLY:HA2   | 2        | 1.53          |
| (1,482)  | 1:10:A:SER:HB3  | 1:75:A:ASN:HD21 | 18       | 1.53          |
| (1,47)   | 1:20:A:LEU:HD11 | 1:34:A:LEU:H    | 6        | 1.53          |
| (1,47)   | 1:20:A:LEU:HD12 | 1:34:A:LEU:H    | 6        | 1.53          |
| (1,47)   | 1:20:A:LEU:HD13 | 1:34:A:LEU:H    | 6        | 1.53          |
| (1,482)  | 1:10:A:SER:HB3  | 1:75:A:ASN:HD21 | 3        | 1.52          |
| (1,397)  | 1:55:A:GLN:HE22 | 1:56:A:ARG:H    | 19       | 1.52          |
| (1,692)  | 1:4:A:PHE:HA    | 1:80:A:VAL:HG21 | 5        | 1.51          |
| (1,692)  | 1:4:A:PHE:HA    | 1:80:A:VAL:HG22 | 5        | 1.51          |
| (1,692)  | 1:4:A:PHE:HA    | 1:80:A:VAL:HG23 | 5        | 1.51          |
| (1,482)  | 1:10:A:SER:HB3  | 1:75:A:ASN:HD21 | 19       | 1.51          |
| (1,396)  | 1:55:A:GLN:HE22 | 1:56:A:ARG:HG2  | 20       | 1.51          |
| (1,809)  | 1:7:A:PHE:HZ    | 1:9:A:GLY:HA2   | 12       | 1.5           |
| (1,803)  | 1:80:A:VAL:HG21 | 1:81:A:GLY:HA3  | 12       | 1.49          |
| (1,803)  | 1:80:A:VAL:HG22 | 1:81:A:GLY:HA3  | 12       | 1.49          |
| (1,803)  | 1:80:A:VAL:HG23 | 1:81:A:GLY:HA3  | 12       | 1.49          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,803)  | 1:80:A:VAL:HG21 | 1:81:A:GLY:HA2  | 12       | 1.49          |
| (1,803)  | 1:80:A:VAL:HG22 | 1:81:A:GLY:HA2  | 12       | 1.49          |
| (1,803)  | 1:80:A:VAL:HG23 | 1:81:A:GLY:HA2  | 12       | 1.49          |
| (1,1200) | 1:69:A:LEU:HD21 | 1:70:A:LYS:HA   | 18       | 1.48          |
| (1,1200) | 1:69:A:LEU:HD22 | 1:70:A:LYS:HA   | 18       | 1.48          |
| (1,1200) | 1:69:A:LEU:HD23 | 1:70:A:LYS:HA   | 18       | 1.48          |
| (1,89)   | 1:8:A:VAL:HG11  | 1:43:A:LEU:H    | 7        | 1.48          |
| (1,89)   | 1:8:A:VAL:HG12  | 1:43:A:LEU:H    | 7        | 1.48          |
| (1,89)   | 1:8:A:VAL:HG13  | 1:43:A:LEU:H    | 7        | 1.48          |
| (1,1200) | 1:69:A:LEU:HD21 | 1:70:A:LYS:HA   | 4        | 1.46          |
| (1,1200) | 1:69:A:LEU:HD22 | 1:70:A:LYS:HA   | 4        | 1.46          |
| (1,1200) | 1:69:A:LEU:HD23 | 1:70:A:LYS:HA   | 4        | 1.46          |
| (1,803)  | 1:80:A:VAL:HG21 | 1:81:A:GLY:HA3  | 19       | 1.46          |
| (1,803)  | 1:80:A:VAL:HG22 | 1:81:A:GLY:HA3  | 19       | 1.46          |
| (1,803)  | 1:80:A:VAL:HG23 | 1:81:A:GLY:HA3  | 19       | 1.46          |
| (1,803)  | 1:80:A:VAL:HG21 | 1:81:A:GLY:HA2  | 19       | 1.46          |
| (1,803)  | 1:80:A:VAL:HG22 | 1:81:A:GLY:HA2  | 19       | 1.46          |
| (1,803)  | 1:80:A:VAL:HG23 | 1:81:A:GLY:HA2  | 19       | 1.46          |
| (1,309)  | 1:58:A:MET:H    | 1:59:A:ASP:HB3  | 15       | 1.45          |
| (1,89)   | 1:8:A:VAL:HG11  | 1:43:A:LEU:H    | 19       | 1.45          |
| (1,89)   | 1:8:A:VAL:HG12  | 1:43:A:LEU:H    | 19       | 1.45          |
| (1,89)   | 1:8:A:VAL:HG13  | 1:43:A:LEU:H    | 19       | 1.45          |
| (1,792)  | 1:11:A:LEU:HB3  | 1:39:A:GLY:HA3  | 4        | 1.44          |
| (1,418)  | 1:80:A:VAL:HG21 | 1:82:A:GLY:H    | 17       | 1.44          |
| (1,418)  | 1:80:A:VAL:HG22 | 1:82:A:GLY:H    | 17       | 1.44          |
| (1,418)  | 1:80:A:VAL:HG23 | 1:82:A:GLY:H    | 17       | 1.44          |
| (1,47)   | 1:20:A:LEU:HD11 | 1:34:A:LEU:H    | 9        | 1.44          |
| (1,47)   | 1:20:A:LEU:HD12 | 1:34:A:LEU:H    | 9        | 1.44          |
| (1,47)   | 1:20:A:LEU:HD13 | 1:34:A:LEU:H    | 9        | 1.44          |
| (1,803)  | 1:80:A:VAL:HG21 | 1:81:A:GLY:HA3  | 9        | 1.43          |
| (1,803)  | 1:80:A:VAL:HG22 | 1:81:A:GLY:HA3  | 9        | 1.43          |
| (1,803)  | 1:80:A:VAL:HG23 | 1:81:A:GLY:HA3  | 9        | 1.43          |
| (1,803)  | 1:80:A:VAL:HG21 | 1:81:A:GLY:HA2  | 9        | 1.43          |
| (1,803)  | 1:80:A:VAL:HG22 | 1:81:A:GLY:HA2  | 9        | 1.43          |
| (1,803)  | 1:80:A:VAL:HG23 | 1:81:A:GLY:HA2  | 9        | 1.43          |
| (1,674)  | 1:68:A:LEU:HB2  | 1:71:A:GLU:HA   | 13       | 1.43          |
| (1,1322) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HD11 | 1        | 1.42          |
| (1,1322) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HD12 | 1        | 1.42          |
| (1,1322) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HD13 | 1        | 1.42          |
| (1,1322) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HD11 | 8        | 1.42          |
| (1,1322) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HD12 | 8        | 1.42          |
| (1,1322) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HD13 | 8        | 1.42          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,397)  | 1:55:A:GLN:HE22 | 1:56:A:ARG:H    | 1        | 1.42          |
| (1,1322) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HD11 | 12       | 1.41          |
| (1,1322) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HD12 | 12       | 1.41          |
| (1,1322) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HD13 | 12       | 1.41          |
| (1,1201) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD21 | 19       | 1.41          |
| (1,1201) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD22 | 19       | 1.41          |
| (1,1201) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD23 | 19       | 1.41          |
| (1,674)  | 1:68:A:LEU:HB2  | 1:71:A:GLU:HA   | 7        | 1.41          |
| (1,89)   | 1:8:A:VAL:HG11  | 1:43:A:LEU:H    | 3        | 1.41          |
| (1,89)   | 1:8:A:VAL:HG12  | 1:43:A:LEU:H    | 3        | 1.41          |
| (1,89)   | 1:8:A:VAL:HG13  | 1:43:A:LEU:H    | 3        | 1.41          |
| (1,1322) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HD11 | 10       | 1.39          |
| (1,1322) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HD12 | 10       | 1.39          |
| (1,1322) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HD13 | 10       | 1.39          |
| (1,1322) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HD11 | 18       | 1.39          |
| (1,1322) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HD12 | 18       | 1.39          |
| (1,1322) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HD13 | 18       | 1.39          |
| (1,590)  | 1:29:A:PRO:HA   | 1:43:A:LEU:HB2  | 2        | 1.39          |
| (1,309)  | 1:58:A:MET:H    | 1:59:A:ASP:HB3  | 11       | 1.39          |
| (1,1322) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HD11 | 5        | 1.38          |
| (1,1322) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HD12 | 5        | 1.38          |
| (1,1322) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HD13 | 5        | 1.38          |
| (1,1322) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HD11 | 19       | 1.38          |
| (1,1322) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HD12 | 19       | 1.38          |
| (1,1322) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HD13 | 19       | 1.38          |
| (1,47)   | 1:20:A:LEU:HD11 | 1:34:A:LEU:H    | 15       | 1.38          |
| (1,47)   | 1:20:A:LEU:HD12 | 1:34:A:LEU:H    | 15       | 1.38          |
| (1,47)   | 1:20:A:LEU:HD13 | 1:34:A:LEU:H    | 15       | 1.38          |
| (1,1322) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HD11 | 2        | 1.37          |
| (1,1322) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HD12 | 2        | 1.37          |
| (1,1322) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HD13 | 2        | 1.37          |
| (1,1322) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HD11 | 20       | 1.37          |
| (1,1322) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HD12 | 20       | 1.37          |
| (1,1322) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HD13 | 20       | 1.37          |
| (1,1258) | 1:79:A:THR:HG21 | 1:80:A:VAL:HG11 | 19       | 1.37          |
| (1,1258) | 1:79:A:THR:HG21 | 1:80:A:VAL:HG12 | 19       | 1.37          |
| (1,1258) | 1:79:A:THR:HG21 | 1:80:A:VAL:HG13 | 19       | 1.37          |
| (1,1258) | 1:79:A:THR:HG22 | 1:80:A:VAL:HG11 | 19       | 1.37          |
| (1,1258) | 1:79:A:THR:HG22 | 1:80:A:VAL:HG12 | 19       | 1.37          |
| (1,1258) | 1:79:A:THR:HG22 | 1:80:A:VAL:HG13 | 19       | 1.37          |
| (1,1258) | 1:79:A:THR:HG23 | 1:80:A:VAL:HG11 | 19       | 1.37          |
| (1,1258) | 1:79:A:THR:HG23 | 1:80:A:VAL:HG12 | 19       | 1.37          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1258) | 1:79:A:THR:HG23 | 1:80:A:VAL:HG13 | 19       | 1.37          |
| (1,397)  | 1:55:A:GLN:HE22 | 1:56:A:ARG:H    | 15       | 1.37          |
| (1,309)  | 1:58:A:MET:H    | 1:59:A:ASP:HB3  | 19       | 1.37          |
| (1,1322) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HD11 | 13       | 1.36          |
| (1,1322) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HD12 | 13       | 1.36          |
| (1,1322) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HD13 | 13       | 1.36          |
| (1,1322) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HD11 | 14       | 1.36          |
| (1,1322) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HD12 | 14       | 1.36          |
| (1,1322) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HD13 | 14       | 1.36          |
| (1,803)  | 1:80:A:VAL:HG21 | 1:81:A:GLY:HA3  | 18       | 1.36          |
| (1,803)  | 1:80:A:VAL:HG22 | 1:81:A:GLY:HA3  | 18       | 1.36          |
| (1,803)  | 1:80:A:VAL:HG23 | 1:81:A:GLY:HA3  | 18       | 1.36          |
| (1,803)  | 1:80:A:VAL:HG21 | 1:81:A:GLY:HA2  | 18       | 1.36          |
| (1,803)  | 1:80:A:VAL:HG22 | 1:81:A:GLY:HA2  | 18       | 1.36          |
| (1,803)  | 1:80:A:VAL:HG23 | 1:81:A:GLY:HA2  | 18       | 1.36          |
| (1,396)  | 1:55:A:GLN:HE22 | 1:56:A:ARG:HG2  | 14       | 1.36          |
| (1,309)  | 1:58:A:MET:H    | 1:59:A:ASP:HB3  | 13       | 1.36          |
| (1,809)  | 1:7:A:PHE:HZ    | 1:9:A:GLY:HA2   | 1        | 1.35          |
| (1,482)  | 1:10:A:SER:HB3  | 1:75:A:ASN:HD21 | 11       | 1.35          |
| (1,309)  | 1:58:A:MET:H    | 1:59:A:ASP:HB3  | 1        | 1.35          |
| (1,1322) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HD11 | 7        | 1.34          |
| (1,1322) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HD12 | 7        | 1.34          |
| (1,1322) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HD13 | 7        | 1.34          |
| (1,692)  | 1:4:A:PHE:HA    | 1:80:A:VAL:HG21 | 15       | 1.34          |
| (1,692)  | 1:4:A:PHE:HA    | 1:80:A:VAL:HG22 | 15       | 1.34          |
| (1,692)  | 1:4:A:PHE:HA    | 1:80:A:VAL:HG23 | 15       | 1.34          |
| (1,536)  | 1:11:A:LEU:HB3  | 1:39:A:GLY:H    | 4        | 1.34          |
| (1,481)  | 1:18:A:VAL:HG11 | 1:22:A:ASN:HD21 | 20       | 1.34          |
| (1,481)  | 1:18:A:VAL:HG12 | 1:22:A:ASN:HD21 | 20       | 1.34          |
| (1,481)  | 1:18:A:VAL:HG13 | 1:22:A:ASN:HD21 | 20       | 1.34          |
| (1,809)  | 1:7:A:PHE:HZ    | 1:9:A:GLY:HA2   | 17       | 1.33          |
| (1,309)  | 1:58:A:MET:H    | 1:59:A:ASP:HB3  | 12       | 1.33          |
| (1,89)   | 1:8:A:VAL:HG11  | 1:43:A:LEU:H    | 12       | 1.33          |
| (1,89)   | 1:8:A:VAL:HG12  | 1:43:A:LEU:H    | 12       | 1.33          |
| (1,89)   | 1:8:A:VAL:HG13  | 1:43:A:LEU:H    | 12       | 1.33          |
| (1,1040) | 1:12:A:PRO:HG2  | 1:70:A:LYS:HB3  | 10       | 1.32          |
| (1,590)  | 1:29:A:PRO:HA   | 1:43:A:LEU:HB2  | 20       | 1.32          |
| (1,309)  | 1:58:A:MET:H    | 1:59:A:ASP:HB3  | 18       | 1.32          |
| (1,1322) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HD11 | 9        | 1.31          |
| (1,1322) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HD12 | 9        | 1.31          |
| (1,1322) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HD13 | 9        | 1.31          |
| (1,1201) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD21 | 1        | 1.31          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1201) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD22 | 1        | 1.31          |
| (1,1201) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD23 | 1        | 1.31          |
| (1,1161) | 1:4:A:PHE:HD1   | 1:78:A:LEU:HD21 | 20       | 1.31          |
| (1,1161) | 1:4:A:PHE:HD1   | 1:78:A:LEU:HD22 | 20       | 1.31          |
| (1,1161) | 1:4:A:PHE:HD1   | 1:78:A:LEU:HD23 | 20       | 1.31          |
| (1,1161) | 1:4:A:PHE:HD2   | 1:78:A:LEU:HD21 | 20       | 1.31          |
| (1,1161) | 1:4:A:PHE:HD2   | 1:78:A:LEU:HD22 | 20       | 1.31          |
| (1,1161) | 1:4:A:PHE:HD2   | 1:78:A:LEU:HD23 | 20       | 1.31          |
| (1,674)  | 1:68:A:LEU:HB2  | 1:71:A:GLU:HA   | 9        | 1.31          |
| (1,1322) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HD11 | 3        | 1.3           |
| (1,1322) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HD12 | 3        | 1.3           |
| (1,1322) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HD13 | 3        | 1.3           |
| (1,1322) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HD11 | 16       | 1.3           |
| (1,1322) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HD12 | 16       | 1.3           |
| (1,1322) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HD13 | 16       | 1.3           |
| (1,1200) | 1:69:A:LEU:HD21 | 1:70:A:LYS:HA   | 3        | 1.3           |
| (1,1200) | 1:69:A:LEU:HD22 | 1:70:A:LYS:HA   | 3        | 1.3           |
| (1,1200) | 1:69:A:LEU:HD23 | 1:70:A:LYS:HA   | 3        | 1.3           |
| (1,482)  | 1:10:A:SER:HB3  | 1:75:A:ASN:HD21 | 13       | 1.3           |
| (1,482)  | 1:10:A:SER:HB3  | 1:75:A:ASN:HD21 | 16       | 1.3           |
| (1,1322) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HD11 | 15       | 1.29          |
| (1,1322) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HD12 | 15       | 1.29          |
| (1,1322) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HD13 | 15       | 1.29          |
| (1,1125) | 1:20:A:LEU:HD11 | 1:34:A:LEU:HB3  | 11       | 1.29          |
| (1,1125) | 1:20:A:LEU:HD12 | 1:34:A:LEU:HB3  | 11       | 1.29          |
| (1,1125) | 1:20:A:LEU:HD13 | 1:34:A:LEU:HB3  | 11       | 1.29          |
| (1,670)  | 1:20:A:LEU:HA   | 1:23:A:HIS:HB3  | 5        | 1.29          |
| (1,670)  | 1:20:A:LEU:HA   | 1:23:A:HIS:HB3  | 13       | 1.29          |
| (1,590)  | 1:29:A:PRO:HA   | 1:43:A:LEU:HB2  | 12       | 1.29          |
| (1,482)  | 1:10:A:SER:HB3  | 1:75:A:ASN:HD21 | 12       | 1.29          |
| (1,309)  | 1:58:A:MET:H    | 1:59:A:ASP:HB3  | 20       | 1.29          |
| (1,1200) | 1:69:A:LEU:HD21 | 1:70:A:LYS:HA   | 16       | 1.28          |
| (1,1200) | 1:69:A:LEU:HD22 | 1:70:A:LYS:HA   | 16       | 1.28          |
| (1,1200) | 1:69:A:LEU:HD23 | 1:70:A:LYS:HA   | 16       | 1.28          |
| (1,670)  | 1:20:A:LEU:HA   | 1:23:A:HIS:HB3  | 10       | 1.28          |
| (1,489)  | 1:10:A:SER:HB3  | 1:75:A:ASN:HD22 | 2        | 1.28          |
| (1,1200) | 1:69:A:LEU:HD21 | 1:70:A:LYS:HA   | 1        | 1.27          |
| (1,1200) | 1:69:A:LEU:HD22 | 1:70:A:LYS:HA   | 1        | 1.27          |
| (1,1200) | 1:69:A:LEU:HD23 | 1:70:A:LYS:HA   | 1        | 1.27          |
| (1,923)  | 1:37:A:ASP:HB3  | 1:38:A:LYS:HG3  | 13       | 1.27          |
| (1,481)  | 1:18:A:VAL:HG11 | 1:22:A:ASN:HD21 | 12       | 1.26          |
| (1,481)  | 1:18:A:VAL:HG12 | 1:22:A:ASN:HD21 | 12       | 1.26          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,481)  | 1:18:A:VAL:HG13 | 1:22:A:ASN:HD21 | 12       | 1.26          |
| (1,309)  | 1:58:A:MET:H    | 1:59:A:ASP:HB3  | 10       | 1.26          |
| (1,1322) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HD11 | 4        | 1.25          |
| (1,1322) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HD12 | 4        | 1.25          |
| (1,1322) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HD13 | 4        | 1.25          |
| (1,1200) | 1:69:A:LEU:HD21 | 1:70:A:LYS:HA   | 6        | 1.25          |
| (1,1200) | 1:69:A:LEU:HD22 | 1:70:A:LYS:HA   | 6        | 1.25          |
| (1,1200) | 1:69:A:LEU:HD23 | 1:70:A:LYS:HA   | 6        | 1.25          |
| (1,1200) | 1:69:A:LEU:HD21 | 1:70:A:LYS:HA   | 7        | 1.25          |
| (1,1200) | 1:69:A:LEU:HD22 | 1:70:A:LYS:HA   | 7        | 1.25          |
| (1,1200) | 1:69:A:LEU:HD23 | 1:70:A:LYS:HA   | 7        | 1.25          |
| (1,1163) | 1:4:A:PHE:HB2   | 1:78:A:LEU:HD21 | 18       | 1.25          |
| (1,1163) | 1:4:A:PHE:HB2   | 1:78:A:LEU:HD22 | 18       | 1.25          |
| (1,1163) | 1:4:A:PHE:HB2   | 1:78:A:LEU:HD23 | 18       | 1.25          |
| (1,1163) | 1:4:A:PHE:HB3   | 1:78:A:LEU:HD21 | 18       | 1.25          |
| (1,1163) | 1:4:A:PHE:HB3   | 1:78:A:LEU:HD22 | 18       | 1.25          |
| (1,1163) | 1:4:A:PHE:HB3   | 1:78:A:LEU:HD23 | 18       | 1.25          |
| (1,946)  | 1:7:A:PHE:HB2   | 1:77:A:GLU:HG2  | 11       | 1.25          |
| (1,489)  | 1:10:A:SER:HB3  | 1:75:A:ASN:HD22 | 19       | 1.25          |
| (1,1322) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HD11 | 11       | 1.24          |
| (1,1322) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HD12 | 11       | 1.24          |
| (1,1322) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HD13 | 11       | 1.24          |
| (1,820)  | 1:68:A:LEU:HB2  | 1:71:A:GLU:H    | 3        | 1.24          |
| (1,708)  | 1:42:A:PHE:HA   | 1:43:A:LEU:HB3  | 19       | 1.24          |
| (1,708)  | 1:42:A:PHE:HA   | 1:43:A:LEU:HB3  | 20       | 1.24          |
| (1,590)  | 1:29:A:PRO:HA   | 1:43:A:LEU:HB2  | 16       | 1.24          |
| (1,489)  | 1:10:A:SER:HB3  | 1:75:A:ASN:HD22 | 5        | 1.24          |
| (1,309)  | 1:58:A:MET:H    | 1:59:A:ASP:HB3  | 6        | 1.24          |
| (1,946)  | 1:7:A:PHE:HB2   | 1:77:A:GLU:HG2  | 7        | 1.23          |
| (1,708)  | 1:42:A:PHE:HA   | 1:43:A:LEU:HB3  | 11       | 1.23          |
| (1,482)  | 1:10:A:SER:HB3  | 1:75:A:ASN:HD21 | 9        | 1.23          |
| (1,304)  | 1:56:A:ARG:H    | 1:59:A:ASP:HB3  | 13       | 1.23          |
| (1,1201) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD21 | 2        | 1.22          |
| (1,1201) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD22 | 2        | 1.22          |
| (1,1201) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD23 | 2        | 1.22          |
| (1,89)   | 1:8:A:VAL:HG11  | 1:43:A:LEU:H    | 11       | 1.22          |
| (1,89)   | 1:8:A:VAL:HG12  | 1:43:A:LEU:H    | 11       | 1.22          |
| (1,89)   | 1:8:A:VAL:HG13  | 1:43:A:LEU:H    | 11       | 1.22          |
| (1,47)   | 1:20:A:LEU:HD11 | 1:34:A:LEU:H    | 7        | 1.22          |
| (1,47)   | 1:20:A:LEU:HD12 | 1:34:A:LEU:H    | 7        | 1.22          |
| (1,47)   | 1:20:A:LEU:HD13 | 1:34:A:LEU:H    | 7        | 1.22          |
| (1,47)   | 1:20:A:LEU:HD11 | 1:34:A:LEU:H    | 13       | 1.22          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,47)   | 1:20:A:LEU:HD12 | 1:34:A:LEU:H    | 13       | 1.22          |
| (1,47)   | 1:20:A:LEU:HD13 | 1:34:A:LEU:H    | 13       | 1.22          |
| (1,1200) | 1:69:A:LEU:HD21 | 1:70:A:LYS:HA   | 9        | 1.21          |
| (1,1200) | 1:69:A:LEU:HD22 | 1:70:A:LYS:HA   | 9        | 1.21          |
| (1,1200) | 1:69:A:LEU:HD23 | 1:70:A:LYS:HA   | 9        | 1.21          |
| (1,708)  | 1:42:A:PHE:HA   | 1:43:A:LEU:HB3  | 9        | 1.21          |
| (1,708)  | 1:42:A:PHE:HA   | 1:43:A:LEU:HB3  | 12       | 1.21          |
| (1,809)  | 1:7:A:PHE:HZ    | 1:9:A:GLY:HA2   | 6        | 1.2           |
| (1,792)  | 1:11:A:LEU:HB3  | 1:39:A:GLY:HA3  | 17       | 1.2           |
| (1,708)  | 1:42:A:PHE:HA   | 1:43:A:LEU:HB3  | 7        | 1.2           |
| (1,708)  | 1:42:A:PHE:HA   | 1:43:A:LEU:HB3  | 10       | 1.2           |
| (1,708)  | 1:42:A:PHE:HA   | 1:43:A:LEU:HB3  | 13       | 1.2           |
| (1,482)  | 1:10:A:SER:HB3  | 1:75:A:ASN:HD21 | 14       | 1.2           |
| (1,1322) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HD11 | 6        | 1.19          |
| (1,1322) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HD12 | 6        | 1.19          |
| (1,1322) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HD13 | 6        | 1.19          |
| (1,819)  | 1:67:A:THR:HA   | 1:68:A:LEU:HB3  | 16       | 1.19          |
| (1,708)  | 1:42:A:PHE:HA   | 1:43:A:LEU:HB3  | 15       | 1.19          |
| (1,708)  | 1:42:A:PHE:HA   | 1:43:A:LEU:HB3  | 18       | 1.19          |
| (1,674)  | 1:68:A:LEU:HB2  | 1:71:A:GLU:HA   | 4        | 1.19          |
| (1,595)  | 1:28:A:SER:HB2  | 1:45:A:PHE:HE1  | 11       | 1.19          |
| (1,595)  | 1:28:A:SER:HB2  | 1:45:A:PHE:HE2  | 11       | 1.19          |
| (1,482)  | 1:10:A:SER:HB3  | 1:75:A:ASN:HD21 | 20       | 1.19          |
| (1,418)  | 1:80:A:VAL:HG21 | 1:82:A:GLY:H    | 13       | 1.19          |
| (1,418)  | 1:80:A:VAL:HG22 | 1:82:A:GLY:H    | 13       | 1.19          |
| (1,418)  | 1:80:A:VAL:HG23 | 1:82:A:GLY:H    | 13       | 1.19          |
| (1,181)  | 1:68:A:LEU:HB2  | 1:72:A:LYS:H    | 3        | 1.19          |
| (1,809)  | 1:7:A:PHE:HZ    | 1:9:A:GLY:HA2   | 8        | 1.18          |
| (1,809)  | 1:7:A:PHE:HZ    | 1:9:A:GLY:HA2   | 11       | 1.18          |
| (1,708)  | 1:42:A:PHE:HA   | 1:43:A:LEU:HB3  | 1        | 1.18          |
| (1,708)  | 1:42:A:PHE:HA   | 1:43:A:LEU:HB3  | 5        | 1.18          |
| (1,708)  | 1:42:A:PHE:HA   | 1:43:A:LEU:HB3  | 8        | 1.18          |
| (1,590)  | 1:29:A:PRO:HA   | 1:43:A:LEU:HB2  | 1        | 1.18          |
| (1,1359) | 1:23:A:HIS:HD2  | 1:64:A:GLN:HB2  | 14       | 1.17          |
| (1,819)  | 1:67:A:THR:HA   | 1:68:A:LEU:HB3  | 9        | 1.17          |
| (1,819)  | 1:67:A:THR:HA   | 1:68:A:LEU:HB3  | 12       | 1.17          |
| (1,819)  | 1:67:A:THR:HA   | 1:68:A:LEU:HB3  | 13       | 1.17          |
| (1,708)  | 1:42:A:PHE:HA   | 1:43:A:LEU:HB3  | 3        | 1.17          |
| (1,708)  | 1:42:A:PHE:HA   | 1:43:A:LEU:HB3  | 4        | 1.17          |
| (1,708)  | 1:42:A:PHE:HA   | 1:43:A:LEU:HB3  | 6        | 1.17          |
| (1,708)  | 1:42:A:PHE:HA   | 1:43:A:LEU:HB3  | 14       | 1.17          |
| (1,708)  | 1:42:A:PHE:HA   | 1:43:A:LEU:HB3  | 17       | 1.17          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,946)  | 1:7:A:PHE:HB2   | 1:77:A:GLU:HG2  | 19       | 1.16          |
| (1,819)  | 1:67:A:THR:HA   | 1:68:A:LEU:HB3  | 7        | 1.16          |
| (1,708)  | 1:42:A:PHE:HA   | 1:43:A:LEU:HB3  | 16       | 1.16          |
| (1,590)  | 1:29:A:PRO:HA   | 1:43:A:LEU:HB2  | 11       | 1.16          |
| (1,590)  | 1:29:A:PRO:HA   | 1:43:A:LEU:HB2  | 18       | 1.16          |
| (1,489)  | 1:10:A:SER:HB3  | 1:75:A:ASN:HD22 | 7        | 1.16          |
| (1,397)  | 1:55:A:GLN:HE22 | 1:56:A:ARG:H    | 12       | 1.16          |
| (1,181)  | 1:68:A:LEU:HB2  | 1:72:A:LYS:H    | 1        | 1.16          |
| (1,819)  | 1:67:A:THR:HA   | 1:68:A:LEU:HB3  | 15       | 1.15          |
| (1,708)  | 1:42:A:PHE:HA   | 1:43:A:LEU:HB3  | 2        | 1.15          |
| (1,482)  | 1:10:A:SER:HB3  | 1:75:A:ASN:HD21 | 6        | 1.15          |
| (1,396)  | 1:55:A:GLN:HE22 | 1:56:A:ARG:HG2  | 11       | 1.15          |
| (1,692)  | 1:4:A:PHE:HA    | 1:80:A:VAL:HG21 | 19       | 1.14          |
| (1,692)  | 1:4:A:PHE:HA    | 1:80:A:VAL:HG22 | 19       | 1.14          |
| (1,692)  | 1:4:A:PHE:HA    | 1:80:A:VAL:HG23 | 19       | 1.14          |
| (1,595)  | 1:28:A:SER:HB2  | 1:45:A:PHE:HE1  | 14       | 1.14          |
| (1,595)  | 1:28:A:SER:HB2  | 1:45:A:PHE:HE2  | 14       | 1.14          |
| (1,590)  | 1:29:A:PRO:HA   | 1:43:A:LEU:HB2  | 19       | 1.14          |
| (1,304)  | 1:56:A:ARG:H    | 1:59:A:ASP:HB3  | 6        | 1.14          |
| (1,1322) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HD11 | 17       | 1.13          |
| (1,1322) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HD12 | 17       | 1.13          |
| (1,1322) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HD13 | 17       | 1.13          |
| (1,1201) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD21 | 15       | 1.13          |
| (1,1201) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD22 | 15       | 1.13          |
| (1,1201) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD23 | 15       | 1.13          |
| (1,1040) | 1:12:A:PRO:HG2  | 1:70:A:LYS:HB3  | 19       | 1.13          |
| (1,819)  | 1:67:A:THR:HA   | 1:68:A:LEU:HB3  | 17       | 1.13          |
| (1,674)  | 1:68:A:LEU:HB2  | 1:71:A:GLU:HA   | 5        | 1.13          |
| (1,590)  | 1:29:A:PRO:HA   | 1:43:A:LEU:HB2  | 5        | 1.13          |
| (1,1201) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD21 | 5        | 1.12          |
| (1,1201) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD22 | 5        | 1.12          |
| (1,1201) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD23 | 5        | 1.12          |
| (1,819)  | 1:67:A:THR:HA   | 1:68:A:LEU:HB3  | 11       | 1.12          |
| (1,309)  | 1:58:A:MET:H    | 1:59:A:ASP:HB3  | 4        | 1.12          |
| (1,47)   | 1:20:A:LEU:HD11 | 1:34:A:LEU:H    | 11       | 1.12          |
| (1,47)   | 1:20:A:LEU:HD12 | 1:34:A:LEU:H    | 11       | 1.12          |
| (1,47)   | 1:20:A:LEU:HD13 | 1:34:A:LEU:H    | 11       | 1.12          |
| (1,1040) | 1:12:A:PRO:HG2  | 1:70:A:LYS:HB3  | 5        | 1.11          |
| (1,819)  | 1:67:A:THR:HA   | 1:68:A:LEU:HB3  | 6        | 1.11          |
| (1,792)  | 1:11:A:LEU:HB3  | 1:39:A:GLY:HA3  | 15       | 1.11          |
| (1,481)  | 1:18:A:VAL:HG11 | 1:22:A:ASN:HD21 | 14       | 1.11          |
| (1,481)  | 1:18:A:VAL:HG12 | 1:22:A:ASN:HD21 | 14       | 1.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,481)  | 1:18:A:VAL:HG13 | 1:22:A:ASN:HD21 | 14       | 1.11          |
| (1,304)  | 1:56:A:ARG:H    | 1:59:A:ASP:HB3  | 1        | 1.11          |
| (1,304)  | 1:56:A:ARG:H    | 1:59:A:ASP:HB3  | 11       | 1.11          |
| (1,1080) | 1:33:A:ARG:HG3  | 1:42:A:PHE:HD1  | 14       | 1.1           |
| (1,1080) | 1:33:A:ARG:HG3  | 1:42:A:PHE:HD2  | 14       | 1.1           |
| (1,819)  | 1:67:A:THR:HA   | 1:68:A:LEU:HB3  | 2        | 1.1           |
| (1,692)  | 1:4:A:PHE:HA    | 1:80:A:VAL:HG21 | 7        | 1.1           |
| (1,692)  | 1:4:A:PHE:HA    | 1:80:A:VAL:HG22 | 7        | 1.1           |
| (1,692)  | 1:4:A:PHE:HA    | 1:80:A:VAL:HG23 | 7        | 1.1           |
| (1,590)  | 1:29:A:PRO:HA   | 1:43:A:LEU:HB2  | 7        | 1.1           |
| (1,590)  | 1:29:A:PRO:HA   | 1:43:A:LEU:HB2  | 9        | 1.1           |
| (1,489)  | 1:10:A:SER:HB3  | 1:75:A:ASN:HD22 | 12       | 1.1           |
| (1,397)  | 1:55:A:GLN:HE22 | 1:56:A:ARG:H    | 2        | 1.1           |
| (1,89)   | 1:8:A:VAL:HG11  | 1:43:A:LEU:H    | 20       | 1.1           |
| (1,89)   | 1:8:A:VAL:HG12  | 1:43:A:LEU:H    | 20       | 1.1           |
| (1,89)   | 1:8:A:VAL:HG13  | 1:43:A:LEU:H    | 20       | 1.1           |
| (1,1040) | 1:12:A:PRO:HG2  | 1:70:A:LYS:HB3  | 4        | 1.09          |
| (1,819)  | 1:67:A:THR:HA   | 1:68:A:LEU:HB3  | 5        | 1.09          |
| (1,819)  | 1:67:A:THR:HA   | 1:68:A:LEU:HB3  | 10       | 1.09          |
| (1,711)  | 1:68:A:LEU:HD11 | 1:73:A:LYS:HA   | 19       | 1.09          |
| (1,711)  | 1:68:A:LEU:HD12 | 1:73:A:LYS:HA   | 19       | 1.09          |
| (1,711)  | 1:68:A:LEU:HD13 | 1:73:A:LYS:HA   | 19       | 1.09          |
| (1,304)  | 1:56:A:ARG:H    | 1:59:A:ASP:HB3  | 20       | 1.09          |
| (1,1201) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD21 | 13       | 1.08          |
| (1,1201) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD22 | 13       | 1.08          |
| (1,1201) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD23 | 13       | 1.08          |
| (1,1198) | 1:69:A:LEU:HD21 | 1:70:A:LYS:H    | 19       | 1.08          |
| (1,1198) | 1:69:A:LEU:HD22 | 1:70:A:LYS:H    | 19       | 1.08          |
| (1,1198) | 1:69:A:LEU:HD23 | 1:70:A:LYS:H    | 19       | 1.08          |
| (1,819)  | 1:67:A:THR:HA   | 1:68:A:LEU:HB3  | 8        | 1.08          |
| (1,819)  | 1:67:A:THR:HA   | 1:68:A:LEU:HB3  | 19       | 1.08          |
| (1,792)  | 1:11:A:LEU:HB3  | 1:39:A:GLY:HA3  | 11       | 1.08          |
| (1,711)  | 1:68:A:LEU:HD11 | 1:73:A:LYS:HA   | 13       | 1.08          |
| (1,711)  | 1:68:A:LEU:HD12 | 1:73:A:LYS:HA   | 13       | 1.08          |
| (1,711)  | 1:68:A:LEU:HD13 | 1:73:A:LYS:HA   | 13       | 1.08          |
| (1,711)  | 1:68:A:LEU:HD11 | 1:73:A:LYS:HA   | 16       | 1.08          |
| (1,711)  | 1:68:A:LEU:HD12 | 1:73:A:LYS:HA   | 16       | 1.08          |
| (1,711)  | 1:68:A:LEU:HD13 | 1:73:A:LYS:HA   | 16       | 1.08          |
| (1,418)  | 1:80:A:VAL:HG21 | 1:82:A:GLY:H    | 19       | 1.08          |
| (1,418)  | 1:80:A:VAL:HG22 | 1:82:A:GLY:H    | 19       | 1.08          |
| (1,418)  | 1:80:A:VAL:HG23 | 1:82:A:GLY:H    | 19       | 1.08          |
| (1,304)  | 1:56:A:ARG:H    | 1:59:A:ASP:HB3  | 12       | 1.08          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,76)   | 1:68:A:LEU:HD11 | 1:73:A:LYS:H    | 1        | 1.08          |
| (1,76)   | 1:68:A:LEU:HD12 | 1:73:A:LYS:H    | 1        | 1.08          |
| (1,76)   | 1:68:A:LEU:HD13 | 1:73:A:LYS:H    | 1        | 1.08          |
| (1,1359) | 1:23:A:HIS:HD2  | 1:64:A:GLN:HB2  | 8        | 1.07          |
| (1,1258) | 1:79:A:THR:HG21 | 1:80:A:VAL:HG11 | 5        | 1.07          |
| (1,1258) | 1:79:A:THR:HG21 | 1:80:A:VAL:HG12 | 5        | 1.07          |
| (1,1258) | 1:79:A:THR:HG21 | 1:80:A:VAL:HG13 | 5        | 1.07          |
| (1,1258) | 1:79:A:THR:HG22 | 1:80:A:VAL:HG11 | 5        | 1.07          |
| (1,1258) | 1:79:A:THR:HG22 | 1:80:A:VAL:HG12 | 5        | 1.07          |
| (1,1258) | 1:79:A:THR:HG22 | 1:80:A:VAL:HG13 | 5        | 1.07          |
| (1,1258) | 1:79:A:THR:HG23 | 1:80:A:VAL:HG11 | 5        | 1.07          |
| (1,1258) | 1:79:A:THR:HG23 | 1:80:A:VAL:HG12 | 5        | 1.07          |
| (1,1258) | 1:79:A:THR:HG23 | 1:80:A:VAL:HG13 | 5        | 1.07          |
| (1,819)  | 1:67:A:THR:HA   | 1:68:A:LEU:HB3  | 18       | 1.07          |
| (1,809)  | 1:7:A:PHE:HZ    | 1:9:A:GLY:HA2   | 16       | 1.07          |
| (1,481)  | 1:18:A:VAL:HG11 | 1:22:A:ASN:HD21 | 16       | 1.07          |
| (1,481)  | 1:18:A:VAL:HG12 | 1:22:A:ASN:HD21 | 16       | 1.07          |
| (1,481)  | 1:18:A:VAL:HG13 | 1:22:A:ASN:HD21 | 16       | 1.07          |
| (1,1201) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD21 | 20       | 1.06          |
| (1,1201) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD22 | 20       | 1.06          |
| (1,1201) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD23 | 20       | 1.06          |
| (1,820)  | 1:68:A:LEU:HB2  | 1:71:A:GLU:H    | 1        | 1.06          |
| (1,711)  | 1:68:A:LEU:HD11 | 1:73:A:LYS:HA   | 11       | 1.06          |
| (1,711)  | 1:68:A:LEU:HD12 | 1:73:A:LYS:HA   | 11       | 1.06          |
| (1,711)  | 1:68:A:LEU:HD13 | 1:73:A:LYS:HA   | 11       | 1.06          |
| (1,692)  | 1:4:A:PHE:HA    | 1:80:A:VAL:HG21 | 16       | 1.06          |
| (1,692)  | 1:4:A:PHE:HA    | 1:80:A:VAL:HG22 | 16       | 1.06          |
| (1,692)  | 1:4:A:PHE:HA    | 1:80:A:VAL:HG23 | 16       | 1.06          |
| (1,304)  | 1:56:A:ARG:H    | 1:59:A:ASP:HB3  | 10       | 1.06          |
| (1,1200) | 1:69:A:LEU:HD21 | 1:70:A:LYS:HA   | 13       | 1.05          |
| (1,1200) | 1:69:A:LEU:HD22 | 1:70:A:LYS:HA   | 13       | 1.05          |
| (1,1200) | 1:69:A:LEU:HD23 | 1:70:A:LYS:HA   | 13       | 1.05          |
| (1,819)  | 1:67:A:THR:HA   | 1:68:A:LEU:HB3  | 14       | 1.05          |
| (1,809)  | 1:7:A:PHE:HZ    | 1:9:A:GLY:HA2   | 9        | 1.05          |
| (1,792)  | 1:11:A:LEU:HB3  | 1:39:A:GLY:HA3  | 7        | 1.05          |
| (1,792)  | 1:11:A:LEU:HB3  | 1:39:A:GLY:HA3  | 18       | 1.05          |
| (1,711)  | 1:68:A:LEU:HD11 | 1:73:A:LYS:HA   | 10       | 1.05          |
| (1,711)  | 1:68:A:LEU:HD12 | 1:73:A:LYS:HA   | 10       | 1.05          |
| (1,711)  | 1:68:A:LEU:HD13 | 1:73:A:LYS:HA   | 10       | 1.05          |
| (1,482)  | 1:10:A:SER:HB3  | 1:75:A:ASN:HD21 | 1        | 1.05          |
| (1,481)  | 1:18:A:VAL:HG11 | 1:22:A:ASN:HD21 | 19       | 1.05          |
| (1,481)  | 1:18:A:VAL:HG12 | 1:22:A:ASN:HD21 | 19       | 1.05          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,481)  | 1:18:A:VAL:HG13 | 1:22:A:ASN:HD21 | 19       | 1.05          |
| (1,304)  | 1:56:A:ARG:H    | 1:59:A:ASP:HB3  | 19       | 1.05          |
| (1,590)  | 1:29:A:PRO:HA   | 1:43:A:LEU:HB2  | 4        | 1.04          |
| (1,590)  | 1:29:A:PRO:HA   | 1:43:A:LEU:HB2  | 10       | 1.04          |
| (1,181)  | 1:68:A:LEU:HB2  | 1:72:A:LYS:H    | 8        | 1.04          |
| (1,811)  | 1:7:A:PHE:HE1   | 1:9:A:GLY:HA2   | 8        | 1.03          |
| (1,811)  | 1:7:A:PHE:HE2   | 1:9:A:GLY:HA2   | 8        | 1.03          |
| (1,481)  | 1:18:A:VAL:HG11 | 1:22:A:ASN:HD21 | 3        | 1.03          |
| (1,481)  | 1:18:A:VAL:HG12 | 1:22:A:ASN:HD21 | 3        | 1.03          |
| (1,481)  | 1:18:A:VAL:HG13 | 1:22:A:ASN:HD21 | 3        | 1.03          |
| (1,481)  | 1:18:A:VAL:HG11 | 1:22:A:ASN:HD21 | 5        | 1.03          |
| (1,481)  | 1:18:A:VAL:HG12 | 1:22:A:ASN:HD21 | 5        | 1.03          |
| (1,481)  | 1:18:A:VAL:HG13 | 1:22:A:ASN:HD21 | 5        | 1.03          |
| (1,397)  | 1:55:A:GLN:HE22 | 1:56:A:ARG:H    | 8        | 1.03          |
| (1,304)  | 1:56:A:ARG:H    | 1:59:A:ASP:HB3  | 18       | 1.03          |
| (1,1163) | 1:4:A:PHE:HB2   | 1:78:A:LEU:HD21 | 3        | 1.02          |
| (1,1163) | 1:4:A:PHE:HB2   | 1:78:A:LEU:HD22 | 3        | 1.02          |
| (1,1163) | 1:4:A:PHE:HB2   | 1:78:A:LEU:HD23 | 3        | 1.02          |
| (1,1163) | 1:4:A:PHE:HB3   | 1:78:A:LEU:HD21 | 3        | 1.02          |
| (1,1163) | 1:4:A:PHE:HB3   | 1:78:A:LEU:HD22 | 3        | 1.02          |
| (1,1163) | 1:4:A:PHE:HB3   | 1:78:A:LEU:HD23 | 3        | 1.02          |
| (1,792)  | 1:11:A:LEU:HB3  | 1:39:A:GLY:HA3  | 5        | 1.02          |
| (1,711)  | 1:68:A:LEU:HD11 | 1:73:A:LYS:HA   | 15       | 1.02          |
| (1,711)  | 1:68:A:LEU:HD12 | 1:73:A:LYS:HA   | 15       | 1.02          |
| (1,711)  | 1:68:A:LEU:HD13 | 1:73:A:LYS:HA   | 15       | 1.02          |
| (1,670)  | 1:20:A:LEU:HA   | 1:23:A:HIS:HB3  | 7        | 1.02          |
| (1,252)  | 1:63:A:LEU:H    | 1:64:A:GLN:HG3  | 18       | 1.02          |
| (1,1201) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD21 | 10       | 1.01          |
| (1,1201) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD22 | 10       | 1.01          |
| (1,1201) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD23 | 10       | 1.01          |
| (1,1198) | 1:69:A:LEU:HD21 | 1:70:A:LYS:H    | 18       | 1.01          |
| (1,1198) | 1:69:A:LEU:HD22 | 1:70:A:LYS:H    | 18       | 1.01          |
| (1,1198) | 1:69:A:LEU:HD23 | 1:70:A:LYS:H    | 18       | 1.01          |
| (1,1152) | 1:68:A:LEU:HD21 | 1:73:A:LYS:HD2  | 3        | 1.01          |
| (1,1152) | 1:68:A:LEU:HD21 | 1:73:A:LYS:HD3  | 3        | 1.01          |
| (1,1152) | 1:68:A:LEU:HD22 | 1:73:A:LYS:HD2  | 3        | 1.01          |
| (1,1152) | 1:68:A:LEU:HD22 | 1:73:A:LYS:HD3  | 3        | 1.01          |
| (1,1152) | 1:68:A:LEU:HD23 | 1:73:A:LYS:HD2  | 3        | 1.01          |
| (1,1152) | 1:68:A:LEU:HD23 | 1:73:A:LYS:HD3  | 3        | 1.01          |
| (1,877)  | 1:7:A:PHE:HB3   | 1:79:A:THR:HB   | 19       | 1.01          |
| (1,809)  | 1:7:A:PHE:HZ    | 1:9:A:GLY:HA2   | 14       | 1.01          |
| (1,792)  | 1:11:A:LEU:HB3  | 1:39:A:GLY:HA3  | 9        | 1.01          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,670)  | 1:20:A:LEU:HA   | 1:23:A:HIS:HB3  | 2        | 1.01          |
| (1,481)  | 1:18:A:VAL:HG11 | 1:22:A:ASN:HD21 | 7        | 1.01          |
| (1,481)  | 1:18:A:VAL:HG12 | 1:22:A:ASN:HD21 | 7        | 1.01          |
| (1,481)  | 1:18:A:VAL:HG13 | 1:22:A:ASN:HD21 | 7        | 1.01          |
| (1,76)   | 1:68:A:LEU:HD11 | 1:73:A:LYS:H    | 19       | 1.01          |
| (1,76)   | 1:68:A:LEU:HD12 | 1:73:A:LYS:H    | 19       | 1.01          |
| (1,76)   | 1:68:A:LEU:HD13 | 1:73:A:LYS:H    | 19       | 1.01          |
| (1,1201) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD21 | 14       | 1.0           |
| (1,1201) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD22 | 14       | 1.0           |
| (1,1201) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD23 | 14       | 1.0           |
| (1,1198) | 1:69:A:LEU:HD21 | 1:70:A:LYS:H    | 4        | 1.0           |
| (1,1198) | 1:69:A:LEU:HD22 | 1:70:A:LYS:H    | 4        | 1.0           |
| (1,1198) | 1:69:A:LEU:HD23 | 1:70:A:LYS:H    | 4        | 1.0           |
| (1,1163) | 1:4:A:PHE:HB2   | 1:78:A:LEU:HD21 | 14       | 1.0           |
| (1,1163) | 1:4:A:PHE:HB2   | 1:78:A:LEU:HD22 | 14       | 1.0           |
| (1,1163) | 1:4:A:PHE:HB2   | 1:78:A:LEU:HD23 | 14       | 1.0           |
| (1,1163) | 1:4:A:PHE:HB3   | 1:78:A:LEU:HD21 | 14       | 1.0           |
| (1,1163) | 1:4:A:PHE:HB3   | 1:78:A:LEU:HD22 | 14       | 1.0           |
| (1,1163) | 1:4:A:PHE:HB3   | 1:78:A:LEU:HD23 | 14       | 1.0           |
| (1,958)  | 1:77:A:GLU:HB2  | 1:78:A:LEU:HD11 | 19       | 1.0           |
| (1,958)  | 1:77:A:GLU:HB2  | 1:78:A:LEU:HD12 | 19       | 1.0           |
| (1,958)  | 1:77:A:GLU:HB2  | 1:78:A:LEU:HD13 | 19       | 1.0           |
| (1,811)  | 1:7:A:PHE:HE1   | 1:9:A:GLY:HA2   | 11       | 1.0           |
| (1,811)  | 1:7:A:PHE:HE2   | 1:9:A:GLY:HA2   | 11       | 1.0           |
| (1,670)  | 1:20:A:LEU:HA   | 1:23:A:HIS:HB3  | 20       | 1.0           |
| (1,598)  | 1:12:A:PRO:HA   | 1:72:A:LYS:HG2  | 6        | 1.0           |
| (1,590)  | 1:29:A:PRO:HA   | 1:43:A:LEU:HB2  | 3        | 1.0           |
| (1,252)  | 1:63:A:LEU:H    | 1:64:A:GLN:HG3  | 4        | 1.0           |
| (1,212)  | 1:8:A:VAL:HG21  | 1:75:A:ASN:H    | 1        | 1.0           |
| (1,212)  | 1:8:A:VAL:HG22  | 1:75:A:ASN:H    | 1        | 1.0           |
| (1,212)  | 1:8:A:VAL:HG23  | 1:75:A:ASN:H    | 1        | 1.0           |
| (1,55)   | 1:68:A:LEU:HD11 | 1:69:A:LEU:H    | 19       | 1.0           |
| (1,55)   | 1:68:A:LEU:HD12 | 1:69:A:LEU:H    | 19       | 1.0           |
| (1,55)   | 1:68:A:LEU:HD13 | 1:69:A:LEU:H    | 19       | 1.0           |
| (1,1201) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD21 | 8        | 0.99          |
| (1,1201) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD22 | 8        | 0.99          |
| (1,1201) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD23 | 8        | 0.99          |
| (1,1161) | 1:4:A:PHE:HD1   | 1:78:A:LEU:HD21 | 14       | 0.99          |
| (1,1161) | 1:4:A:PHE:HD1   | 1:78:A:LEU:HD22 | 14       | 0.99          |
| (1,1161) | 1:4:A:PHE:HD1   | 1:78:A:LEU:HD23 | 14       | 0.99          |
| (1,1161) | 1:4:A:PHE:HD2   | 1:78:A:LEU:HD21 | 14       | 0.99          |
| (1,1161) | 1:4:A:PHE:HD2   | 1:78:A:LEU:HD22 | 14       | 0.99          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1161) | 1:4:A:PHE:HD2   | 1:78:A:LEU:HD23 | 14       | 0.99          |
| (1,819)  | 1:67:A:THR:HA   | 1:68:A:LEU:HB3  | 4        | 0.99          |
| (1,711)  | 1:68:A:LEU:HD11 | 1:73:A:LYS:HA   | 12       | 0.99          |
| (1,711)  | 1:68:A:LEU:HD12 | 1:73:A:LYS:HA   | 12       | 0.99          |
| (1,711)  | 1:68:A:LEU:HD13 | 1:73:A:LYS:HA   | 12       | 0.99          |
| (1,304)  | 1:56:A:ARG:H    | 1:59:A:ASP:HB3  | 15       | 0.99          |
| (1,252)  | 1:63:A:LEU:H    | 1:64:A:GLN:HG3  | 20       | 0.99          |
| (1,1004) | 1:54:A:ILE:HD11 | 1:58:A:MET:HB3  | 20       | 0.98          |
| (1,1004) | 1:54:A:ILE:HD12 | 1:58:A:MET:HB3  | 20       | 0.98          |
| (1,1004) | 1:54:A:ILE:HD13 | 1:58:A:MET:HB3  | 20       | 0.98          |
| (1,819)  | 1:67:A:THR:HA   | 1:68:A:LEU:HB3  | 3        | 0.98          |
| (1,792)  | 1:11:A:LEU:HB3  | 1:39:A:GLY:HA3  | 16       | 0.98          |
| (1,711)  | 1:68:A:LEU:HD11 | 1:73:A:LYS:HA   | 6        | 0.98          |
| (1,711)  | 1:68:A:LEU:HD12 | 1:73:A:LYS:HA   | 6        | 0.98          |
| (1,711)  | 1:68:A:LEU:HD13 | 1:73:A:LYS:HA   | 6        | 0.98          |
| (1,482)  | 1:10:A:SER:HB3  | 1:75:A:ASN:HD21 | 10       | 0.98          |
| (1,76)   | 1:68:A:LEU:HD11 | 1:73:A:LYS:H    | 6        | 0.98          |
| (1,76)   | 1:68:A:LEU:HD12 | 1:73:A:LYS:H    | 6        | 0.98          |
| (1,76)   | 1:68:A:LEU:HD13 | 1:73:A:LYS:H    | 6        | 0.98          |
| (1,958)  | 1:77:A:GLU:HB2  | 1:78:A:LEU:HD11 | 12       | 0.97          |
| (1,958)  | 1:77:A:GLU:HB2  | 1:78:A:LEU:HD12 | 12       | 0.97          |
| (1,958)  | 1:77:A:GLU:HB2  | 1:78:A:LEU:HD13 | 12       | 0.97          |
| (1,644)  | 1:56:A:ARG:HA   | 1:59:A:ASP:HB3  | 20       | 0.97          |
| (1,536)  | 1:11:A:LEU:HB3  | 1:39:A:GLY:H    | 11       | 0.97          |
| (1,489)  | 1:10:A:SER:HB3  | 1:75:A:ASN:HD22 | 11       | 0.97          |
| (1,489)  | 1:10:A:SER:HB3  | 1:75:A:ASN:HD22 | 18       | 0.97          |
| (1,481)  | 1:18:A:VAL:HG11 | 1:22:A:ASN:HD21 | 9        | 0.97          |
| (1,481)  | 1:18:A:VAL:HG12 | 1:22:A:ASN:HD21 | 9        | 0.97          |
| (1,481)  | 1:18:A:VAL:HG13 | 1:22:A:ASN:HD21 | 9        | 0.97          |
| (1,252)  | 1:63:A:LEU:H    | 1:64:A:GLN:HG3  | 2        | 0.97          |
| (1,89)   | 1:8:A:VAL:HG11  | 1:43:A:LEU:H    | 2        | 0.97          |
| (1,89)   | 1:8:A:VAL:HG12  | 1:43:A:LEU:H    | 2        | 0.97          |
| (1,89)   | 1:8:A:VAL:HG13  | 1:43:A:LEU:H    | 2        | 0.97          |
| (1,1248) | 1:8:A:VAL:HG11  | 1:43:A:LEU:HD21 | 4        | 0.96          |
| (1,1248) | 1:8:A:VAL:HG11  | 1:43:A:LEU:HD22 | 4        | 0.96          |
| (1,1248) | 1:8:A:VAL:HG11  | 1:43:A:LEU:HD23 | 4        | 0.96          |
| (1,1248) | 1:8:A:VAL:HG12  | 1:43:A:LEU:HD21 | 4        | 0.96          |
| (1,1248) | 1:8:A:VAL:HG12  | 1:43:A:LEU:HD22 | 4        | 0.96          |
| (1,1248) | 1:8:A:VAL:HG12  | 1:43:A:LEU:HD23 | 4        | 0.96          |
| (1,1248) | 1:8:A:VAL:HG13  | 1:43:A:LEU:HD21 | 4        | 0.96          |
| (1,1248) | 1:8:A:VAL:HG13  | 1:43:A:LEU:HD22 | 4        | 0.96          |
| (1,1248) | 1:8:A:VAL:HG13  | 1:43:A:LEU:HD23 | 4        | 0.96          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1215) | 1:23:A:HIS:H    | 1:69:A:LEU:HD21 | 1        | 0.96          |
| (1,1215) | 1:23:A:HIS:H    | 1:69:A:LEU:HD22 | 1        | 0.96          |
| (1,1215) | 1:23:A:HIS:H    | 1:69:A:LEU:HD23 | 1        | 0.96          |
| (1,1080) | 1:33:A:ARG:HG3  | 1:42:A:PHE:HD1  | 9        | 0.96          |
| (1,1080) | 1:33:A:ARG:HG3  | 1:42:A:PHE:HD2  | 9        | 0.96          |
| (1,1040) | 1:12:A:PRO:HG2  | 1:70:A:LYS:HB3  | 1        | 0.96          |
| (1,674)  | 1:68:A:LEU:HB2  | 1:71:A:GLU:HA   | 6        | 0.96          |
| (1,644)  | 1:56:A:ARG:HA   | 1:59:A:ASP:HB3  | 11       | 0.96          |
| (1,590)  | 1:29:A:PRO:HA   | 1:43:A:LEU:HB2  | 13       | 0.96          |
| (1,489)  | 1:10:A:SER:HB3  | 1:75:A:ASN:HD22 | 3        | 0.96          |
| (1,481)  | 1:18:A:VAL:HG11 | 1:22:A:ASN:HD21 | 2        | 0.96          |
| (1,481)  | 1:18:A:VAL:HG12 | 1:22:A:ASN:HD21 | 2        | 0.96          |
| (1,481)  | 1:18:A:VAL:HG13 | 1:22:A:ASN:HD21 | 2        | 0.96          |
| (1,55)   | 1:68:A:LEU:HD11 | 1:69:A:LEU:H    | 10       | 0.96          |
| (1,55)   | 1:68:A:LEU:HD12 | 1:69:A:LEU:H    | 10       | 0.96          |
| (1,55)   | 1:68:A:LEU:HD13 | 1:69:A:LEU:H    | 10       | 0.96          |
| (1,819)  | 1:67:A:THR:HA   | 1:68:A:LEU:HB3  | 1        | 0.95          |
| (1,674)  | 1:68:A:LEU:HB2  | 1:71:A:GLU:HA   | 2        | 0.95          |
| (1,670)  | 1:20:A:LEU:HA   | 1:23:A:HIS:HB3  | 18       | 0.95          |
| (1,644)  | 1:56:A:ARG:HA   | 1:59:A:ASP:HB3  | 6        | 0.95          |
| (1,644)  | 1:56:A:ARG:HA   | 1:59:A:ASP:HB3  | 13       | 0.95          |
| (1,644)  | 1:56:A:ARG:HA   | 1:59:A:ASP:HB3  | 19       | 0.95          |
| (1,482)  | 1:10:A:SER:HB3  | 1:75:A:ASN:HD21 | 15       | 0.95          |
| (1,55)   | 1:68:A:LEU:HD11 | 1:69:A:LEU:H    | 15       | 0.95          |
| (1,55)   | 1:68:A:LEU:HD12 | 1:69:A:LEU:H    | 15       | 0.95          |
| (1,55)   | 1:68:A:LEU:HD13 | 1:69:A:LEU:H    | 15       | 0.95          |
| (1,1359) | 1:23:A:HIS:HD2  | 1:64:A:GLN:HB2  | 15       | 0.94          |
| (1,1040) | 1:12:A:PRO:HG2  | 1:70:A:LYS:HB3  | 14       | 0.94          |
| (1,958)  | 1:77:A:GLU:HB2  | 1:78:A:LEU:HD11 | 20       | 0.94          |
| (1,958)  | 1:77:A:GLU:HB2  | 1:78:A:LEU:HD12 | 20       | 0.94          |
| (1,958)  | 1:77:A:GLU:HB2  | 1:78:A:LEU:HD13 | 20       | 0.94          |
| (1,819)  | 1:67:A:THR:HA   | 1:68:A:LEU:HB3  | 20       | 0.94          |
| (1,792)  | 1:11:A:LEU:HB3  | 1:39:A:GLY:HA3  | 19       | 0.94          |
| (1,711)  | 1:68:A:LEU:HD11 | 1:73:A:LYS:HA   | 9        | 0.94          |
| (1,711)  | 1:68:A:LEU:HD12 | 1:73:A:LYS:HA   | 9        | 0.94          |
| (1,711)  | 1:68:A:LEU:HD13 | 1:73:A:LYS:HA   | 9        | 0.94          |
| (1,711)  | 1:68:A:LEU:HD11 | 1:73:A:LYS:HA   | 17       | 0.94          |
| (1,711)  | 1:68:A:LEU:HD12 | 1:73:A:LYS:HA   | 17       | 0.94          |
| (1,711)  | 1:68:A:LEU:HD13 | 1:73:A:LYS:HA   | 17       | 0.94          |
| (1,670)  | 1:20:A:LEU:HA   | 1:23:A:HIS:HB3  | 15       | 0.94          |
| (1,252)  | 1:63:A:LEU:H    | 1:64:A:GLN:HG3  | 3        | 0.94          |
| (1,252)  | 1:63:A:LEU:H    | 1:64:A:GLN:HG3  | 11       | 0.94          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,55)   | 1:68:A:LEU:HD11 | 1:69:A:LEU:H    | 16       | 0.94          |
| (1,55)   | 1:68:A:LEU:HD12 | 1:69:A:LEU:H    | 16       | 0.94          |
| (1,55)   | 1:68:A:LEU:HD13 | 1:69:A:LEU:H    | 16       | 0.94          |
| (1,1163) | 1:4:A:PHE:HB2   | 1:78:A:LEU:HD21 | 8        | 0.93          |
| (1,1163) | 1:4:A:PHE:HB2   | 1:78:A:LEU:HD22 | 8        | 0.93          |
| (1,1163) | 1:4:A:PHE:HB2   | 1:78:A:LEU:HD23 | 8        | 0.93          |
| (1,1163) | 1:4:A:PHE:HB3   | 1:78:A:LEU:HD21 | 8        | 0.93          |
| (1,1163) | 1:4:A:PHE:HB3   | 1:78:A:LEU:HD22 | 8        | 0.93          |
| (1,1163) | 1:4:A:PHE:HB3   | 1:78:A:LEU:HD23 | 8        | 0.93          |
| (1,877)  | 1:7:A:PHE:HB3   | 1:79:A:THR:HB   | 16       | 0.93          |
| (1,809)  | 1:7:A:PHE:HZ    | 1:9:A:GLY:HA2   | 4        | 0.93          |
| (1,536)  | 1:11:A:LEU:HB3  | 1:39:A:GLY:H    | 3        | 0.93          |
| (1,1040) | 1:12:A:PRO:HG2  | 1:70:A:LYS:HB3  | 11       | 0.92          |
| (1,595)  | 1:28:A:SER:HB2  | 1:45:A:PHE:HE1  | 9        | 0.92          |
| (1,595)  | 1:28:A:SER:HB2  | 1:45:A:PHE:HE2  | 9        | 0.92          |
| (1,590)  | 1:29:A:PRO:HA   | 1:43:A:LEU:HB2  | 15       | 0.92          |
| (1,309)  | 1:58:A:MET:H    | 1:59:A:ASP:HB3  | 3        | 0.92          |
| (1,252)  | 1:63:A:LEU:H    | 1:64:A:GLN:HG3  | 17       | 0.92          |
| (1,1248) | 1:8:A:VAL:HG11  | 1:43:A:LEU:HD21 | 18       | 0.91          |
| (1,1248) | 1:8:A:VAL:HG11  | 1:43:A:LEU:HD22 | 18       | 0.91          |
| (1,1248) | 1:8:A:VAL:HG11  | 1:43:A:LEU:HD23 | 18       | 0.91          |
| (1,1248) | 1:8:A:VAL:HG12  | 1:43:A:LEU:HD21 | 18       | 0.91          |
| (1,1248) | 1:8:A:VAL:HG12  | 1:43:A:LEU:HD22 | 18       | 0.91          |
| (1,1248) | 1:8:A:VAL:HG12  | 1:43:A:LEU:HD23 | 18       | 0.91          |
| (1,1248) | 1:8:A:VAL:HG13  | 1:43:A:LEU:HD21 | 18       | 0.91          |
| (1,1248) | 1:8:A:VAL:HG13  | 1:43:A:LEU:HD22 | 18       | 0.91          |
| (1,1248) | 1:8:A:VAL:HG13  | 1:43:A:LEU:HD23 | 18       | 0.91          |
| (1,1198) | 1:69:A:LEU:HD21 | 1:70:A:LYS:H    | 7        | 0.91          |
| (1,1198) | 1:69:A:LEU:HD22 | 1:70:A:LYS:H    | 7        | 0.91          |
| (1,1198) | 1:69:A:LEU:HD23 | 1:70:A:LYS:H    | 7        | 0.91          |
| (1,958)  | 1:77:A:GLU:HB2  | 1:78:A:LEU:HD11 | 13       | 0.91          |
| (1,958)  | 1:77:A:GLU:HB2  | 1:78:A:LEU:HD12 | 13       | 0.91          |
| (1,958)  | 1:77:A:GLU:HB2  | 1:78:A:LEU:HD13 | 13       | 0.91          |
| (1,670)  | 1:20:A:LEU:HA   | 1:23:A:HIS:HB3  | 11       | 0.91          |
| (1,644)  | 1:56:A:ARG:HA   | 1:59:A:ASP:HB3  | 12       | 0.91          |
| (1,644)  | 1:56:A:ARG:HA   | 1:59:A:ASP:HB3  | 15       | 0.91          |
| (1,536)  | 1:11:A:LEU:HB3  | 1:39:A:GLY:H    | 15       | 0.91          |
| (1,252)  | 1:63:A:LEU:H    | 1:64:A:GLN:HG3  | 5        | 0.91          |
| (1,252)  | 1:63:A:LEU:H    | 1:64:A:GLN:HG3  | 6        | 0.91          |
| (1,212)  | 1:8:A:VAL:HG21  | 1:75:A:ASN:H    | 3        | 0.91          |
| (1,212)  | 1:8:A:VAL:HG22  | 1:75:A:ASN:H    | 3        | 0.91          |
| (1,212)  | 1:8:A:VAL:HG23  | 1:75:A:ASN:H    | 3        | 0.91          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1161) | 1:4:A:PHE:HD1   | 1:78:A:LEU:HD21 | 16       | 0.9           |
| (1,1161) | 1:4:A:PHE:HD1   | 1:78:A:LEU:HD22 | 16       | 0.9           |
| (1,1161) | 1:4:A:PHE:HD1   | 1:78:A:LEU:HD23 | 16       | 0.9           |
| (1,1161) | 1:4:A:PHE:HD2   | 1:78:A:LEU:HD21 | 16       | 0.9           |
| (1,1161) | 1:4:A:PHE:HD2   | 1:78:A:LEU:HD22 | 16       | 0.9           |
| (1,1161) | 1:4:A:PHE:HD2   | 1:78:A:LEU:HD23 | 16       | 0.9           |
| (1,1040) | 1:12:A:PRO:HG2  | 1:70:A:LYS:HB3  | 15       | 0.9           |
| (1,958)  | 1:77:A:GLU:HB2  | 1:78:A:LEU:HD11 | 11       | 0.9           |
| (1,958)  | 1:77:A:GLU:HB2  | 1:78:A:LEU:HD12 | 11       | 0.9           |
| (1,958)  | 1:77:A:GLU:HB2  | 1:78:A:LEU:HD13 | 11       | 0.9           |
| (1,811)  | 1:7:A:PHE:HE1   | 1:9:A:GLY:HA2   | 12       | 0.9           |
| (1,811)  | 1:7:A:PHE:HE2   | 1:9:A:GLY:HA2   | 12       | 0.9           |
| (1,644)  | 1:56:A:ARG:HA   | 1:59:A:ASP:HB3  | 18       | 0.9           |
| (1,536)  | 1:11:A:LEU:HB3  | 1:39:A:GLY:H    | 18       | 0.9           |
| (1,55)   | 1:68:A:LEU:HD11 | 1:69:A:LEU:H    | 12       | 0.9           |
| (1,55)   | 1:68:A:LEU:HD12 | 1:69:A:LEU:H    | 12       | 0.9           |
| (1,55)   | 1:68:A:LEU:HD13 | 1:69:A:LEU:H    | 12       | 0.9           |
| (1,1313) | 1:58:A:MET:HB3  | 1:58:A:MET:HE1  | 20       | 0.89          |
| (1,1313) | 1:58:A:MET:HB3  | 1:58:A:MET:HE2  | 20       | 0.89          |
| (1,1313) | 1:58:A:MET:HB3  | 1:58:A:MET:HE3  | 20       | 0.89          |
| (1,1163) | 1:4:A:PHE:HB2   | 1:78:A:LEU:HD21 | 4        | 0.89          |
| (1,1163) | 1:4:A:PHE:HB2   | 1:78:A:LEU:HD22 | 4        | 0.89          |
| (1,1163) | 1:4:A:PHE:HB2   | 1:78:A:LEU:HD23 | 4        | 0.89          |
| (1,1163) | 1:4:A:PHE:HB3   | 1:78:A:LEU:HD21 | 4        | 0.89          |
| (1,1163) | 1:4:A:PHE:HB3   | 1:78:A:LEU:HD22 | 4        | 0.89          |
| (1,1163) | 1:4:A:PHE:HB3   | 1:78:A:LEU:HD23 | 4        | 0.89          |
| (1,958)  | 1:77:A:GLU:HB2  | 1:78:A:LEU:HD11 | 8        | 0.89          |
| (1,958)  | 1:77:A:GLU:HB2  | 1:78:A:LEU:HD12 | 8        | 0.89          |
| (1,958)  | 1:77:A:GLU:HB2  | 1:78:A:LEU:HD13 | 8        | 0.89          |
| (1,958)  | 1:77:A:GLU:HB2  | 1:78:A:LEU:HD11 | 17       | 0.89          |
| (1,958)  | 1:77:A:GLU:HB2  | 1:78:A:LEU:HD12 | 17       | 0.89          |
| (1,958)  | 1:77:A:GLU:HB2  | 1:78:A:LEU:HD13 | 17       | 0.89          |
| (1,874)  | 1:74:A:ILE:HA   | 1:75:A:ASN:HB2  | 9        | 0.89          |
| (1,874)  | 1:74:A:ILE:HA   | 1:75:A:ASN:HB2  | 19       | 0.89          |
| (1,644)  | 1:56:A:ARG:HA   | 1:59:A:ASP:HB3  | 1        | 0.89          |
| (1,212)  | 1:8:A:VAL:HG21  | 1:75:A:ASN:H    | 9        | 0.89          |
| (1,212)  | 1:8:A:VAL:HG22  | 1:75:A:ASN:H    | 9        | 0.89          |
| (1,212)  | 1:8:A:VAL:HG23  | 1:75:A:ASN:H    | 9        | 0.89          |
| (1,1198) | 1:69:A:LEU:HD21 | 1:70:A:LYS:H    | 3        | 0.88          |
| (1,1198) | 1:69:A:LEU:HD22 | 1:70:A:LYS:H    | 3        | 0.88          |
| (1,1198) | 1:69:A:LEU:HD23 | 1:70:A:LYS:H    | 3        | 0.88          |
| (1,1198) | 1:69:A:LEU:HD21 | 1:70:A:LYS:H    | 16       | 0.88          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1198) | 1:69:A:LEU:HD22 | 1:70:A:LYS:H    | 16       | 0.88          |
| (1,1198) | 1:69:A:LEU:HD23 | 1:70:A:LYS:H    | 16       | 0.88          |
| (1,874)  | 1:74:A:ILE:HA   | 1:75:A:ASN:HB2  | 2        | 0.88          |
| (1,874)  | 1:74:A:ILE:HA   | 1:75:A:ASN:HB2  | 17       | 0.88          |
| (1,792)  | 1:11:A:LEU:HB3  | 1:39:A:GLY:HA3  | 2        | 0.88          |
| (1,792)  | 1:11:A:LEU:HB3  | 1:39:A:GLY:HA3  | 13       | 0.88          |
| (1,1040) | 1:12:A:PRO:HG2  | 1:70:A:LYS:HB3  | 20       | 0.87          |
| (1,1030) | 1:29:A:PRO:HB2  | 1:43:A:LEU:HB2  | 12       | 0.87          |
| (1,1012) | 1:65:A:HIS:HB3  | 1:76:A:VAL:HG21 | 5        | 0.87          |
| (1,1012) | 1:65:A:HIS:HB3  | 1:76:A:VAL:HG22 | 5        | 0.87          |
| (1,1012) | 1:65:A:HIS:HB3  | 1:76:A:VAL:HG23 | 5        | 0.87          |
| (1,874)  | 1:74:A:ILE:HA   | 1:75:A:ASN:HB2  | 5        | 0.87          |
| (1,692)  | 1:4:A:PHE:HA    | 1:80:A:VAL:HG21 | 13       | 0.87          |
| (1,692)  | 1:4:A:PHE:HA    | 1:80:A:VAL:HG22 | 13       | 0.87          |
| (1,692)  | 1:4:A:PHE:HA    | 1:80:A:VAL:HG23 | 13       | 0.87          |
| (1,101)  | 1:17:A:ALA:H    | 1:20:A:LEU:HD11 | 9        | 0.87          |
| (1,101)  | 1:17:A:ALA:H    | 1:20:A:LEU:HD12 | 9        | 0.87          |
| (1,101)  | 1:17:A:ALA:H    | 1:20:A:LEU:HD13 | 9        | 0.87          |
| (1,76)   | 1:68:A:LEU:HD11 | 1:73:A:LYS:H    | 10       | 0.87          |
| (1,76)   | 1:68:A:LEU:HD12 | 1:73:A:LYS:H    | 10       | 0.87          |
| (1,76)   | 1:68:A:LEU:HD13 | 1:73:A:LYS:H    | 10       | 0.87          |
| (1,1258) | 1:79:A:THR:HG21 | 1:80:A:VAL:HG11 | 12       | 0.86          |
| (1,1258) | 1:79:A:THR:HG21 | 1:80:A:VAL:HG12 | 12       | 0.86          |
| (1,1258) | 1:79:A:THR:HG21 | 1:80:A:VAL:HG13 | 12       | 0.86          |
| (1,1258) | 1:79:A:THR:HG22 | 1:80:A:VAL:HG11 | 12       | 0.86          |
| (1,1258) | 1:79:A:THR:HG22 | 1:80:A:VAL:HG12 | 12       | 0.86          |
| (1,1258) | 1:79:A:THR:HG22 | 1:80:A:VAL:HG13 | 12       | 0.86          |
| (1,1258) | 1:79:A:THR:HG23 | 1:80:A:VAL:HG11 | 12       | 0.86          |
| (1,1258) | 1:79:A:THR:HG23 | 1:80:A:VAL:HG12 | 12       | 0.86          |
| (1,1258) | 1:79:A:THR:HG23 | 1:80:A:VAL:HG13 | 12       | 0.86          |
| (1,1248) | 1:8:A:VAL:HG11  | 1:43:A:LEU:HD21 | 17       | 0.86          |
| (1,1248) | 1:8:A:VAL:HG11  | 1:43:A:LEU:HD22 | 17       | 0.86          |
| (1,1248) | 1:8:A:VAL:HG11  | 1:43:A:LEU:HD23 | 17       | 0.86          |
| (1,1248) | 1:8:A:VAL:HG12  | 1:43:A:LEU:HD21 | 17       | 0.86          |
| (1,1248) | 1:8:A:VAL:HG12  | 1:43:A:LEU:HD22 | 17       | 0.86          |
| (1,1248) | 1:8:A:VAL:HG12  | 1:43:A:LEU:HD23 | 17       | 0.86          |
| (1,1248) | 1:8:A:VAL:HG13  | 1:43:A:LEU:HD21 | 17       | 0.86          |
| (1,1248) | 1:8:A:VAL:HG13  | 1:43:A:LEU:HD22 | 17       | 0.86          |
| (1,1248) | 1:8:A:VAL:HG13  | 1:43:A:LEU:HD23 | 17       | 0.86          |
| (1,1201) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD21 | 11       | 0.86          |
| (1,1201) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD22 | 11       | 0.86          |
| (1,1201) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD23 | 11       | 0.86          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1198) | 1:69:A:LEU:HD21 | 1:70:A:LYS:H    | 9        | 0.86          |
| (1,1198) | 1:69:A:LEU:HD22 | 1:70:A:LYS:H    | 9        | 0.86          |
| (1,1198) | 1:69:A:LEU:HD23 | 1:70:A:LYS:H    | 9        | 0.86          |
| (1,874)  | 1:74:A:ILE:HA   | 1:75:A:ASN:HB2  | 3        | 0.86          |
| (1,874)  | 1:74:A:ILE:HA   | 1:75:A:ASN:HB2  | 11       | 0.86          |
| (1,874)  | 1:74:A:ILE:HA   | 1:75:A:ASN:HB2  | 12       | 0.86          |
| (1,874)  | 1:74:A:ILE:HA   | 1:75:A:ASN:HB2  | 14       | 0.86          |
| (1,868)  | 1:9:A:GLY:H     | 1:75:A:ASN:HB3  | 8        | 0.86          |
| (1,811)  | 1:7:A:PHE:HE1   | 1:9:A:GLY:HA2   | 1        | 0.86          |
| (1,811)  | 1:7:A:PHE:HE2   | 1:9:A:GLY:HA2   | 1        | 0.86          |
| (1,670)  | 1:20:A:LEU:HA   | 1:23:A:HIS:HB3  | 14       | 0.86          |
| (1,536)  | 1:11:A:LEU:HB3  | 1:39:A:GLY:H    | 9        | 0.86          |
| (1,536)  | 1:11:A:LEU:HB3  | 1:39:A:GLY:H    | 17       | 0.86          |
| (1,252)  | 1:63:A:LEU:H    | 1:64:A:GLN:HG3  | 9        | 0.86          |
| (1,1198) | 1:69:A:LEU:HD21 | 1:70:A:LYS:H    | 1        | 0.85          |
| (1,1198) | 1:69:A:LEU:HD22 | 1:70:A:LYS:H    | 1        | 0.85          |
| (1,1198) | 1:69:A:LEU:HD23 | 1:70:A:LYS:H    | 1        | 0.85          |
| (1,1161) | 1:4:A:PHE:HD1   | 1:78:A:LEU:HD21 | 15       | 0.85          |
| (1,1161) | 1:4:A:PHE:HD1   | 1:78:A:LEU:HD22 | 15       | 0.85          |
| (1,1161) | 1:4:A:PHE:HD1   | 1:78:A:LEU:HD23 | 15       | 0.85          |
| (1,1161) | 1:4:A:PHE:HD2   | 1:78:A:LEU:HD21 | 15       | 0.85          |
| (1,1161) | 1:4:A:PHE:HD2   | 1:78:A:LEU:HD22 | 15       | 0.85          |
| (1,1161) | 1:4:A:PHE:HD2   | 1:78:A:LEU:HD23 | 15       | 0.85          |
| (1,874)  | 1:74:A:ILE:HA   | 1:75:A:ASN:HB2  | 20       | 0.85          |
| (1,792)  | 1:11:A:LEU:HB3  | 1:39:A:GLY:HA3  | 10       | 0.85          |
| (1,773)  | 1:65:A:HIS:HB3  | 1:75:A:ASN:HA   | 19       | 0.85          |
| (1,644)  | 1:56:A:ARG:HA   | 1:59:A:ASP:HB3  | 10       | 0.85          |
| (1,590)  | 1:29:A:PRO:HA   | 1:43:A:LEU:HB2  | 17       | 0.85          |
| (1,489)  | 1:10:A:SER:HB3  | 1:75:A:ASN:HD22 | 16       | 0.85          |
| (1,252)  | 1:63:A:LEU:H    | 1:64:A:GLN:HG3  | 13       | 0.85          |
| (1,212)  | 1:8:A:VAL:HG21  | 1:75:A:ASN:H    | 13       | 0.85          |
| (1,212)  | 1:8:A:VAL:HG22  | 1:75:A:ASN:H    | 13       | 0.85          |
| (1,212)  | 1:8:A:VAL:HG23  | 1:75:A:ASN:H    | 13       | 0.85          |
| (1,181)  | 1:68:A:LEU:HB2  | 1:72:A:LYS:H    | 18       | 0.85          |
| (1,1359) | 1:23:A:HIS:HD2  | 1:64:A:GLN:HB2  | 20       | 0.84          |
| (1,1280) | 1:36:A:ALA:HB1  | 1:37:A:ASP:HB3  | 18       | 0.84          |
| (1,1280) | 1:36:A:ALA:HB2  | 1:37:A:ASP:HB3  | 18       | 0.84          |
| (1,1280) | 1:36:A:ALA:HB3  | 1:37:A:ASP:HB3  | 18       | 0.84          |
| (1,1201) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD21 | 17       | 0.84          |
| (1,1201) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD22 | 17       | 0.84          |
| (1,1201) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD23 | 17       | 0.84          |
| (1,1198) | 1:69:A:LEU:HD21 | 1:70:A:LYS:H    | 6        | 0.84          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1198) | 1:69:A:LEU:HD22 | 1:70:A:LYS:H    | 6        | 0.84          |
| (1,1198) | 1:69:A:LEU:HD23 | 1:70:A:LYS:H    | 6        | 0.84          |
| (1,1040) | 1:12:A:PRO:HG2  | 1:70:A:LYS:HB3  | 18       | 0.84          |
| (1,958)  | 1:77:A:GLU:HB2  | 1:78:A:LEU:HD11 | 5        | 0.84          |
| (1,958)  | 1:77:A:GLU:HB2  | 1:78:A:LEU:HD12 | 5        | 0.84          |
| (1,958)  | 1:77:A:GLU:HB2  | 1:78:A:LEU:HD13 | 5        | 0.84          |
| (1,890)  | 1:59:A:ASP:HA   | 1:62:A:LEU:HB3  | 2        | 0.84          |
| (1,874)  | 1:74:A:ILE:HA   | 1:75:A:ASN:HB2  | 16       | 0.84          |
| (1,868)  | 1:9:A:GLY:H     | 1:75:A:ASN:HB3  | 4        | 0.84          |
| (1,692)  | 1:4:A:PHE:HA    | 1:80:A:VAL:HG21 | 12       | 0.84          |
| (1,692)  | 1:4:A:PHE:HA    | 1:80:A:VAL:HG22 | 12       | 0.84          |
| (1,692)  | 1:4:A:PHE:HA    | 1:80:A:VAL:HG23 | 12       | 0.84          |
| (1,674)  | 1:68:A:LEU:HB2  | 1:71:A:GLU:HA   | 20       | 0.84          |
| (1,590)  | 1:29:A:PRO:HA   | 1:43:A:LEU:HB2  | 6        | 0.84          |
| (1,252)  | 1:63:A:LEU:H    | 1:64:A:GLN:HG3  | 7        | 0.84          |
| (1,212)  | 1:8:A:VAL:HG21  | 1:75:A:ASN:H    | 5        | 0.84          |
| (1,212)  | 1:8:A:VAL:HG22  | 1:75:A:ASN:H    | 5        | 0.84          |
| (1,212)  | 1:8:A:VAL:HG23  | 1:75:A:ASN:H    | 5        | 0.84          |
| (1,1359) | 1:23:A:HIS:HD2  | 1:64:A:GLN:HB2  | 17       | 0.83          |
| (1,1313) | 1:58:A:MET:HB3  | 1:58:A:MET:HE1  | 13       | 0.83          |
| (1,1313) | 1:58:A:MET:HB3  | 1:58:A:MET:HE2  | 13       | 0.83          |
| (1,1313) | 1:58:A:MET:HB3  | 1:58:A:MET:HE3  | 13       | 0.83          |
| (1,1040) | 1:12:A:PRO:HG2  | 1:70:A:LYS:HB3  | 2        | 0.83          |
| (1,877)  | 1:7:A:PHE:HB3   | 1:79:A:THR:HB   | 13       | 0.83          |
| (1,874)  | 1:74:A:ILE:HA   | 1:75:A:ASN:HB2  | 6        | 0.83          |
| (1,711)  | 1:68:A:LEU:HD11 | 1:73:A:LYS:HA   | 4        | 0.83          |
| (1,711)  | 1:68:A:LEU:HD12 | 1:73:A:LYS:HA   | 4        | 0.83          |
| (1,711)  | 1:68:A:LEU:HD13 | 1:73:A:LYS:HA   | 4        | 0.83          |
| (1,309)  | 1:58:A:MET:H    | 1:59:A:ASP:HB3  | 17       | 0.83          |
| (1,55)   | 1:68:A:LEU:HD11 | 1:69:A:LEU:H    | 4        | 0.83          |
| (1,55)   | 1:68:A:LEU:HD12 | 1:69:A:LEU:H    | 4        | 0.83          |
| (1,55)   | 1:68:A:LEU:HD13 | 1:69:A:LEU:H    | 4        | 0.83          |
| (1,30)   | 1:32:A:ILE:HG12 | 1:33:A:ARG:H    | 18       | 0.83          |
| (1,958)  | 1:77:A:GLU:HB2  | 1:78:A:LEU:HD11 | 6        | 0.82          |
| (1,958)  | 1:77:A:GLU:HB2  | 1:78:A:LEU:HD12 | 6        | 0.82          |
| (1,958)  | 1:77:A:GLU:HB2  | 1:78:A:LEU:HD13 | 6        | 0.82          |
| (1,958)  | 1:77:A:GLU:HB2  | 1:78:A:LEU:HD11 | 16       | 0.82          |
| (1,958)  | 1:77:A:GLU:HB2  | 1:78:A:LEU:HD12 | 16       | 0.82          |
| (1,958)  | 1:77:A:GLU:HB2  | 1:78:A:LEU:HD13 | 16       | 0.82          |
| (1,874)  | 1:74:A:ILE:HA   | 1:75:A:ASN:HB2  | 8        | 0.82          |
| (1,806)  | 1:68:A:LEU:HA   | 1:69:A:LEU:HB3  | 12       | 0.82          |
| (1,792)  | 1:11:A:LEU:HB3  | 1:39:A:GLY:HA3  | 12       | 0.82          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,674)  | 1:68:A:LEU:HB2  | 1:71:A:GLU:HA   | 18       | 0.82          |
| (1,536)  | 1:11:A:LEU:HB3  | 1:39:A:GLY:H    | 7        | 0.82          |
| (1,481)  | 1:18:A:VAL:HG11 | 1:22:A:ASN:HD21 | 18       | 0.82          |
| (1,481)  | 1:18:A:VAL:HG12 | 1:22:A:ASN:HD21 | 18       | 0.82          |
| (1,481)  | 1:18:A:VAL:HG13 | 1:22:A:ASN:HD21 | 18       | 0.82          |
| (1,181)  | 1:68:A:LEU:HB2  | 1:72:A:LYS:H    | 13       | 0.82          |
| (1,55)   | 1:68:A:LEU:HD11 | 1:69:A:LEU:H    | 9        | 0.82          |
| (1,55)   | 1:68:A:LEU:HD12 | 1:69:A:LEU:H    | 9        | 0.82          |
| (1,55)   | 1:68:A:LEU:HD13 | 1:69:A:LEU:H    | 9        | 0.82          |
| (1,1163) | 1:4:A:PHE:HB2   | 1:78:A:LEU:HD21 | 12       | 0.81          |
| (1,1163) | 1:4:A:PHE:HB2   | 1:78:A:LEU:HD22 | 12       | 0.81          |
| (1,1163) | 1:4:A:PHE:HB2   | 1:78:A:LEU:HD23 | 12       | 0.81          |
| (1,1163) | 1:4:A:PHE:HB3   | 1:78:A:LEU:HD21 | 12       | 0.81          |
| (1,1163) | 1:4:A:PHE:HB3   | 1:78:A:LEU:HD22 | 12       | 0.81          |
| (1,1163) | 1:4:A:PHE:HB3   | 1:78:A:LEU:HD23 | 12       | 0.81          |
| (1,1080) | 1:33:A:ARG:HG3  | 1:42:A:PHE:HD1  | 1        | 0.81          |
| (1,1080) | 1:33:A:ARG:HG3  | 1:42:A:PHE:HD2  | 1        | 0.81          |
| (1,1080) | 1:33:A:ARG:HG3  | 1:42:A:PHE:HD1  | 20       | 0.81          |
| (1,1080) | 1:33:A:ARG:HG3  | 1:42:A:PHE:HD2  | 20       | 0.81          |
| (1,961)  | 1:7:A:PHE:HB2   | 1:77:A:GLU:HB2  | 2        | 0.81          |
| (1,961)  | 1:7:A:PHE:HB2   | 1:77:A:GLU:HB2  | 4        | 0.81          |
| (1,961)  | 1:7:A:PHE:HB2   | 1:77:A:GLU:HB2  | 5        | 0.81          |
| (1,961)  | 1:7:A:PHE:HB2   | 1:77:A:GLU:HB2  | 9        | 0.81          |
| (1,961)  | 1:7:A:PHE:HB2   | 1:77:A:GLU:HB2  | 10       | 0.81          |
| (1,961)  | 1:7:A:PHE:HB2   | 1:77:A:GLU:HB2  | 14       | 0.81          |
| (1,961)  | 1:7:A:PHE:HB2   | 1:77:A:GLU:HB2  | 15       | 0.81          |
| (1,961)  | 1:7:A:PHE:HB2   | 1:77:A:GLU:HB2  | 16       | 0.81          |
| (1,874)  | 1:74:A:ILE:HA   | 1:75:A:ASN:HB2  | 1        | 0.81          |
| (1,874)  | 1:74:A:ILE:HA   | 1:75:A:ASN:HB2  | 7        | 0.81          |
| (1,874)  | 1:74:A:ILE:HA   | 1:75:A:ASN:HB2  | 15       | 0.81          |
| (1,868)  | 1:9:A:GLY:H     | 1:75:A:ASN:HB3  | 10       | 0.81          |
| (1,820)  | 1:68:A:LEU:HB2  | 1:71:A:GLU:H    | 13       | 0.81          |
| (1,785)  | 1:11:A:LEU:HB2  | 1:12:A:PRO:HD3  | 4        | 0.81          |
| (1,785)  | 1:11:A:LEU:HB2  | 1:12:A:PRO:HD3  | 10       | 0.81          |
| (1,711)  | 1:68:A:LEU:HD11 | 1:73:A:LYS:HA   | 18       | 0.81          |
| (1,711)  | 1:68:A:LEU:HD12 | 1:73:A:LYS:HA   | 18       | 0.81          |
| (1,711)  | 1:68:A:LEU:HD13 | 1:73:A:LYS:HA   | 18       | 0.81          |
| (1,181)  | 1:68:A:LEU:HB2  | 1:72:A:LYS:H    | 7        | 0.81          |
| (1,55)   | 1:68:A:LEU:HD11 | 1:69:A:LEU:H    | 11       | 0.81          |
| (1,55)   | 1:68:A:LEU:HD12 | 1:69:A:LEU:H    | 11       | 0.81          |
| (1,55)   | 1:68:A:LEU:HD13 | 1:69:A:LEU:H    | 11       | 0.81          |
| (1,55)   | 1:68:A:LEU:HD11 | 1:69:A:LEU:H    | 17       | 0.81          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,55)   | 1:68:A:LEU:HD12 | 1:69:A:LEU:H    | 17       | 0.81          |
| (1,55)   | 1:68:A:LEU:HD13 | 1:69:A:LEU:H    | 17       | 0.81          |
| (1,961)  | 1:7:A:PHE:HB2   | 1:77:A:GLU:HB2  | 1        | 0.8           |
| (1,961)  | 1:7:A:PHE:HB2   | 1:77:A:GLU:HB2  | 3        | 0.8           |
| (1,961)  | 1:7:A:PHE:HB2   | 1:77:A:GLU:HB2  | 6        | 0.8           |
| (1,961)  | 1:7:A:PHE:HB2   | 1:77:A:GLU:HB2  | 13       | 0.8           |
| (1,961)  | 1:7:A:PHE:HB2   | 1:77:A:GLU:HB2  | 17       | 0.8           |
| (1,961)  | 1:7:A:PHE:HB2   | 1:77:A:GLU:HB2  | 18       | 0.8           |
| (1,958)  | 1:77:A:GLU:HB2  | 1:78:A:LEU:HD11 | 2        | 0.8           |
| (1,958)  | 1:77:A:GLU:HB2  | 1:78:A:LEU:HD12 | 2        | 0.8           |
| (1,958)  | 1:77:A:GLU:HB2  | 1:78:A:LEU:HD13 | 2        | 0.8           |
| (1,874)  | 1:74:A:ILE:HA   | 1:75:A:ASN:HB2  | 10       | 0.8           |
| (1,874)  | 1:74:A:ILE:HA   | 1:75:A:ASN:HB2  | 18       | 0.8           |
| (1,792)  | 1:11:A:LEU:HB3  | 1:39:A:GLY:HA3  | 20       | 0.8           |
| (1,785)  | 1:11:A:LEU:HB2  | 1:12:A:PRO:HD3  | 5        | 0.8           |
| (1,773)  | 1:65:A:HIS:HB3  | 1:75:A:ASN:HA   | 2        | 0.8           |
| (1,711)  | 1:68:A:LEU:HD11 | 1:73:A:LYS:HA   | 7        | 0.8           |
| (1,711)  | 1:68:A:LEU:HD12 | 1:73:A:LYS:HA   | 7        | 0.8           |
| (1,711)  | 1:68:A:LEU:HD13 | 1:73:A:LYS:HA   | 7        | 0.8           |
| (1,536)  | 1:11:A:LEU:HB3  | 1:39:A:GLY:H    | 16       | 0.8           |
| (1,536)  | 1:11:A:LEU:HB3  | 1:39:A:GLY:H    | 20       | 0.8           |
| (1,252)  | 1:63:A:LEU:H    | 1:64:A:GLN:HG3  | 19       | 0.8           |
| (1,181)  | 1:68:A:LEU:HB2  | 1:72:A:LYS:H    | 2        | 0.8           |
| (1,55)   | 1:68:A:LEU:HD11 | 1:69:A:LEU:H    | 14       | 0.8           |
| (1,55)   | 1:68:A:LEU:HD12 | 1:69:A:LEU:H    | 14       | 0.8           |
| (1,55)   | 1:68:A:LEU:HD13 | 1:69:A:LEU:H    | 14       | 0.8           |
| (1,1336) | 1:59:A:ASP:HB3  | 1:60:A:ILE:HD11 | 6        | 0.79          |
| (1,1336) | 1:59:A:ASP:HB3  | 1:60:A:ILE:HD12 | 6        | 0.79          |
| (1,1336) | 1:59:A:ASP:HB3  | 1:60:A:ILE:HD13 | 6        | 0.79          |
| (1,1313) | 1:58:A:MET:HB3  | 1:58:A:MET:HE1  | 11       | 0.79          |
| (1,1313) | 1:58:A:MET:HB3  | 1:58:A:MET:HE2  | 11       | 0.79          |
| (1,1313) | 1:58:A:MET:HB3  | 1:58:A:MET:HE3  | 11       | 0.79          |
| (1,1246) | 1:7:A:PHE:HA    | 1:8:A:VAL:HG11  | 8        | 0.79          |
| (1,1246) | 1:7:A:PHE:HA    | 1:8:A:VAL:HG12  | 8        | 0.79          |
| (1,1246) | 1:7:A:PHE:HA    | 1:8:A:VAL:HG13  | 8        | 0.79          |
| (1,1040) | 1:12:A:PRO:HG2  | 1:70:A:LYS:HB3  | 16       | 0.79          |
| (1,874)  | 1:74:A:ILE:HA   | 1:75:A:ASN:HB2  | 4        | 0.79          |
| (1,874)  | 1:74:A:ILE:HA   | 1:75:A:ASN:HB2  | 13       | 0.79          |
| (1,792)  | 1:11:A:LEU:HB3  | 1:39:A:GLY:HA3  | 8        | 0.79          |
| (1,785)  | 1:11:A:LEU:HB2  | 1:12:A:PRO:HD3  | 2        | 0.79          |
| (1,785)  | 1:11:A:LEU:HB2  | 1:12:A:PRO:HD3  | 11       | 0.79          |
| (1,785)  | 1:11:A:LEU:HB2  | 1:12:A:PRO:HD3  | 17       | 0.79          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,489)  | 1:10:A:SER:HB3  | 1:75:A:ASN:HD22 | 20       | 0.79          |
| (1,55)   | 1:68:A:LEU:HD11 | 1:69:A:LEU:H    | 7        | 0.79          |
| (1,55)   | 1:68:A:LEU:HD12 | 1:69:A:LEU:H    | 7        | 0.79          |
| (1,55)   | 1:68:A:LEU:HD13 | 1:69:A:LEU:H    | 7        | 0.79          |
| (1,1313) | 1:58:A:MET:HB3  | 1:58:A:MET:HE1  | 18       | 0.78          |
| (1,1313) | 1:58:A:MET:HB3  | 1:58:A:MET:HE2  | 18       | 0.78          |
| (1,1313) | 1:58:A:MET:HB3  | 1:58:A:MET:HE3  | 18       | 0.78          |
| (1,958)  | 1:77:A:GLU:HB2  | 1:78:A:LEU:HD11 | 4        | 0.78          |
| (1,958)  | 1:77:A:GLU:HB2  | 1:78:A:LEU:HD12 | 4        | 0.78          |
| (1,958)  | 1:77:A:GLU:HB2  | 1:78:A:LEU:HD13 | 4        | 0.78          |
| (1,958)  | 1:77:A:GLU:HB2  | 1:78:A:LEU:HD11 | 15       | 0.78          |
| (1,958)  | 1:77:A:GLU:HB2  | 1:78:A:LEU:HD12 | 15       | 0.78          |
| (1,958)  | 1:77:A:GLU:HB2  | 1:78:A:LEU:HD13 | 15       | 0.78          |
| (1,868)  | 1:9:A:GLY:H     | 1:75:A:ASN:HB3  | 17       | 0.78          |
| (1,789)  | 1:11:A:LEU:HB3  | 1:39:A:GLY:HA2  | 4        | 0.78          |
| (1,785)  | 1:11:A:LEU:HB2  | 1:12:A:PRO:HD3  | 14       | 0.78          |
| (1,670)  | 1:20:A:LEU:HA   | 1:23:A:HIS:HB3  | 4        | 0.78          |
| (1,598)  | 1:12:A:PRO:HA   | 1:72:A:LYS:HG2  | 16       | 0.78          |
| (1,396)  | 1:55:A:GLN:HE22 | 1:56:A:ARG:HG2  | 6        | 0.78          |
| (1,252)  | 1:63:A:LEU:H    | 1:64:A:GLN:HG3  | 16       | 0.78          |
| (1,181)  | 1:68:A:LEU:HB2  | 1:72:A:LYS:H    | 11       | 0.78          |
| (1,1313) | 1:58:A:MET:HB3  | 1:58:A:MET:HE1  | 19       | 0.77          |
| (1,1313) | 1:58:A:MET:HB3  | 1:58:A:MET:HE2  | 19       | 0.77          |
| (1,1313) | 1:58:A:MET:HB3  | 1:58:A:MET:HE3  | 19       | 0.77          |
| (1,1246) | 1:7:A:PHE:HA    | 1:8:A:VAL:HG11  | 1        | 0.77          |
| (1,1246) | 1:7:A:PHE:HA    | 1:8:A:VAL:HG12  | 1        | 0.77          |
| (1,1246) | 1:7:A:PHE:HA    | 1:8:A:VAL:HG13  | 1        | 0.77          |
| (1,1201) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD21 | 7        | 0.77          |
| (1,1201) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD22 | 7        | 0.77          |
| (1,1201) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD23 | 7        | 0.77          |
| (1,1198) | 1:69:A:LEU:HD21 | 1:70:A:LYS:H    | 13       | 0.77          |
| (1,1198) | 1:69:A:LEU:HD22 | 1:70:A:LYS:H    | 13       | 0.77          |
| (1,1198) | 1:69:A:LEU:HD23 | 1:70:A:LYS:H    | 13       | 0.77          |
| (1,1161) | 1:4:A:PHE:HD1   | 1:78:A:LEU:HD21 | 11       | 0.77          |
| (1,1161) | 1:4:A:PHE:HD1   | 1:78:A:LEU:HD22 | 11       | 0.77          |
| (1,1161) | 1:4:A:PHE:HD1   | 1:78:A:LEU:HD23 | 11       | 0.77          |
| (1,1161) | 1:4:A:PHE:HD2   | 1:78:A:LEU:HD21 | 11       | 0.77          |
| (1,1161) | 1:4:A:PHE:HD2   | 1:78:A:LEU:HD22 | 11       | 0.77          |
| (1,1161) | 1:4:A:PHE:HD2   | 1:78:A:LEU:HD23 | 11       | 0.77          |
| (1,1030) | 1:29:A:PRO:HB2  | 1:43:A:LEU:HB2  | 11       | 0.77          |
| (1,958)  | 1:77:A:GLU:HB2  | 1:78:A:LEU:HD11 | 9        | 0.77          |
| (1,958)  | 1:77:A:GLU:HB2  | 1:78:A:LEU:HD12 | 9        | 0.77          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,958)  | 1:77:A:GLU:HB2  | 1:78:A:LEU:HD13 | 9        | 0.77          |
| (1,785)  | 1:11:A:LEU:HB2  | 1:12:A:PRO:HD3  | 15       | 0.77          |
| (1,711)  | 1:68:A:LEU:HD11 | 1:73:A:LYS:HA   | 2        | 0.77          |
| (1,711)  | 1:68:A:LEU:HD12 | 1:73:A:LYS:HA   | 2        | 0.77          |
| (1,711)  | 1:68:A:LEU:HD13 | 1:73:A:LYS:HA   | 2        | 0.77          |
| (1,598)  | 1:12:A:PRO:HA   | 1:72:A:LYS:HG2  | 13       | 0.77          |
| (1,536)  | 1:11:A:LEU:HB3  | 1:39:A:GLY:H    | 19       | 0.77          |
| (1,489)  | 1:10:A:SER:HB3  | 1:75:A:ASN:HD22 | 13       | 0.77          |
| (1,181)  | 1:68:A:LEU:HB2  | 1:72:A:LYS:H    | 9        | 0.77          |
| (1,55)   | 1:68:A:LEU:HD11 | 1:69:A:LEU:H    | 6        | 0.77          |
| (1,55)   | 1:68:A:LEU:HD12 | 1:69:A:LEU:H    | 6        | 0.77          |
| (1,55)   | 1:68:A:LEU:HD13 | 1:69:A:LEU:H    | 6        | 0.77          |
| (1,1280) | 1:36:A:ALA:HB1  | 1:37:A:ASP:HB3  | 3        | 0.76          |
| (1,1280) | 1:36:A:ALA:HB2  | 1:37:A:ASP:HB3  | 3        | 0.76          |
| (1,1280) | 1:36:A:ALA:HB3  | 1:37:A:ASP:HB3  | 3        | 0.76          |
| (1,1280) | 1:36:A:ALA:HB1  | 1:37:A:ASP:HB3  | 4        | 0.76          |
| (1,1280) | 1:36:A:ALA:HB2  | 1:37:A:ASP:HB3  | 4        | 0.76          |
| (1,1280) | 1:36:A:ALA:HB3  | 1:37:A:ASP:HB3  | 4        | 0.76          |
| (1,1160) | 1:78:A:LEU:HD21 | 1:79:A:THR:H    | 7        | 0.76          |
| (1,1160) | 1:78:A:LEU:HD22 | 1:79:A:THR:H    | 7        | 0.76          |
| (1,1160) | 1:78:A:LEU:HD23 | 1:79:A:THR:H    | 7        | 0.76          |
| (1,958)  | 1:77:A:GLU:HB2  | 1:78:A:LEU:HD11 | 18       | 0.76          |
| (1,958)  | 1:77:A:GLU:HB2  | 1:78:A:LEU:HD12 | 18       | 0.76          |
| (1,958)  | 1:77:A:GLU:HB2  | 1:78:A:LEU:HD13 | 18       | 0.76          |
| (1,785)  | 1:11:A:LEU:HB2  | 1:12:A:PRO:HD3  | 13       | 0.76          |
| (1,773)  | 1:65:A:HIS:HB3  | 1:75:A:ASN:HA   | 3        | 0.76          |
| (1,773)  | 1:65:A:HIS:HB3  | 1:75:A:ASN:HA   | 18       | 0.76          |
| (1,590)  | 1:29:A:PRO:HA   | 1:43:A:LEU:HB2  | 8        | 0.76          |
| (1,378)  | 1:38:A:LYS:H    | 1:38:A:LYS:HG3  | 1        | 0.76          |
| (1,378)  | 1:38:A:LYS:H    | 1:38:A:LYS:HG3  | 19       | 0.76          |
| (1,76)   | 1:68:A:LEU:HD11 | 1:73:A:LYS:H    | 12       | 0.76          |
| (1,76)   | 1:68:A:LEU:HD12 | 1:73:A:LYS:H    | 12       | 0.76          |
| (1,76)   | 1:68:A:LEU:HD13 | 1:73:A:LYS:H    | 12       | 0.76          |
| (1,1336) | 1:59:A:ASP:HB3  | 1:60:A:ILE:HD11 | 20       | 0.75          |
| (1,1336) | 1:59:A:ASP:HB3  | 1:60:A:ILE:HD12 | 20       | 0.75          |
| (1,1336) | 1:59:A:ASP:HB3  | 1:60:A:ILE:HD13 | 20       | 0.75          |
| (1,1280) | 1:36:A:ALA:HB1  | 1:37:A:ASP:HB3  | 6        | 0.75          |
| (1,1280) | 1:36:A:ALA:HB2  | 1:37:A:ASP:HB3  | 6        | 0.75          |
| (1,1280) | 1:36:A:ALA:HB3  | 1:37:A:ASP:HB3  | 6        | 0.75          |
| (1,1280) | 1:36:A:ALA:HB1  | 1:37:A:ASP:HB3  | 10       | 0.75          |
| (1,1280) | 1:36:A:ALA:HB2  | 1:37:A:ASP:HB3  | 10       | 0.75          |
| (1,1280) | 1:36:A:ALA:HB3  | 1:37:A:ASP:HB3  | 10       | 0.75          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1246) | 1:7:A:PHE:HA    | 1:8:A:VAL:HG11 | 11       | 0.75          |
| (1,1246) | 1:7:A:PHE:HA    | 1:8:A:VAL:HG12 | 11       | 0.75          |
| (1,1246) | 1:7:A:PHE:HA    | 1:8:A:VAL:HG13 | 11       | 0.75          |
| (1,1040) | 1:12:A:PRO:HG2  | 1:70:A:LYS:HB3 | 12       | 0.75          |
| (1,820)  | 1:68:A:LEU:HB2  | 1:71:A:GLU:H   | 7        | 0.75          |
| (1,806)  | 1:68:A:LEU:HA   | 1:69:A:LEU:HB3 | 11       | 0.75          |
| (1,792)  | 1:11:A:LEU:HB3  | 1:39:A:GLY:HA3 | 14       | 0.75          |
| (1,785)  | 1:11:A:LEU:HB2  | 1:12:A:PRO:HD3 | 19       | 0.75          |
| (1,773)  | 1:65:A:HIS:HB3  | 1:75:A:ASN:HA  | 17       | 0.75          |
| (1,378)  | 1:38:A:LYS:H    | 1:38:A:LYS:HG3 | 14       | 0.75          |
| (1,378)  | 1:38:A:LYS:H    | 1:38:A:LYS:HG3 | 17       | 0.75          |
| (1,212)  | 1:8:A:VAL:HG21  | 1:75:A:ASN:H   | 6        | 0.75          |
| (1,212)  | 1:8:A:VAL:HG22  | 1:75:A:ASN:H   | 6        | 0.75          |
| (1,212)  | 1:8:A:VAL:HG23  | 1:75:A:ASN:H   | 6        | 0.75          |
| (1,212)  | 1:8:A:VAL:HG21  | 1:75:A:ASN:H   | 10       | 0.75          |
| (1,212)  | 1:8:A:VAL:HG22  | 1:75:A:ASN:H   | 10       | 0.75          |
| (1,212)  | 1:8:A:VAL:HG23  | 1:75:A:ASN:H   | 10       | 0.75          |
| (1,181)  | 1:68:A:LEU:HB2  | 1:72:A:LYS:H   | 5        | 0.75          |
| (1,76)   | 1:68:A:LEU:HD11 | 1:73:A:LYS:H   | 11       | 0.75          |
| (1,76)   | 1:68:A:LEU:HD12 | 1:73:A:LYS:H   | 11       | 0.75          |
| (1,76)   | 1:68:A:LEU:HD13 | 1:73:A:LYS:H   | 11       | 0.75          |
| (1,55)   | 1:68:A:LEU:HD11 | 1:69:A:LEU:H   | 8        | 0.75          |
| (1,55)   | 1:68:A:LEU:HD12 | 1:69:A:LEU:H   | 8        | 0.75          |
| (1,55)   | 1:68:A:LEU:HD13 | 1:69:A:LEU:H   | 8        | 0.75          |
| (1,55)   | 1:68:A:LEU:HD11 | 1:69:A:LEU:H   | 13       | 0.75          |
| (1,55)   | 1:68:A:LEU:HD12 | 1:69:A:LEU:H   | 13       | 0.75          |
| (1,55)   | 1:68:A:LEU:HD13 | 1:69:A:LEU:H   | 13       | 0.75          |
| (1,55)   | 1:68:A:LEU:HD11 | 1:69:A:LEU:H   | 18       | 0.75          |
| (1,55)   | 1:68:A:LEU:HD12 | 1:69:A:LEU:H   | 18       | 0.75          |
| (1,55)   | 1:68:A:LEU:HD13 | 1:69:A:LEU:H   | 18       | 0.75          |
| (1,1313) | 1:58:A:MET:HB3  | 1:58:A:MET:HE1 | 15       | 0.74          |
| (1,1313) | 1:58:A:MET:HB3  | 1:58:A:MET:HE2 | 15       | 0.74          |
| (1,1313) | 1:58:A:MET:HB3  | 1:58:A:MET:HE3 | 15       | 0.74          |
| (1,1280) | 1:36:A:ALA:HB1  | 1:37:A:ASP:HB3 | 5        | 0.74          |
| (1,1280) | 1:36:A:ALA:HB2  | 1:37:A:ASP:HB3 | 5        | 0.74          |
| (1,1280) | 1:36:A:ALA:HB3  | 1:37:A:ASP:HB3 | 5        | 0.74          |
| (1,1280) | 1:36:A:ALA:HB1  | 1:37:A:ASP:HB3 | 15       | 0.74          |
| (1,1280) | 1:36:A:ALA:HB2  | 1:37:A:ASP:HB3 | 15       | 0.74          |
| (1,1280) | 1:36:A:ALA:HB3  | 1:37:A:ASP:HB3 | 15       | 0.74          |
| (1,1280) | 1:36:A:ALA:HB1  | 1:37:A:ASP:HB3 | 17       | 0.74          |
| (1,1280) | 1:36:A:ALA:HB2  | 1:37:A:ASP:HB3 | 17       | 0.74          |
| (1,1280) | 1:36:A:ALA:HB3  | 1:37:A:ASP:HB3 | 17       | 0.74          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1258) | 1:79:A:THR:HG21 | 1:80:A:VAL:HG11 | 7        | 0.74          |
| (1,1258) | 1:79:A:THR:HG21 | 1:80:A:VAL:HG12 | 7        | 0.74          |
| (1,1258) | 1:79:A:THR:HG21 | 1:80:A:VAL:HG13 | 7        | 0.74          |
| (1,1258) | 1:79:A:THR:HG22 | 1:80:A:VAL:HG11 | 7        | 0.74          |
| (1,1258) | 1:79:A:THR:HG22 | 1:80:A:VAL:HG12 | 7        | 0.74          |
| (1,1258) | 1:79:A:THR:HG22 | 1:80:A:VAL:HG13 | 7        | 0.74          |
| (1,1258) | 1:79:A:THR:HG23 | 1:80:A:VAL:HG11 | 7        | 0.74          |
| (1,1258) | 1:79:A:THR:HG23 | 1:80:A:VAL:HG12 | 7        | 0.74          |
| (1,1258) | 1:79:A:THR:HG23 | 1:80:A:VAL:HG13 | 7        | 0.74          |
| (1,1248) | 1:8:A:VAL:HG11  | 1:43:A:LEU:HD21 | 14       | 0.74          |
| (1,1248) | 1:8:A:VAL:HG11  | 1:43:A:LEU:HD22 | 14       | 0.74          |
| (1,1248) | 1:8:A:VAL:HG11  | 1:43:A:LEU:HD23 | 14       | 0.74          |
| (1,1248) | 1:8:A:VAL:HG12  | 1:43:A:LEU:HD21 | 14       | 0.74          |
| (1,1248) | 1:8:A:VAL:HG12  | 1:43:A:LEU:HD22 | 14       | 0.74          |
| (1,1248) | 1:8:A:VAL:HG12  | 1:43:A:LEU:HD23 | 14       | 0.74          |
| (1,1248) | 1:8:A:VAL:HG13  | 1:43:A:LEU:HD21 | 14       | 0.74          |
| (1,1248) | 1:8:A:VAL:HG13  | 1:43:A:LEU:HD22 | 14       | 0.74          |
| (1,1248) | 1:8:A:VAL:HG13  | 1:43:A:LEU:HD23 | 14       | 0.74          |
| (1,1224) | 1:8:A:VAL:HG21  | 1:9:A:GLY:H     | 9        | 0.74          |
| (1,1224) | 1:8:A:VAL:HG22  | 1:9:A:GLY:H     | 9        | 0.74          |
| (1,1224) | 1:8:A:VAL:HG23  | 1:9:A:GLY:H     | 9        | 0.74          |
| (1,1040) | 1:12:A:PRO:HG2  | 1:70:A:LYS:HB3  | 17       | 0.74          |
| (1,958)  | 1:77:A:GLU:HB2  | 1:78:A:LEU:HD11 | 10       | 0.74          |
| (1,958)  | 1:77:A:GLU:HB2  | 1:78:A:LEU:HD12 | 10       | 0.74          |
| (1,958)  | 1:77:A:GLU:HB2  | 1:78:A:LEU:HD13 | 10       | 0.74          |
| (1,877)  | 1:7:A:PHE:HB3   | 1:79:A:THR:HB   | 2        | 0.74          |
| (1,811)  | 1:7:A:PHE:HE1   | 1:9:A:GLY:HA2   | 7        | 0.74          |
| (1,811)  | 1:7:A:PHE:HE2   | 1:9:A:GLY:HA2   | 7        | 0.74          |
| (1,792)  | 1:11:A:LEU:HB3  | 1:39:A:GLY:HA3  | 3        | 0.74          |
| (1,785)  | 1:11:A:LEU:HB2  | 1:12:A:PRO:HD3  | 16       | 0.74          |
| (1,773)  | 1:65:A:HIS:HB3  | 1:75:A:ASN:HA   | 16       | 0.74          |
| (1,536)  | 1:11:A:LEU:HB3  | 1:39:A:GLY:H    | 14       | 0.74          |
| (1,489)  | 1:10:A:SER:HB3  | 1:75:A:ASN:HD22 | 6        | 0.74          |
| (1,378)  | 1:38:A:LYS:H    | 1:38:A:LYS:HG3  | 6        | 0.74          |
| (1,378)  | 1:38:A:LYS:H    | 1:38:A:LYS:HG3  | 11       | 0.74          |
| (1,378)  | 1:38:A:LYS:H    | 1:38:A:LYS:HG3  | 13       | 0.74          |
| (1,55)   | 1:68:A:LEU:HD11 | 1:69:A:LEU:H    | 2        | 0.74          |
| (1,55)   | 1:68:A:LEU:HD12 | 1:69:A:LEU:H    | 2        | 0.74          |
| (1,55)   | 1:68:A:LEU:HD13 | 1:69:A:LEU:H    | 2        | 0.74          |
| (1,55)   | 1:68:A:LEU:HD11 | 1:69:A:LEU:H    | 20       | 0.74          |
| (1,55)   | 1:68:A:LEU:HD12 | 1:69:A:LEU:H    | 20       | 0.74          |
| (1,55)   | 1:68:A:LEU:HD13 | 1:69:A:LEU:H    | 20       | 0.74          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1246) | 1:7:A:PHE:HA    | 1:8:A:VAL:HG11  | 7        | 0.73          |
| (1,1246) | 1:7:A:PHE:HA    | 1:8:A:VAL:HG12  | 7        | 0.73          |
| (1,1246) | 1:7:A:PHE:HA    | 1:8:A:VAL:HG13  | 7        | 0.73          |
| (1,785)  | 1:11:A:LEU:HB2  | 1:12:A:PRO:HD3  | 18       | 0.73          |
| (1,674)  | 1:68:A:LEU:HB2  | 1:71:A:GLU:HA   | 12       | 0.73          |
| (1,595)  | 1:28:A:SER:HB2  | 1:45:A:PHE:HE1  | 18       | 0.73          |
| (1,595)  | 1:28:A:SER:HB2  | 1:45:A:PHE:HE2  | 18       | 0.73          |
| (1,536)  | 1:11:A:LEU:HB3  | 1:39:A:GLY:H    | 12       | 0.73          |
| (1,101)  | 1:17:A:ALA:H    | 1:20:A:LEU:HD11 | 6        | 0.73          |
| (1,101)  | 1:17:A:ALA:H    | 1:20:A:LEU:HD12 | 6        | 0.73          |
| (1,101)  | 1:17:A:ALA:H    | 1:20:A:LEU:HD13 | 6        | 0.73          |
| (1,76)   | 1:68:A:LEU:HD11 | 1:73:A:LYS:H    | 13       | 0.73          |
| (1,76)   | 1:68:A:LEU:HD12 | 1:73:A:LYS:H    | 13       | 0.73          |
| (1,76)   | 1:68:A:LEU:HD13 | 1:73:A:LYS:H    | 13       | 0.73          |
| (1,1359) | 1:23:A:HIS:HD2  | 1:64:A:GLN:HB2  | 4        | 0.72          |
| (1,1313) | 1:58:A:MET:HB3  | 1:58:A:MET:HE1  | 6        | 0.72          |
| (1,1313) | 1:58:A:MET:HB3  | 1:58:A:MET:HE2  | 6        | 0.72          |
| (1,1313) | 1:58:A:MET:HB3  | 1:58:A:MET:HE3  | 6        | 0.72          |
| (1,1280) | 1:36:A:ALA:HB1  | 1:37:A:ASP:HB3  | 1        | 0.72          |
| (1,1280) | 1:36:A:ALA:HB2  | 1:37:A:ASP:HB3  | 1        | 0.72          |
| (1,1280) | 1:36:A:ALA:HB3  | 1:37:A:ASP:HB3  | 1        | 0.72          |
| (1,1246) | 1:7:A:PHE:HA    | 1:8:A:VAL:HG11  | 20       | 0.72          |
| (1,1246) | 1:7:A:PHE:HA    | 1:8:A:VAL:HG12  | 20       | 0.72          |
| (1,1246) | 1:7:A:PHE:HA    | 1:8:A:VAL:HG13  | 20       | 0.72          |
| (1,1189) | 1:20:A:LEU:HD21 | 1:34:A:LEU:HD11 | 9        | 0.72          |
| (1,1189) | 1:20:A:LEU:HD21 | 1:34:A:LEU:HD12 | 9        | 0.72          |
| (1,1189) | 1:20:A:LEU:HD21 | 1:34:A:LEU:HD13 | 9        | 0.72          |
| (1,1189) | 1:20:A:LEU:HD22 | 1:34:A:LEU:HD11 | 9        | 0.72          |
| (1,1189) | 1:20:A:LEU:HD22 | 1:34:A:LEU:HD12 | 9        | 0.72          |
| (1,1189) | 1:20:A:LEU:HD22 | 1:34:A:LEU:HD13 | 9        | 0.72          |
| (1,1189) | 1:20:A:LEU:HD23 | 1:34:A:LEU:HD11 | 9        | 0.72          |
| (1,1189) | 1:20:A:LEU:HD23 | 1:34:A:LEU:HD12 | 9        | 0.72          |
| (1,1189) | 1:20:A:LEU:HD23 | 1:34:A:LEU:HD13 | 9        | 0.72          |
| (1,809)  | 1:7:A:PHE:HZ    | 1:9:A:GLY:HA2   | 3        | 0.72          |
| (1,806)  | 1:68:A:LEU:HA   | 1:69:A:LEU:HB3  | 2        | 0.72          |
| (1,785)  | 1:11:A:LEU:HB2  | 1:12:A:PRO:HD3  | 20       | 0.72          |
| (1,711)  | 1:68:A:LEU:HD11 | 1:73:A:LYS:HA   | 1        | 0.72          |
| (1,711)  | 1:68:A:LEU:HD12 | 1:73:A:LYS:HA   | 1        | 0.72          |
| (1,711)  | 1:68:A:LEU:HD13 | 1:73:A:LYS:HA   | 1        | 0.72          |
| (1,536)  | 1:11:A:LEU:HB3  | 1:39:A:GLY:H    | 5        | 0.72          |
| (1,481)  | 1:18:A:VAL:HG11 | 1:22:A:ASN:HD21 | 4        | 0.72          |
| (1,481)  | 1:18:A:VAL:HG12 | 1:22:A:ASN:HD21 | 4        | 0.72          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,481)  | 1:18:A:VAL:HG13 | 1:22:A:ASN:HD21 | 4        | 0.72          |
| (1,181)  | 1:68:A:LEU:HB2  | 1:72:A:LYS:H    | 17       | 0.72          |
| (1,1246) | 1:7:A:PHE:HA    | 1:8:A:VAL:HG11  | 3        | 0.71          |
| (1,1246) | 1:7:A:PHE:HA    | 1:8:A:VAL:HG12  | 3        | 0.71          |
| (1,1246) | 1:7:A:PHE:HA    | 1:8:A:VAL:HG13  | 3        | 0.71          |
| (1,1246) | 1:7:A:PHE:HA    | 1:8:A:VAL:HG11  | 16       | 0.71          |
| (1,1246) | 1:7:A:PHE:HA    | 1:8:A:VAL:HG12  | 16       | 0.71          |
| (1,1246) | 1:7:A:PHE:HA    | 1:8:A:VAL:HG13  | 16       | 0.71          |
| (1,1224) | 1:8:A:VAL:HG21  | 1:9:A:GLY:H     | 3        | 0.71          |
| (1,1224) | 1:8:A:VAL:HG22  | 1:9:A:GLY:H     | 3        | 0.71          |
| (1,1224) | 1:8:A:VAL:HG23  | 1:9:A:GLY:H     | 3        | 0.71          |
| (1,877)  | 1:7:A:PHE:HB3   | 1:79:A:THR:HB   | 15       | 0.71          |
| (1,785)  | 1:11:A:LEU:HB2  | 1:12:A:PRO:HD3  | 6        | 0.71          |
| (1,711)  | 1:68:A:LEU:HD11 | 1:73:A:LYS:HA   | 20       | 0.71          |
| (1,711)  | 1:68:A:LEU:HD12 | 1:73:A:LYS:HA   | 20       | 0.71          |
| (1,711)  | 1:68:A:LEU:HD13 | 1:73:A:LYS:HA   | 20       | 0.71          |
| (1,590)  | 1:29:A:PRO:HA   | 1:43:A:LEU:HB2  | 14       | 0.71          |
| (1,536)  | 1:11:A:LEU:HB3  | 1:39:A:GLY:H    | 1        | 0.71          |
| (1,536)  | 1:11:A:LEU:HB3  | 1:39:A:GLY:H    | 2        | 0.71          |
| (1,536)  | 1:11:A:LEU:HB3  | 1:39:A:GLY:H    | 10       | 0.71          |
| (1,489)  | 1:10:A:SER:HB3  | 1:75:A:ASN:HD22 | 15       | 0.71          |
| (1,1280) | 1:36:A:ALA:HB1  | 1:37:A:ASP:HB3  | 16       | 0.7           |
| (1,1280) | 1:36:A:ALA:HB2  | 1:37:A:ASP:HB3  | 16       | 0.7           |
| (1,1280) | 1:36:A:ALA:HB3  | 1:37:A:ASP:HB3  | 16       | 0.7           |
| (1,1248) | 1:8:A:VAL:HG11  | 1:43:A:LEU:HD21 | 5        | 0.7           |
| (1,1248) | 1:8:A:VAL:HG11  | 1:43:A:LEU:HD22 | 5        | 0.7           |
| (1,1248) | 1:8:A:VAL:HG11  | 1:43:A:LEU:HD23 | 5        | 0.7           |
| (1,1248) | 1:8:A:VAL:HG12  | 1:43:A:LEU:HD21 | 5        | 0.7           |
| (1,1248) | 1:8:A:VAL:HG12  | 1:43:A:LEU:HD22 | 5        | 0.7           |
| (1,1248) | 1:8:A:VAL:HG12  | 1:43:A:LEU:HD23 | 5        | 0.7           |
| (1,1248) | 1:8:A:VAL:HG13  | 1:43:A:LEU:HD21 | 5        | 0.7           |
| (1,1248) | 1:8:A:VAL:HG13  | 1:43:A:LEU:HD22 | 5        | 0.7           |
| (1,1248) | 1:8:A:VAL:HG13  | 1:43:A:LEU:HD23 | 5        | 0.7           |
| (1,1248) | 1:8:A:VAL:HG11  | 1:43:A:LEU:HD21 | 10       | 0.7           |
| (1,1248) | 1:8:A:VAL:HG11  | 1:43:A:LEU:HD22 | 10       | 0.7           |
| (1,1248) | 1:8:A:VAL:HG11  | 1:43:A:LEU:HD23 | 10       | 0.7           |
| (1,1248) | 1:8:A:VAL:HG12  | 1:43:A:LEU:HD21 | 10       | 0.7           |
| (1,1248) | 1:8:A:VAL:HG12  | 1:43:A:LEU:HD22 | 10       | 0.7           |
| (1,1248) | 1:8:A:VAL:HG12  | 1:43:A:LEU:HD23 | 10       | 0.7           |
| (1,1248) | 1:8:A:VAL:HG13  | 1:43:A:LEU:HD21 | 10       | 0.7           |
| (1,1248) | 1:8:A:VAL:HG13  | 1:43:A:LEU:HD22 | 10       | 0.7           |
| (1,1248) | 1:8:A:VAL:HG13  | 1:43:A:LEU:HD23 | 10       | 0.7           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1246) | 1:7:A:PHE:HA    | 1:8:A:VAL:HG11  | 12       | 0.7           |
| (1,1246) | 1:7:A:PHE:HA    | 1:8:A:VAL:HG12  | 12       | 0.7           |
| (1,1246) | 1:7:A:PHE:HA    | 1:8:A:VAL:HG13  | 12       | 0.7           |
| (1,1246) | 1:7:A:PHE:HA    | 1:8:A:VAL:HG11  | 15       | 0.7           |
| (1,1246) | 1:7:A:PHE:HA    | 1:8:A:VAL:HG12  | 15       | 0.7           |
| (1,1246) | 1:7:A:PHE:HA    | 1:8:A:VAL:HG13  | 15       | 0.7           |
| (1,1224) | 1:8:A:VAL:HG21  | 1:9:A:GLY:H     | 5        | 0.7           |
| (1,1224) | 1:8:A:VAL:HG22  | 1:9:A:GLY:H     | 5        | 0.7           |
| (1,1224) | 1:8:A:VAL:HG23  | 1:9:A:GLY:H     | 5        | 0.7           |
| (1,877)  | 1:7:A:PHE:HB3   | 1:79:A:THR:HB   | 6        | 0.7           |
| (1,820)  | 1:68:A:LEU:HB2  | 1:71:A:GLU:H    | 9        | 0.7           |
| (1,809)  | 1:7:A:PHE:HZ    | 1:9:A:GLY:HA2   | 15       | 0.7           |
| (1,806)  | 1:68:A:LEU:HA   | 1:69:A:LEU:HB3  | 20       | 0.7           |
| (1,378)  | 1:38:A:LYS:H    | 1:38:A:LYS:HG3  | 2        | 0.7           |
| (1,212)  | 1:8:A:VAL:HG21  | 1:75:A:ASN:H    | 7        | 0.7           |
| (1,212)  | 1:8:A:VAL:HG22  | 1:75:A:ASN:H    | 7        | 0.7           |
| (1,212)  | 1:8:A:VAL:HG23  | 1:75:A:ASN:H    | 7        | 0.7           |
| (1,212)  | 1:8:A:VAL:HG21  | 1:75:A:ASN:H    | 18       | 0.7           |
| (1,212)  | 1:8:A:VAL:HG22  | 1:75:A:ASN:H    | 18       | 0.7           |
| (1,212)  | 1:8:A:VAL:HG23  | 1:75:A:ASN:H    | 18       | 0.7           |
| (1,76)   | 1:68:A:LEU:HD11 | 1:73:A:LYS:H    | 20       | 0.7           |
| (1,76)   | 1:68:A:LEU:HD12 | 1:73:A:LYS:H    | 20       | 0.7           |
| (1,76)   | 1:68:A:LEU:HD13 | 1:73:A:LYS:H    | 20       | 0.7           |
| (1,1248) | 1:8:A:VAL:HG11  | 1:43:A:LEU:HD21 | 8        | 0.69          |
| (1,1248) | 1:8:A:VAL:HG11  | 1:43:A:LEU:HD22 | 8        | 0.69          |
| (1,1248) | 1:8:A:VAL:HG11  | 1:43:A:LEU:HD23 | 8        | 0.69          |
| (1,1248) | 1:8:A:VAL:HG12  | 1:43:A:LEU:HD21 | 8        | 0.69          |
| (1,1248) | 1:8:A:VAL:HG12  | 1:43:A:LEU:HD22 | 8        | 0.69          |
| (1,1248) | 1:8:A:VAL:HG12  | 1:43:A:LEU:HD23 | 8        | 0.69          |
| (1,1248) | 1:8:A:VAL:HG13  | 1:43:A:LEU:HD21 | 8        | 0.69          |
| (1,1248) | 1:8:A:VAL:HG13  | 1:43:A:LEU:HD22 | 8        | 0.69          |
| (1,1248) | 1:8:A:VAL:HG13  | 1:43:A:LEU:HD23 | 8        | 0.69          |
| (1,1128) | 1:20:A:LEU:HD11 | 1:34:A:LEU:HB2  | 9        | 0.69          |
| (1,1128) | 1:20:A:LEU:HD12 | 1:34:A:LEU:HB2  | 9        | 0.69          |
| (1,1128) | 1:20:A:LEU:HD13 | 1:34:A:LEU:HB2  | 9        | 0.69          |
| (1,1004) | 1:54:A:ILE:HD11 | 1:58:A:MET:HB3  | 13       | 0.69          |
| (1,1004) | 1:54:A:ILE:HD12 | 1:58:A:MET:HB3  | 13       | 0.69          |
| (1,1004) | 1:54:A:ILE:HD13 | 1:58:A:MET:HB3  | 13       | 0.69          |
| (1,785)  | 1:11:A:LEU:HB2  | 1:12:A:PRO:HD3  | 12       | 0.69          |
| (1,598)  | 1:12:A:PRO:HA   | 1:72:A:LYS:HG2  | 8        | 0.69          |
| (1,595)  | 1:28:A:SER:HB2  | 1:45:A:PHE:HE1  | 4        | 0.69          |
| (1,595)  | 1:28:A:SER:HB2  | 1:45:A:PHE:HE2  | 4        | 0.69          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,595)  | 1:28:A:SER:HB2  | 1:45:A:PHE:HE1  | 16       | 0.69          |
| (1,595)  | 1:28:A:SER:HB2  | 1:45:A:PHE:HE2  | 16       | 0.69          |
| (1,489)  | 1:10:A:SER:HB3  | 1:75:A:ASN:HD22 | 9        | 0.69          |
| (1,423)  | 1:55:A:GLN:HE22 | 1:59:A:ASP:HB3  | 20       | 0.69          |
| (1,76)   | 1:68:A:LEU:HD11 | 1:73:A:LYS:H    | 9        | 0.69          |
| (1,76)   | 1:68:A:LEU:HD12 | 1:73:A:LYS:H    | 9        | 0.69          |
| (1,76)   | 1:68:A:LEU:HD13 | 1:73:A:LYS:H    | 9        | 0.69          |
| (1,1248) | 1:8:A:VAL:HG11  | 1:43:A:LEU:HD21 | 16       | 0.68          |
| (1,1248) | 1:8:A:VAL:HG11  | 1:43:A:LEU:HD22 | 16       | 0.68          |
| (1,1248) | 1:8:A:VAL:HG11  | 1:43:A:LEU:HD23 | 16       | 0.68          |
| (1,1248) | 1:8:A:VAL:HG12  | 1:43:A:LEU:HD21 | 16       | 0.68          |
| (1,1248) | 1:8:A:VAL:HG12  | 1:43:A:LEU:HD22 | 16       | 0.68          |
| (1,1248) | 1:8:A:VAL:HG12  | 1:43:A:LEU:HD23 | 16       | 0.68          |
| (1,1248) | 1:8:A:VAL:HG13  | 1:43:A:LEU:HD21 | 16       | 0.68          |
| (1,1248) | 1:8:A:VAL:HG13  | 1:43:A:LEU:HD22 | 16       | 0.68          |
| (1,1248) | 1:8:A:VAL:HG13  | 1:43:A:LEU:HD23 | 16       | 0.68          |
| (1,1246) | 1:7:A:PHE:HA    | 1:8:A:VAL:HG11  | 10       | 0.68          |
| (1,1246) | 1:7:A:PHE:HA    | 1:8:A:VAL:HG12  | 10       | 0.68          |
| (1,1246) | 1:7:A:PHE:HA    | 1:8:A:VAL:HG13  | 10       | 0.68          |
| (1,1246) | 1:7:A:PHE:HA    | 1:8:A:VAL:HG11  | 17       | 0.68          |
| (1,1246) | 1:7:A:PHE:HA    | 1:8:A:VAL:HG12  | 17       | 0.68          |
| (1,1246) | 1:7:A:PHE:HA    | 1:8:A:VAL:HG13  | 17       | 0.68          |
| (1,1246) | 1:7:A:PHE:HA    | 1:8:A:VAL:HG11  | 19       | 0.68          |
| (1,1246) | 1:7:A:PHE:HA    | 1:8:A:VAL:HG12  | 19       | 0.68          |
| (1,1246) | 1:7:A:PHE:HA    | 1:8:A:VAL:HG13  | 19       | 0.68          |
| (1,1215) | 1:23:A:HIS:H    | 1:69:A:LEU:HD21 | 19       | 0.68          |
| (1,1215) | 1:23:A:HIS:H    | 1:69:A:LEU:HD22 | 19       | 0.68          |
| (1,1215) | 1:23:A:HIS:H    | 1:69:A:LEU:HD23 | 19       | 0.68          |
| (1,958)  | 1:77:A:GLU:HB2  | 1:78:A:LEU:HD11 | 7        | 0.68          |
| (1,958)  | 1:77:A:GLU:HB2  | 1:78:A:LEU:HD12 | 7        | 0.68          |
| (1,958)  | 1:77:A:GLU:HB2  | 1:78:A:LEU:HD13 | 7        | 0.68          |
| (1,773)  | 1:65:A:HIS:HB3  | 1:75:A:ASN:HA   | 15       | 0.68          |
| (1,378)  | 1:38:A:LYS:H    | 1:38:A:LYS:HG3  | 8        | 0.68          |
| (1,252)  | 1:63:A:LEU:H    | 1:64:A:GLN:HG3  | 8        | 0.68          |
| (1,252)  | 1:63:A:LEU:H    | 1:64:A:GLN:HG3  | 14       | 0.68          |
| (1,1248) | 1:8:A:VAL:HG11  | 1:43:A:LEU:HD21 | 12       | 0.67          |
| (1,1248) | 1:8:A:VAL:HG11  | 1:43:A:LEU:HD22 | 12       | 0.67          |
| (1,1248) | 1:8:A:VAL:HG11  | 1:43:A:LEU:HD23 | 12       | 0.67          |
| (1,1248) | 1:8:A:VAL:HG12  | 1:43:A:LEU:HD21 | 12       | 0.67          |
| (1,1248) | 1:8:A:VAL:HG12  | 1:43:A:LEU:HD22 | 12       | 0.67          |
| (1,1248) | 1:8:A:VAL:HG12  | 1:43:A:LEU:HD23 | 12       | 0.67          |
| (1,1248) | 1:8:A:VAL:HG13  | 1:43:A:LEU:HD21 | 12       | 0.67          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1248) | 1:8:A:VAL:HG13 | 1:43:A:LEU:HD22 | 12       | 0.67          |
| (1,1248) | 1:8:A:VAL:HG13 | 1:43:A:LEU:HD23 | 12       | 0.67          |
| (1,1246) | 1:7:A:PHE:HA   | 1:8:A:VAL:HG11  | 13       | 0.67          |
| (1,1246) | 1:7:A:PHE:HA   | 1:8:A:VAL:HG12  | 13       | 0.67          |
| (1,1246) | 1:7:A:PHE:HA   | 1:8:A:VAL:HG13  | 13       | 0.67          |
| (1,1224) | 1:8:A:VAL:HG21 | 1:9:A:GLY:H     | 18       | 0.67          |
| (1,1224) | 1:8:A:VAL:HG22 | 1:9:A:GLY:H     | 18       | 0.67          |
| (1,1224) | 1:8:A:VAL:HG23 | 1:9:A:GLY:H     | 18       | 0.67          |
| (1,890)  | 1:59:A:ASP:HA  | 1:62:A:LEU:HB3  | 7        | 0.67          |
| (1,868)  | 1:9:A:GLY:H    | 1:75:A:ASN:HB3  | 9        | 0.67          |
| (1,811)  | 1:7:A:PHE:HE1  | 1:9:A:GLY:HA2   | 15       | 0.67          |
| (1,811)  | 1:7:A:PHE:HE2  | 1:9:A:GLY:HA2   | 15       | 0.67          |
| (1,806)  | 1:68:A:LEU:HA  | 1:69:A:LEU:HB3  | 10       | 0.67          |
| (1,792)  | 1:11:A:LEU:HB3 | 1:39:A:GLY:HA3  | 1        | 0.67          |
| (1,785)  | 1:11:A:LEU:HB2 | 1:12:A:PRO:HD3  | 3        | 0.67          |
| (1,252)  | 1:63:A:LEU:H   | 1:64:A:GLN:HG3  | 1        | 0.67          |
| (1,252)  | 1:63:A:LEU:H   | 1:64:A:GLN:HG3  | 12       | 0.67          |
| (1,101)  | 1:17:A:ALA:H   | 1:20:A:LEU:HD11 | 7        | 0.67          |
| (1,101)  | 1:17:A:ALA:H   | 1:20:A:LEU:HD12 | 7        | 0.67          |
| (1,101)  | 1:17:A:ALA:H   | 1:20:A:LEU:HD13 | 7        | 0.67          |
| (1,1359) | 1:23:A:HIS:HD2 | 1:64:A:GLN:HB2  | 18       | 0.66          |
| (1,1336) | 1:59:A:ASP:HB3 | 1:60:A:ILE:HD11 | 13       | 0.66          |
| (1,1336) | 1:59:A:ASP:HB3 | 1:60:A:ILE:HD12 | 13       | 0.66          |
| (1,1336) | 1:59:A:ASP:HB3 | 1:60:A:ILE:HD13 | 13       | 0.66          |
| (1,1280) | 1:36:A:ALA:HB1 | 1:37:A:ASP:HB3  | 9        | 0.66          |
| (1,1280) | 1:36:A:ALA:HB2 | 1:37:A:ASP:HB3  | 9        | 0.66          |
| (1,1280) | 1:36:A:ALA:HB3 | 1:37:A:ASP:HB3  | 9        | 0.66          |
| (1,1280) | 1:36:A:ALA:HB1 | 1:37:A:ASP:HB3  | 20       | 0.66          |
| (1,1280) | 1:36:A:ALA:HB2 | 1:37:A:ASP:HB3  | 20       | 0.66          |
| (1,1280) | 1:36:A:ALA:HB3 | 1:37:A:ASP:HB3  | 20       | 0.66          |
| (1,1246) | 1:7:A:PHE:HA   | 1:8:A:VAL:HG11  | 14       | 0.66          |
| (1,1246) | 1:7:A:PHE:HA   | 1:8:A:VAL:HG12  | 14       | 0.66          |
| (1,1246) | 1:7:A:PHE:HA   | 1:8:A:VAL:HG13  | 14       | 0.66          |
| (1,1224) | 1:8:A:VAL:HG21 | 1:9:A:GLY:H     | 13       | 0.66          |
| (1,1224) | 1:8:A:VAL:HG22 | 1:9:A:GLY:H     | 13       | 0.66          |
| (1,1224) | 1:8:A:VAL:HG23 | 1:9:A:GLY:H     | 13       | 0.66          |
| (1,1224) | 1:8:A:VAL:HG21 | 1:9:A:GLY:H     | 14       | 0.66          |
| (1,1224) | 1:8:A:VAL:HG22 | 1:9:A:GLY:H     | 14       | 0.66          |
| (1,1224) | 1:8:A:VAL:HG23 | 1:9:A:GLY:H     | 14       | 0.66          |
| (1,1161) | 1:4:A:PHE:HD1  | 1:78:A:LEU:HD21 | 3        | 0.66          |
| (1,1161) | 1:4:A:PHE:HD1  | 1:78:A:LEU:HD22 | 3        | 0.66          |
| (1,1161) | 1:4:A:PHE:HD1  | 1:78:A:LEU:HD23 | 3        | 0.66          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1161) | 1:4:A:PHE:HD2   | 1:78:A:LEU:HD21 | 3        | 0.66          |
| (1,1161) | 1:4:A:PHE:HD2   | 1:78:A:LEU:HD22 | 3        | 0.66          |
| (1,1161) | 1:4:A:PHE:HD2   | 1:78:A:LEU:HD23 | 3        | 0.66          |
| (1,1128) | 1:20:A:LEU:HD11 | 1:34:A:LEU:HB2  | 6        | 0.66          |
| (1,1128) | 1:20:A:LEU:HD12 | 1:34:A:LEU:HB2  | 6        | 0.66          |
| (1,1128) | 1:20:A:LEU:HD13 | 1:34:A:LEU:HB2  | 6        | 0.66          |
| (1,958)  | 1:77:A:GLU:HB2  | 1:78:A:LEU:HD11 | 14       | 0.66          |
| (1,958)  | 1:77:A:GLU:HB2  | 1:78:A:LEU:HD12 | 14       | 0.66          |
| (1,958)  | 1:77:A:GLU:HB2  | 1:78:A:LEU:HD13 | 14       | 0.66          |
| (1,773)  | 1:65:A:HIS:HB3  | 1:75:A:ASN:HA   | 6        | 0.66          |
| (1,773)  | 1:65:A:HIS:HB3  | 1:75:A:ASN:HA   | 7        | 0.66          |
| (1,711)  | 1:68:A:LEU:HD11 | 1:73:A:LYS:HA   | 5        | 0.66          |
| (1,711)  | 1:68:A:LEU:HD12 | 1:73:A:LYS:HA   | 5        | 0.66          |
| (1,711)  | 1:68:A:LEU:HD13 | 1:73:A:LYS:HA   | 5        | 0.66          |
| (1,674)  | 1:68:A:LEU:HB2  | 1:71:A:GLU:HA   | 14       | 0.66          |
| (1,482)  | 1:10:A:SER:HB3  | 1:75:A:ASN:HD21 | 17       | 0.66          |
| (1,309)  | 1:58:A:MET:H    | 1:59:A:ASP:HB3  | 5        | 0.66          |
| (1,1246) | 1:7:A:PHE:HA    | 1:8:A:VAL:HG11  | 4        | 0.65          |
| (1,1246) | 1:7:A:PHE:HA    | 1:8:A:VAL:HG12  | 4        | 0.65          |
| (1,1246) | 1:7:A:PHE:HA    | 1:8:A:VAL:HG13  | 4        | 0.65          |
| (1,1246) | 1:7:A:PHE:HA    | 1:8:A:VAL:HG11  | 18       | 0.65          |
| (1,1246) | 1:7:A:PHE:HA    | 1:8:A:VAL:HG12  | 18       | 0.65          |
| (1,1246) | 1:7:A:PHE:HA    | 1:8:A:VAL:HG13  | 18       | 0.65          |
| (1,1224) | 1:8:A:VAL:HG21  | 1:9:A:GLY:H     | 15       | 0.65          |
| (1,1224) | 1:8:A:VAL:HG22  | 1:9:A:GLY:H     | 15       | 0.65          |
| (1,1224) | 1:8:A:VAL:HG23  | 1:9:A:GLY:H     | 15       | 0.65          |
| (1,1189) | 1:20:A:LEU:HD21 | 1:34:A:LEU:HD11 | 13       | 0.65          |
| (1,1189) | 1:20:A:LEU:HD21 | 1:34:A:LEU:HD12 | 13       | 0.65          |
| (1,1189) | 1:20:A:LEU:HD21 | 1:34:A:LEU:HD13 | 13       | 0.65          |
| (1,1189) | 1:20:A:LEU:HD22 | 1:34:A:LEU:HD11 | 13       | 0.65          |
| (1,1189) | 1:20:A:LEU:HD22 | 1:34:A:LEU:HD12 | 13       | 0.65          |
| (1,1189) | 1:20:A:LEU:HD22 | 1:34:A:LEU:HD13 | 13       | 0.65          |
| (1,1189) | 1:20:A:LEU:HD23 | 1:34:A:LEU:HD11 | 13       | 0.65          |
| (1,1189) | 1:20:A:LEU:HD23 | 1:34:A:LEU:HD12 | 13       | 0.65          |
| (1,1189) | 1:20:A:LEU:HD23 | 1:34:A:LEU:HD13 | 13       | 0.65          |
| (1,846)  | 1:20:A:LEU:HB2  | 1:20:A:LEU:HG   | 6        | 0.65          |
| (1,846)  | 1:20:A:LEU:HB2  | 1:20:A:LEU:HG   | 7        | 0.65          |
| (1,846)  | 1:20:A:LEU:HB2  | 1:20:A:LEU:HG   | 13       | 0.65          |
| (1,846)  | 1:20:A:LEU:HB2  | 1:20:A:LEU:HG   | 15       | 0.65          |
| (1,811)  | 1:7:A:PHE:HE1   | 1:9:A:GLY:HA2   | 19       | 0.65          |
| (1,811)  | 1:7:A:PHE:HE2   | 1:9:A:GLY:HA2   | 19       | 0.65          |
| (1,809)  | 1:7:A:PHE:HZ    | 1:9:A:GLY:HA2   | 7        | 0.65          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,809)  | 1:7:A:PHE:HZ    | 1:9:A:GLY:HA2   | 13       | 0.65          |
| (1,806)  | 1:68:A:LEU:HA   | 1:69:A:LEU:HB3  | 17       | 0.65          |
| (1,773)  | 1:65:A:HIS:HB3  | 1:75:A:ASN:HA   | 5        | 0.65          |
| (1,674)  | 1:68:A:LEU:HB2  | 1:71:A:GLU:HA   | 16       | 0.65          |
| (1,378)  | 1:38:A:LYS:H    | 1:38:A:LYS:HG3  | 4        | 0.65          |
| (1,101)  | 1:17:A:ALA:H    | 1:20:A:LEU:HD11 | 15       | 0.65          |
| (1,101)  | 1:17:A:ALA:H    | 1:20:A:LEU:HD12 | 15       | 0.65          |
| (1,101)  | 1:17:A:ALA:H    | 1:20:A:LEU:HD13 | 15       | 0.65          |
| (1,1280) | 1:36:A:ALA:HB1  | 1:37:A:ASP:HB3  | 2        | 0.64          |
| (1,1280) | 1:36:A:ALA:HB2  | 1:37:A:ASP:HB3  | 2        | 0.64          |
| (1,1280) | 1:36:A:ALA:HB3  | 1:37:A:ASP:HB3  | 2        | 0.64          |
| (1,1248) | 1:8:A:VAL:HG11  | 1:43:A:LEU:HD21 | 9        | 0.64          |
| (1,1248) | 1:8:A:VAL:HG11  | 1:43:A:LEU:HD22 | 9        | 0.64          |
| (1,1248) | 1:8:A:VAL:HG11  | 1:43:A:LEU:HD23 | 9        | 0.64          |
| (1,1248) | 1:8:A:VAL:HG12  | 1:43:A:LEU:HD21 | 9        | 0.64          |
| (1,1248) | 1:8:A:VAL:HG12  | 1:43:A:LEU:HD22 | 9        | 0.64          |
| (1,1248) | 1:8:A:VAL:HG12  | 1:43:A:LEU:HD23 | 9        | 0.64          |
| (1,1248) | 1:8:A:VAL:HG13  | 1:43:A:LEU:HD21 | 9        | 0.64          |
| (1,1248) | 1:8:A:VAL:HG13  | 1:43:A:LEU:HD22 | 9        | 0.64          |
| (1,1248) | 1:8:A:VAL:HG13  | 1:43:A:LEU:HD23 | 9        | 0.64          |
| (1,1246) | 1:7:A:PHE:HA    | 1:8:A:VAL:HG11  | 6        | 0.64          |
| (1,1246) | 1:7:A:PHE:HA    | 1:8:A:VAL:HG12  | 6        | 0.64          |
| (1,1246) | 1:7:A:PHE:HA    | 1:8:A:VAL:HG13  | 6        | 0.64          |
| (1,1246) | 1:7:A:PHE:HA    | 1:8:A:VAL:HG11  | 9        | 0.64          |
| (1,1246) | 1:7:A:PHE:HA    | 1:8:A:VAL:HG12  | 9        | 0.64          |
| (1,1246) | 1:7:A:PHE:HA    | 1:8:A:VAL:HG13  | 9        | 0.64          |
| (1,1224) | 1:8:A:VAL:HG21  | 1:9:A:GLY:H     | 7        | 0.64          |
| (1,1224) | 1:8:A:VAL:HG22  | 1:9:A:GLY:H     | 7        | 0.64          |
| (1,1224) | 1:8:A:VAL:HG23  | 1:9:A:GLY:H     | 7        | 0.64          |
| (1,1224) | 1:8:A:VAL:HG21  | 1:9:A:GLY:H     | 12       | 0.64          |
| (1,1224) | 1:8:A:VAL:HG22  | 1:9:A:GLY:H     | 12       | 0.64          |
| (1,1224) | 1:8:A:VAL:HG23  | 1:9:A:GLY:H     | 12       | 0.64          |
| (1,1224) | 1:8:A:VAL:HG21  | 1:9:A:GLY:H     | 17       | 0.64          |
| (1,1224) | 1:8:A:VAL:HG22  | 1:9:A:GLY:H     | 17       | 0.64          |
| (1,1224) | 1:8:A:VAL:HG23  | 1:9:A:GLY:H     | 17       | 0.64          |
| (1,1224) | 1:8:A:VAL:HG21  | 1:9:A:GLY:H     | 20       | 0.64          |
| (1,1224) | 1:8:A:VAL:HG22  | 1:9:A:GLY:H     | 20       | 0.64          |
| (1,1224) | 1:8:A:VAL:HG23  | 1:9:A:GLY:H     | 20       | 0.64          |
| (1,1134) | 1:69:A:LEU:HD11 | 1:74:A:ILE:HD11 | 3        | 0.64          |
| (1,1134) | 1:69:A:LEU:HD11 | 1:74:A:ILE:HD12 | 3        | 0.64          |
| (1,1134) | 1:69:A:LEU:HD11 | 1:74:A:ILE:HD13 | 3        | 0.64          |
| (1,1134) | 1:69:A:LEU:HD12 | 1:74:A:ILE:HD11 | 3        | 0.64          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1134) | 1:69:A:LEU:HD12 | 1:74:A:ILE:HD12 | 3        | 0.64          |
| (1,1134) | 1:69:A:LEU:HD12 | 1:74:A:ILE:HD13 | 3        | 0.64          |
| (1,1134) | 1:69:A:LEU:HD13 | 1:74:A:ILE:HD11 | 3        | 0.64          |
| (1,1134) | 1:69:A:LEU:HD13 | 1:74:A:ILE:HD12 | 3        | 0.64          |
| (1,1134) | 1:69:A:LEU:HD13 | 1:74:A:ILE:HD13 | 3        | 0.64          |
| (1,1134) | 1:69:A:LEU:HD11 | 1:74:A:ILE:HD11 | 4        | 0.64          |
| (1,1134) | 1:69:A:LEU:HD11 | 1:74:A:ILE:HD12 | 4        | 0.64          |
| (1,1134) | 1:69:A:LEU:HD11 | 1:74:A:ILE:HD13 | 4        | 0.64          |
| (1,1134) | 1:69:A:LEU:HD12 | 1:74:A:ILE:HD11 | 4        | 0.64          |
| (1,1134) | 1:69:A:LEU:HD12 | 1:74:A:ILE:HD12 | 4        | 0.64          |
| (1,1134) | 1:69:A:LEU:HD12 | 1:74:A:ILE:HD13 | 4        | 0.64          |
| (1,1134) | 1:69:A:LEU:HD13 | 1:74:A:ILE:HD11 | 4        | 0.64          |
| (1,1134) | 1:69:A:LEU:HD13 | 1:74:A:ILE:HD12 | 4        | 0.64          |
| (1,1134) | 1:69:A:LEU:HD13 | 1:74:A:ILE:HD13 | 4        | 0.64          |
| (1,1080) | 1:33:A:ARG:HG3  | 1:42:A:PHE:HD1  | 4        | 0.64          |
| (1,1080) | 1:33:A:ARG:HG3  | 1:42:A:PHE:HD2  | 4        | 0.64          |
| (1,890)  | 1:59:A:ASP:HA   | 1:62:A:LEU:HB3  | 15       | 0.64          |
| (1,846)  | 1:20:A:LEU:HB2  | 1:20:A:LEU:HG   | 9        | 0.64          |
| (1,846)  | 1:20:A:LEU:HB2  | 1:20:A:LEU:HG   | 11       | 0.64          |
| (1,820)  | 1:68:A:LEU:HB2  | 1:71:A:GLU:H    | 6        | 0.64          |
| (1,806)  | 1:68:A:LEU:HA   | 1:69:A:LEU:HB3  | 5        | 0.64          |
| (1,773)  | 1:65:A:HIS:HB3  | 1:75:A:ASN:HA   | 4        | 0.64          |
| (1,773)  | 1:65:A:HIS:HB3  | 1:75:A:ASN:HA   | 9        | 0.64          |
| (1,773)  | 1:65:A:HIS:HB3  | 1:75:A:ASN:HA   | 12       | 0.64          |
| (1,674)  | 1:68:A:LEU:HB2  | 1:71:A:GLU:HA   | 8        | 0.64          |
| (1,674)  | 1:68:A:LEU:HB2  | 1:71:A:GLU:HA   | 11       | 0.64          |
| (1,181)  | 1:68:A:LEU:HB2  | 1:72:A:LYS:H    | 4        | 0.64          |
| (1,76)   | 1:68:A:LEU:HD11 | 1:73:A:LYS:H    | 4        | 0.64          |
| (1,76)   | 1:68:A:LEU:HD12 | 1:73:A:LYS:H    | 4        | 0.64          |
| (1,76)   | 1:68:A:LEU:HD13 | 1:73:A:LYS:H    | 4        | 0.64          |
| (1,1255) | 1:18:A:VAL:HG11 | 1:22:A:ASN:HB2  | 9        | 0.63          |
| (1,1255) | 1:18:A:VAL:HG11 | 1:22:A:ASN:HB3  | 9        | 0.63          |
| (1,1255) | 1:18:A:VAL:HG12 | 1:22:A:ASN:HB2  | 9        | 0.63          |
| (1,1255) | 1:18:A:VAL:HG12 | 1:22:A:ASN:HB3  | 9        | 0.63          |
| (1,1255) | 1:18:A:VAL:HG13 | 1:22:A:ASN:HB2  | 9        | 0.63          |
| (1,1255) | 1:18:A:VAL:HG13 | 1:22:A:ASN:HB3  | 9        | 0.63          |
| (1,1224) | 1:8:A:VAL:HG21  | 1:9:A:GLY:H     | 1        | 0.63          |
| (1,1224) | 1:8:A:VAL:HG22  | 1:9:A:GLY:H     | 1        | 0.63          |
| (1,1224) | 1:8:A:VAL:HG23  | 1:9:A:GLY:H     | 1        | 0.63          |
| (1,1224) | 1:8:A:VAL:HG21  | 1:9:A:GLY:H     | 10       | 0.63          |
| (1,1224) | 1:8:A:VAL:HG22  | 1:9:A:GLY:H     | 10       | 0.63          |
| (1,1224) | 1:8:A:VAL:HG23  | 1:9:A:GLY:H     | 10       | 0.63          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1012) | 1:65:A:HIS:HB3  | 1:76:A:VAL:HG21 | 9        | 0.63          |
| (1,1012) | 1:65:A:HIS:HB3  | 1:76:A:VAL:HG22 | 9        | 0.63          |
| (1,1012) | 1:65:A:HIS:HB3  | 1:76:A:VAL:HG23 | 9        | 0.63          |
| (1,890)  | 1:59:A:ASP:HA   | 1:62:A:LEU:HB3  | 12       | 0.63          |
| (1,890)  | 1:59:A:ASP:HA   | 1:62:A:LEU:HB3  | 13       | 0.63          |
| (1,868)  | 1:9:A:GLY:H     | 1:75:A:ASN:HB3  | 14       | 0.63          |
| (1,809)  | 1:7:A:PHE:HZ    | 1:9:A:GLY:HA2   | 10       | 0.63          |
| (1,785)  | 1:11:A:LEU:HB2  | 1:12:A:PRO:HD3  | 9        | 0.63          |
| (1,773)  | 1:65:A:HIS:HB3  | 1:75:A:ASN:HA   | 8        | 0.63          |
| (1,378)  | 1:38:A:LYS:H    | 1:38:A:LYS:HG3  | 18       | 0.63          |
| (1,1336) | 1:59:A:ASP:HB3  | 1:60:A:ILE:HD11 | 12       | 0.62          |
| (1,1336) | 1:59:A:ASP:HB3  | 1:60:A:ILE:HD12 | 12       | 0.62          |
| (1,1336) | 1:59:A:ASP:HB3  | 1:60:A:ILE:HD13 | 12       | 0.62          |
| (1,1224) | 1:8:A:VAL:HG21  | 1:9:A:GLY:H     | 19       | 0.62          |
| (1,1224) | 1:8:A:VAL:HG22  | 1:9:A:GLY:H     | 19       | 0.62          |
| (1,1224) | 1:8:A:VAL:HG23  | 1:9:A:GLY:H     | 19       | 0.62          |
| (1,1189) | 1:20:A:LEU:HD21 | 1:34:A:LEU:HD11 | 11       | 0.62          |
| (1,1189) | 1:20:A:LEU:HD21 | 1:34:A:LEU:HD12 | 11       | 0.62          |
| (1,1189) | 1:20:A:LEU:HD21 | 1:34:A:LEU:HD13 | 11       | 0.62          |
| (1,1189) | 1:20:A:LEU:HD22 | 1:34:A:LEU:HD11 | 11       | 0.62          |
| (1,1189) | 1:20:A:LEU:HD22 | 1:34:A:LEU:HD12 | 11       | 0.62          |
| (1,1189) | 1:20:A:LEU:HD22 | 1:34:A:LEU:HD13 | 11       | 0.62          |
| (1,1189) | 1:20:A:LEU:HD23 | 1:34:A:LEU:HD11 | 11       | 0.62          |
| (1,1189) | 1:20:A:LEU:HD23 | 1:34:A:LEU:HD12 | 11       | 0.62          |
| (1,1189) | 1:20:A:LEU:HD23 | 1:34:A:LEU:HD13 | 11       | 0.62          |
| (1,1189) | 1:20:A:LEU:HD21 | 1:34:A:LEU:HD11 | 15       | 0.62          |
| (1,1189) | 1:20:A:LEU:HD21 | 1:34:A:LEU:HD12 | 15       | 0.62          |
| (1,1189) | 1:20:A:LEU:HD21 | 1:34:A:LEU:HD13 | 15       | 0.62          |
| (1,1189) | 1:20:A:LEU:HD22 | 1:34:A:LEU:HD11 | 15       | 0.62          |
| (1,1189) | 1:20:A:LEU:HD22 | 1:34:A:LEU:HD12 | 15       | 0.62          |
| (1,1189) | 1:20:A:LEU:HD22 | 1:34:A:LEU:HD13 | 15       | 0.62          |
| (1,1189) | 1:20:A:LEU:HD23 | 1:34:A:LEU:HD11 | 15       | 0.62          |
| (1,1189) | 1:20:A:LEU:HD23 | 1:34:A:LEU:HD12 | 15       | 0.62          |
| (1,1189) | 1:20:A:LEU:HD23 | 1:34:A:LEU:HD13 | 15       | 0.62          |
| (1,1030) | 1:29:A:PRO:HB2  | 1:43:A:LEU:HB2  | 16       | 0.62          |
| (1,785)  | 1:11:A:LEU:HB2  | 1:12:A:PRO:HD3  | 7        | 0.62          |
| (1,536)  | 1:11:A:LEU:HB3  | 1:39:A:GLY:H    | 13       | 0.62          |
| (1,489)  | 1:10:A:SER:HB3  | 1:75:A:ASN:HD22 | 1        | 0.62          |
| (1,304)  | 1:56:A:ARG:H    | 1:59:A:ASP:HB3  | 4        | 0.62          |
| (1,180)  | 1:72:A:LYS:H    | 1:72:A:LYS:HG3  | 4        | 0.62          |
| (1,180)  | 1:72:A:LYS:H    | 1:72:A:LYS:HG3  | 16       | 0.62          |
| (1,1280) | 1:36:A:ALA:HB1  | 1:37:A:ASP:HB3  | 7        | 0.61          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1280) | 1:36:A:ALA:HB2  | 1:37:A:ASP:HB3  | 7        | 0.61          |
| (1,1280) | 1:36:A:ALA:HB3  | 1:37:A:ASP:HB3  | 7        | 0.61          |
| (1,1248) | 1:8:A:VAL:HG11  | 1:43:A:LEU:HD21 | 7        | 0.61          |
| (1,1248) | 1:8:A:VAL:HG11  | 1:43:A:LEU:HD22 | 7        | 0.61          |
| (1,1248) | 1:8:A:VAL:HG11  | 1:43:A:LEU:HD23 | 7        | 0.61          |
| (1,1248) | 1:8:A:VAL:HG12  | 1:43:A:LEU:HD21 | 7        | 0.61          |
| (1,1248) | 1:8:A:VAL:HG12  | 1:43:A:LEU:HD22 | 7        | 0.61          |
| (1,1248) | 1:8:A:VAL:HG12  | 1:43:A:LEU:HD23 | 7        | 0.61          |
| (1,1248) | 1:8:A:VAL:HG13  | 1:43:A:LEU:HD21 | 7        | 0.61          |
| (1,1248) | 1:8:A:VAL:HG13  | 1:43:A:LEU:HD22 | 7        | 0.61          |
| (1,1248) | 1:8:A:VAL:HG13  | 1:43:A:LEU:HD23 | 7        | 0.61          |
| (1,1224) | 1:8:A:VAL:HG21  | 1:9:A:GLY:H     | 4        | 0.61          |
| (1,1224) | 1:8:A:VAL:HG22  | 1:9:A:GLY:H     | 4        | 0.61          |
| (1,1224) | 1:8:A:VAL:HG23  | 1:9:A:GLY:H     | 4        | 0.61          |
| (1,1224) | 1:8:A:VAL:HG21  | 1:9:A:GLY:H     | 11       | 0.61          |
| (1,1224) | 1:8:A:VAL:HG22  | 1:9:A:GLY:H     | 11       | 0.61          |
| (1,1224) | 1:8:A:VAL:HG23  | 1:9:A:GLY:H     | 11       | 0.61          |
| (1,1121) | 1:40:A:ILE:HG12 | 1:42:A:PHE:HE1  | 10       | 0.61          |
| (1,1121) | 1:40:A:ILE:HG12 | 1:42:A:PHE:HE2  | 10       | 0.61          |
| (1,877)  | 1:7:A:PHE:HB3   | 1:79:A:THR:HB   | 17       | 0.61          |
| (1,809)  | 1:7:A:PHE:HZ    | 1:9:A:GLY:HA2   | 19       | 0.61          |
| (1,792)  | 1:11:A:LEU:HB3  | 1:39:A:GLY:HA3  | 6        | 0.61          |
| (1,785)  | 1:11:A:LEU:HB2  | 1:12:A:PRO:HD3  | 8        | 0.61          |
| (1,536)  | 1:11:A:LEU:HB3  | 1:39:A:GLY:H    | 6        | 0.61          |
| (1,76)   | 1:68:A:LEU:HD11 | 1:73:A:LYS:H    | 7        | 0.61          |
| (1,76)   | 1:68:A:LEU:HD12 | 1:73:A:LYS:H    | 7        | 0.61          |
| (1,76)   | 1:68:A:LEU:HD13 | 1:73:A:LYS:H    | 7        | 0.61          |
| (1,55)   | 1:68:A:LEU:HD11 | 1:69:A:LEU:H    | 5        | 0.61          |
| (1,55)   | 1:68:A:LEU:HD12 | 1:69:A:LEU:H    | 5        | 0.61          |
| (1,55)   | 1:68:A:LEU:HD13 | 1:69:A:LEU:H    | 5        | 0.61          |
| (1,1280) | 1:36:A:ALA:HB1  | 1:37:A:ASP:HB3  | 8        | 0.6           |
| (1,1280) | 1:36:A:ALA:HB2  | 1:37:A:ASP:HB3  | 8        | 0.6           |
| (1,1280) | 1:36:A:ALA:HB3  | 1:37:A:ASP:HB3  | 8        | 0.6           |
| (1,1246) | 1:7:A:PHE:HA    | 1:8:A:VAL:HG11  | 5        | 0.6           |
| (1,1246) | 1:7:A:PHE:HA    | 1:8:A:VAL:HG12  | 5        | 0.6           |
| (1,1246) | 1:7:A:PHE:HA    | 1:8:A:VAL:HG13  | 5        | 0.6           |
| (1,1224) | 1:8:A:VAL:HG21  | 1:9:A:GLY:H     | 6        | 0.6           |
| (1,1224) | 1:8:A:VAL:HG22  | 1:9:A:GLY:H     | 6        | 0.6           |
| (1,1224) | 1:8:A:VAL:HG23  | 1:9:A:GLY:H     | 6        | 0.6           |
| (1,1201) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD21 | 12       | 0.6           |
| (1,1201) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD22 | 12       | 0.6           |
| (1,1201) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD23 | 12       | 0.6           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1148) | 1:68:A:LEU:HD21 | 1:71:A:GLU:HA   | 5        | 0.6           |
| (1,1148) | 1:68:A:LEU:HD22 | 1:71:A:GLU:HA   | 5        | 0.6           |
| (1,1148) | 1:68:A:LEU:HD23 | 1:71:A:GLU:HA   | 5        | 0.6           |
| (1,1134) | 1:69:A:LEU:HD11 | 1:74:A:ILE:HD11 | 16       | 0.6           |
| (1,1134) | 1:69:A:LEU:HD11 | 1:74:A:ILE:HD12 | 16       | 0.6           |
| (1,1134) | 1:69:A:LEU:HD11 | 1:74:A:ILE:HD13 | 16       | 0.6           |
| (1,1134) | 1:69:A:LEU:HD12 | 1:74:A:ILE:HD11 | 16       | 0.6           |
| (1,1134) | 1:69:A:LEU:HD12 | 1:74:A:ILE:HD12 | 16       | 0.6           |
| (1,1134) | 1:69:A:LEU:HD12 | 1:74:A:ILE:HD13 | 16       | 0.6           |
| (1,1134) | 1:69:A:LEU:HD13 | 1:74:A:ILE:HD11 | 16       | 0.6           |
| (1,1134) | 1:69:A:LEU:HD13 | 1:74:A:ILE:HD12 | 16       | 0.6           |
| (1,1134) | 1:69:A:LEU:HD13 | 1:74:A:ILE:HD13 | 16       | 0.6           |
| (1,890)  | 1:59:A:ASP:HA   | 1:62:A:LEU:HB3  | 18       | 0.6           |
| (1,890)  | 1:59:A:ASP:HA   | 1:62:A:LEU:HB3  | 19       | 0.6           |
| (1,868)  | 1:9:A:GLY:H     | 1:75:A:ASN:HB3  | 3        | 0.6           |
| (1,773)  | 1:65:A:HIS:HB3  | 1:75:A:ASN:HA   | 1        | 0.6           |
| (1,711)  | 1:68:A:LEU:HD11 | 1:73:A:LYS:HA   | 14       | 0.6           |
| (1,711)  | 1:68:A:LEU:HD12 | 1:73:A:LYS:HA   | 14       | 0.6           |
| (1,711)  | 1:68:A:LEU:HD13 | 1:73:A:LYS:HA   | 14       | 0.6           |
| (1,212)  | 1:8:A:VAL:HG21  | 1:75:A:ASN:H    | 2        | 0.6           |
| (1,212)  | 1:8:A:VAL:HG22  | 1:75:A:ASN:H    | 2        | 0.6           |
| (1,212)  | 1:8:A:VAL:HG23  | 1:75:A:ASN:H    | 2        | 0.6           |
| (1,212)  | 1:8:A:VAL:HG21  | 1:75:A:ASN:H    | 17       | 0.6           |
| (1,212)  | 1:8:A:VAL:HG22  | 1:75:A:ASN:H    | 17       | 0.6           |
| (1,212)  | 1:8:A:VAL:HG23  | 1:75:A:ASN:H    | 17       | 0.6           |
| (1,181)  | 1:68:A:LEU:HB2  | 1:72:A:LYS:H    | 6        | 0.6           |
| (1,76)   | 1:68:A:LEU:HD11 | 1:73:A:LYS:H    | 17       | 0.6           |
| (1,76)   | 1:68:A:LEU:HD12 | 1:73:A:LYS:H    | 17       | 0.6           |
| (1,76)   | 1:68:A:LEU:HD13 | 1:73:A:LYS:H    | 17       | 0.6           |
| (1,1248) | 1:8:A:VAL:HG11  | 1:43:A:LEU:HD21 | 13       | 0.59          |
| (1,1248) | 1:8:A:VAL:HG11  | 1:43:A:LEU:HD22 | 13       | 0.59          |
| (1,1248) | 1:8:A:VAL:HG11  | 1:43:A:LEU:HD23 | 13       | 0.59          |
| (1,1248) | 1:8:A:VAL:HG12  | 1:43:A:LEU:HD21 | 13       | 0.59          |
| (1,1248) | 1:8:A:VAL:HG12  | 1:43:A:LEU:HD22 | 13       | 0.59          |
| (1,1248) | 1:8:A:VAL:HG12  | 1:43:A:LEU:HD23 | 13       | 0.59          |
| (1,1248) | 1:8:A:VAL:HG13  | 1:43:A:LEU:HD21 | 13       | 0.59          |
| (1,1248) | 1:8:A:VAL:HG13  | 1:43:A:LEU:HD22 | 13       | 0.59          |
| (1,1248) | 1:8:A:VAL:HG13  | 1:43:A:LEU:HD23 | 13       | 0.59          |
| (1,1246) | 1:7:A:PHE:HA    | 1:8:A:VAL:HG11  | 2        | 0.59          |
| (1,1246) | 1:7:A:PHE:HA    | 1:8:A:VAL:HG12  | 2        | 0.59          |
| (1,1246) | 1:7:A:PHE:HA    | 1:8:A:VAL:HG13  | 2        | 0.59          |
| (1,1148) | 1:68:A:LEU:HD21 | 1:71:A:GLU:HA   | 1        | 0.59          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1148) | 1:68:A:LEU:HD22 | 1:71:A:GLU:HA   | 1        | 0.59          |
| (1,1148) | 1:68:A:LEU:HD23 | 1:71:A:GLU:HA   | 1        | 0.59          |
| (1,1148) | 1:68:A:LEU:HD21 | 1:71:A:GLU:HA   | 8        | 0.59          |
| (1,1148) | 1:68:A:LEU:HD22 | 1:71:A:GLU:HA   | 8        | 0.59          |
| (1,1148) | 1:68:A:LEU:HD23 | 1:71:A:GLU:HA   | 8        | 0.59          |
| (1,1080) | 1:33:A:ARG:HG3  | 1:42:A:PHE:HD1  | 19       | 0.59          |
| (1,1080) | 1:33:A:ARG:HG3  | 1:42:A:PHE:HD2  | 19       | 0.59          |
| (1,1030) | 1:29:A:PRO:HB2  | 1:43:A:LEU:HB2  | 20       | 0.59          |
| (1,901)  | 1:49:A:LYS:HG2  | 1:50:A:ASP:HB2  | 12       | 0.59          |
| (1,901)  | 1:49:A:LYS:HG2  | 1:50:A:ASP:HB3  | 12       | 0.59          |
| (1,773)  | 1:65:A:HIS:HB3  | 1:75:A:ASN:HA   | 13       | 0.59          |
| (1,212)  | 1:8:A:VAL:HG21  | 1:75:A:ASN:H    | 4        | 0.59          |
| (1,212)  | 1:8:A:VAL:HG22  | 1:75:A:ASN:H    | 4        | 0.59          |
| (1,212)  | 1:8:A:VAL:HG23  | 1:75:A:ASN:H    | 4        | 0.59          |
| (1,181)  | 1:68:A:LEU:HB2  | 1:72:A:LYS:H    | 20       | 0.59          |
| (1,55)   | 1:68:A:LEU:HD11 | 1:69:A:LEU:H    | 3        | 0.59          |
| (1,55)   | 1:68:A:LEU:HD12 | 1:69:A:LEU:H    | 3        | 0.59          |
| (1,55)   | 1:68:A:LEU:HD13 | 1:69:A:LEU:H    | 3        | 0.59          |
| (1,1280) | 1:36:A:ALA:HB1  | 1:37:A:ASP:HB3  | 14       | 0.58          |
| (1,1280) | 1:36:A:ALA:HB2  | 1:37:A:ASP:HB3  | 14       | 0.58          |
| (1,1280) | 1:36:A:ALA:HB3  | 1:37:A:ASP:HB3  | 14       | 0.58          |
| (1,1160) | 1:78:A:LEU:HD21 | 1:79:A:THR:H    | 3        | 0.58          |
| (1,1160) | 1:78:A:LEU:HD22 | 1:79:A:THR:H    | 3        | 0.58          |
| (1,1160) | 1:78:A:LEU:HD23 | 1:79:A:THR:H    | 3        | 0.58          |
| (1,820)  | 1:68:A:LEU:HB2  | 1:71:A:GLU:H    | 4        | 0.58          |
| (1,785)  | 1:11:A:LEU:HB2  | 1:12:A:PRO:HD3  | 1        | 0.58          |
| (1,773)  | 1:65:A:HIS:HB3  | 1:75:A:ASN:HA   | 14       | 0.58          |
| (1,536)  | 1:11:A:LEU:HB3  | 1:39:A:GLY:H    | 8        | 0.58          |
| (1,481)  | 1:18:A:VAL:HG11 | 1:22:A:ASN:HD21 | 6        | 0.58          |
| (1,481)  | 1:18:A:VAL:HG12 | 1:22:A:ASN:HD21 | 6        | 0.58          |
| (1,481)  | 1:18:A:VAL:HG13 | 1:22:A:ASN:HD21 | 6        | 0.58          |
| (1,418)  | 1:80:A:VAL:HG21 | 1:82:A:GLY:H    | 2        | 0.58          |
| (1,418)  | 1:80:A:VAL:HG22 | 1:82:A:GLY:H    | 2        | 0.58          |
| (1,418)  | 1:80:A:VAL:HG23 | 1:82:A:GLY:H    | 2        | 0.58          |
| (1,418)  | 1:80:A:VAL:HG21 | 1:82:A:GLY:H    | 6        | 0.58          |
| (1,418)  | 1:80:A:VAL:HG22 | 1:82:A:GLY:H    | 6        | 0.58          |
| (1,418)  | 1:80:A:VAL:HG23 | 1:82:A:GLY:H    | 6        | 0.58          |
| (1,378)  | 1:38:A:LYS:H    | 1:38:A:LYS:HG3  | 12       | 0.58          |
| (1,309)  | 1:58:A:MET:H    | 1:59:A:ASP:HB3  | 9        | 0.58          |
| (1,212)  | 1:8:A:VAL:HG21  | 1:75:A:ASN:H    | 11       | 0.58          |
| (1,212)  | 1:8:A:VAL:HG22  | 1:75:A:ASN:H    | 11       | 0.58          |
| (1,212)  | 1:8:A:VAL:HG23  | 1:75:A:ASN:H    | 11       | 0.58          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,212)  | 1:8:A:VAL:HG21  | 1:75:A:ASN:H    | 14       | 0.58          |
| (1,212)  | 1:8:A:VAL:HG22  | 1:75:A:ASN:H    | 14       | 0.58          |
| (1,212)  | 1:8:A:VAL:HG23  | 1:75:A:ASN:H    | 14       | 0.58          |
| (1,180)  | 1:72:A:LYS:H    | 1:72:A:LYS:HG3  | 10       | 0.58          |
| (1,1313) | 1:58:A:MET:HB3  | 1:58:A:MET:HE1  | 10       | 0.57          |
| (1,1313) | 1:58:A:MET:HB3  | 1:58:A:MET:HE2  | 10       | 0.57          |
| (1,1313) | 1:58:A:MET:HB3  | 1:58:A:MET:HE3  | 10       | 0.57          |
| (1,1280) | 1:36:A:ALA:HB1  | 1:37:A:ASP:HB3  | 19       | 0.57          |
| (1,1280) | 1:36:A:ALA:HB2  | 1:37:A:ASP:HB3  | 19       | 0.57          |
| (1,1280) | 1:36:A:ALA:HB3  | 1:37:A:ASP:HB3  | 19       | 0.57          |
| (1,1224) | 1:8:A:VAL:HG21  | 1:9:A:GLY:H     | 8        | 0.57          |
| (1,1224) | 1:8:A:VAL:HG22  | 1:9:A:GLY:H     | 8        | 0.57          |
| (1,1224) | 1:8:A:VAL:HG23  | 1:9:A:GLY:H     | 8        | 0.57          |
| (1,1160) | 1:78:A:LEU:HD21 | 1:79:A:THR:H    | 14       | 0.57          |
| (1,1160) | 1:78:A:LEU:HD22 | 1:79:A:THR:H    | 14       | 0.57          |
| (1,1160) | 1:78:A:LEU:HD23 | 1:79:A:THR:H    | 14       | 0.57          |
| (1,1030) | 1:29:A:PRO:HB2  | 1:43:A:LEU:HB2  | 10       | 0.57          |
| (1,1030) | 1:29:A:PRO:HB2  | 1:43:A:LEU:HB2  | 19       | 0.57          |
| (1,721)  | 1:17:A:ALA:HA   | 1:20:A:LEU:HD11 | 9        | 0.57          |
| (1,721)  | 1:17:A:ALA:HA   | 1:20:A:LEU:HD12 | 9        | 0.57          |
| (1,721)  | 1:17:A:ALA:HA   | 1:20:A:LEU:HD13 | 9        | 0.57          |
| (1,598)  | 1:12:A:PRO:HA   | 1:72:A:LYS:HG2  | 15       | 0.57          |
| (1,212)  | 1:8:A:VAL:HG21  | 1:75:A:ASN:H    | 8        | 0.57          |
| (1,212)  | 1:8:A:VAL:HG22  | 1:75:A:ASN:H    | 8        | 0.57          |
| (1,212)  | 1:8:A:VAL:HG23  | 1:75:A:ASN:H    | 8        | 0.57          |
| (1,212)  | 1:8:A:VAL:HG21  | 1:75:A:ASN:H    | 12       | 0.57          |
| (1,212)  | 1:8:A:VAL:HG22  | 1:75:A:ASN:H    | 12       | 0.57          |
| (1,212)  | 1:8:A:VAL:HG23  | 1:75:A:ASN:H    | 12       | 0.57          |
| (1,212)  | 1:8:A:VAL:HG21  | 1:75:A:ASN:H    | 19       | 0.57          |
| (1,212)  | 1:8:A:VAL:HG22  | 1:75:A:ASN:H    | 19       | 0.57          |
| (1,212)  | 1:8:A:VAL:HG23  | 1:75:A:ASN:H    | 19       | 0.57          |
| (1,212)  | 1:8:A:VAL:HG21  | 1:75:A:ASN:H    | 20       | 0.57          |
| (1,212)  | 1:8:A:VAL:HG22  | 1:75:A:ASN:H    | 20       | 0.57          |
| (1,212)  | 1:8:A:VAL:HG23  | 1:75:A:ASN:H    | 20       | 0.57          |
| (1,181)  | 1:68:A:LEU:HB2  | 1:72:A:LYS:H    | 14       | 0.57          |
| (1,101)  | 1:17:A:ALA:H    | 1:20:A:LEU:HD11 | 13       | 0.57          |
| (1,101)  | 1:17:A:ALA:H    | 1:20:A:LEU:HD12 | 13       | 0.57          |
| (1,101)  | 1:17:A:ALA:H    | 1:20:A:LEU:HD13 | 13       | 0.57          |
| (1,1224) | 1:8:A:VAL:HG21  | 1:9:A:GLY:H     | 16       | 0.56          |
| (1,1224) | 1:8:A:VAL:HG22  | 1:9:A:GLY:H     | 16       | 0.56          |
| (1,1224) | 1:8:A:VAL:HG23  | 1:9:A:GLY:H     | 16       | 0.56          |
| (1,1199) | 1:69:A:LEU:HA   | 1:69:A:LEU:HD21 | 7        | 0.56          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1199) | 1:69:A:LEU:HA   | 1:69:A:LEU:HD22 | 7        | 0.56          |
| (1,1199) | 1:69:A:LEU:HA   | 1:69:A:LEU:HD23 | 7        | 0.56          |
| (1,1160) | 1:78:A:LEU:HD21 | 1:79:A:THR:H    | 11       | 0.56          |
| (1,1160) | 1:78:A:LEU:HD22 | 1:79:A:THR:H    | 11       | 0.56          |
| (1,1160) | 1:78:A:LEU:HD23 | 1:79:A:THR:H    | 11       | 0.56          |
| (1,877)  | 1:7:A:PHE:HB3   | 1:79:A:THR:HB   | 5        | 0.56          |
| (1,877)  | 1:7:A:PHE:HB3   | 1:79:A:THR:HB   | 18       | 0.56          |
| (1,868)  | 1:9:A:GLY:H     | 1:75:A:ASN:HB3  | 20       | 0.56          |
| (1,811)  | 1:7:A:PHE:HE1   | 1:9:A:GLY:HA2   | 4        | 0.56          |
| (1,811)  | 1:7:A:PHE:HE2   | 1:9:A:GLY:HA2   | 4        | 0.56          |
| (1,721)  | 1:17:A:ALA:HA   | 1:20:A:LEU:HD11 | 7        | 0.56          |
| (1,721)  | 1:17:A:ALA:HA   | 1:20:A:LEU:HD12 | 7        | 0.56          |
| (1,721)  | 1:17:A:ALA:HA   | 1:20:A:LEU:HD13 | 7        | 0.56          |
| (1,197)  | 1:23:A:HIS:H    | 1:23:A:HIS:HB3  | 19       | 0.56          |
| (1,1359) | 1:23:A:HIS:HD2  | 1:64:A:GLN:HB2  | 12       | 0.55          |
| (1,1030) | 1:29:A:PRO:HB2  | 1:43:A:LEU:HB2  | 9        | 0.55          |
| (1,711)  | 1:68:A:LEU:HD11 | 1:73:A:LYS:HA   | 8        | 0.55          |
| (1,711)  | 1:68:A:LEU:HD12 | 1:73:A:LYS:HA   | 8        | 0.55          |
| (1,711)  | 1:68:A:LEU:HD13 | 1:73:A:LYS:HA   | 8        | 0.55          |
| (1,692)  | 1:4:A:PHE:HA    | 1:80:A:VAL:HG21 | 2        | 0.55          |
| (1,692)  | 1:4:A:PHE:HA    | 1:80:A:VAL:HG22 | 2        | 0.55          |
| (1,692)  | 1:4:A:PHE:HA    | 1:80:A:VAL:HG23 | 2        | 0.55          |
| (1,674)  | 1:68:A:LEU:HB2  | 1:71:A:GLU:HA   | 17       | 0.55          |
| (1,222)  | 1:19:A:GLU:HB3  | 1:20:A:LEU:H    | 1        | 0.55          |
| (1,76)   | 1:68:A:LEU:HD11 | 1:73:A:LYS:H    | 16       | 0.55          |
| (1,76)   | 1:68:A:LEU:HD12 | 1:73:A:LYS:H    | 16       | 0.55          |
| (1,76)   | 1:68:A:LEU:HD13 | 1:73:A:LYS:H    | 16       | 0.55          |
| (1,1378) | 1:23:A:HIS:HB3  | 1:23:A:HIS:HE1  | 16       | 0.54          |
| (1,1336) | 1:59:A:ASP:HB3  | 1:60:A:ILE:HD11 | 11       | 0.54          |
| (1,1336) | 1:59:A:ASP:HB3  | 1:60:A:ILE:HD12 | 11       | 0.54          |
| (1,1336) | 1:59:A:ASP:HB3  | 1:60:A:ILE:HD13 | 11       | 0.54          |
| (1,1128) | 1:20:A:LEU:HD11 | 1:34:A:LEU:HB2  | 15       | 0.54          |
| (1,1128) | 1:20:A:LEU:HD12 | 1:34:A:LEU:HB2  | 15       | 0.54          |
| (1,1128) | 1:20:A:LEU:HD13 | 1:34:A:LEU:HB2  | 15       | 0.54          |
| (1,1004) | 1:54:A:ILE:HD11 | 1:58:A:MET:HB3  | 6        | 0.54          |
| (1,1004) | 1:54:A:ILE:HD12 | 1:58:A:MET:HB3  | 6        | 0.54          |
| (1,1004) | 1:54:A:ILE:HD13 | 1:58:A:MET:HB3  | 6        | 0.54          |
| (1,958)  | 1:77:A:GLU:HB2  | 1:78:A:LEU:HD11 | 3        | 0.54          |
| (1,958)  | 1:77:A:GLU:HB2  | 1:78:A:LEU:HD12 | 3        | 0.54          |
| (1,958)  | 1:77:A:GLU:HB2  | 1:78:A:LEU:HD13 | 3        | 0.54          |
| (1,890)  | 1:59:A:ASP:HA   | 1:62:A:LEU:HB3  | 9        | 0.54          |
| (1,820)  | 1:68:A:LEU:HB2  | 1:71:A:GLU:H    | 5        | 0.54          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,820)  | 1:68:A:LEU:HB2  | 1:71:A:GLU:H    | 8        | 0.54          |
| (1,670)  | 1:20:A:LEU:HA   | 1:23:A:HIS:HB3  | 8        | 0.54          |
| (1,309)  | 1:58:A:MET:H    | 1:59:A:ASP:HB3  | 14       | 0.54          |
| (1,304)  | 1:56:A:ARG:H    | 1:59:A:ASP:HB3  | 3        | 0.54          |
| (1,212)  | 1:8:A:VAL:HG21  | 1:75:A:ASN:H    | 16       | 0.54          |
| (1,212)  | 1:8:A:VAL:HG22  | 1:75:A:ASN:H    | 16       | 0.54          |
| (1,212)  | 1:8:A:VAL:HG23  | 1:75:A:ASN:H    | 16       | 0.54          |
| (1,180)  | 1:72:A:LYS:H    | 1:72:A:LYS:HG3  | 19       | 0.54          |
| (1,1378) | 1:23:A:HIS:HB3  | 1:23:A:HIS:HE1  | 3        | 0.53          |
| (1,1378) | 1:23:A:HIS:HB3  | 1:23:A:HIS:HE1  | 8        | 0.53          |
| (1,1378) | 1:23:A:HIS:HB3  | 1:23:A:HIS:HE1  | 10       | 0.53          |
| (1,1199) | 1:69:A:LEU:HA   | 1:69:A:LEU:HD21 | 9        | 0.53          |
| (1,1199) | 1:69:A:LEU:HA   | 1:69:A:LEU:HD22 | 9        | 0.53          |
| (1,1199) | 1:69:A:LEU:HA   | 1:69:A:LEU:HD23 | 9        | 0.53          |
| (1,1199) | 1:69:A:LEU:HA   | 1:69:A:LEU:HD21 | 13       | 0.53          |
| (1,1199) | 1:69:A:LEU:HA   | 1:69:A:LEU:HD22 | 13       | 0.53          |
| (1,1199) | 1:69:A:LEU:HA   | 1:69:A:LEU:HD23 | 13       | 0.53          |
| (1,1148) | 1:68:A:LEU:HD21 | 1:71:A:GLU:HA   | 2        | 0.53          |
| (1,1148) | 1:68:A:LEU:HD22 | 1:71:A:GLU:HA   | 2        | 0.53          |
| (1,1148) | 1:68:A:LEU:HD23 | 1:71:A:GLU:HA   | 2        | 0.53          |
| (1,1148) | 1:68:A:LEU:HD21 | 1:71:A:GLU:HA   | 14       | 0.53          |
| (1,1148) | 1:68:A:LEU:HD22 | 1:71:A:GLU:HA   | 14       | 0.53          |
| (1,1148) | 1:68:A:LEU:HD23 | 1:71:A:GLU:HA   | 14       | 0.53          |
| (1,1030) | 1:29:A:PRO:HB2  | 1:43:A:LEU:HB2  | 5        | 0.53          |
| (1,1030) | 1:29:A:PRO:HB2  | 1:43:A:LEU:HB2  | 7        | 0.53          |
| (1,773)  | 1:65:A:HIS:HB3  | 1:75:A:ASN:HA   | 20       | 0.53          |
| (1,744)  | 1:38:A:LYS:HA   | 1:38:A:LYS:HG3  | 18       | 0.53          |
| (1,595)  | 1:28:A:SER:HB2  | 1:45:A:PHE:HE1  | 7        | 0.53          |
| (1,595)  | 1:28:A:SER:HB2  | 1:45:A:PHE:HE2  | 7        | 0.53          |
| (1,181)  | 1:68:A:LEU:HB2  | 1:72:A:LYS:H    | 12       | 0.53          |
| (1,180)  | 1:72:A:LYS:H    | 1:72:A:LYS:HG3  | 13       | 0.53          |
| (1,1378) | 1:23:A:HIS:HB3  | 1:23:A:HIS:HE1  | 1        | 0.52          |
| (1,1378) | 1:23:A:HIS:HB3  | 1:23:A:HIS:HE1  | 2        | 0.52          |
| (1,1378) | 1:23:A:HIS:HB3  | 1:23:A:HIS:HE1  | 5        | 0.52          |
| (1,1378) | 1:23:A:HIS:HB3  | 1:23:A:HIS:HE1  | 6        | 0.52          |
| (1,1378) | 1:23:A:HIS:HB3  | 1:23:A:HIS:HE1  | 7        | 0.52          |
| (1,1378) | 1:23:A:HIS:HB3  | 1:23:A:HIS:HE1  | 11       | 0.52          |
| (1,1378) | 1:23:A:HIS:HB3  | 1:23:A:HIS:HE1  | 15       | 0.52          |
| (1,1336) | 1:59:A:ASP:HB3  | 1:60:A:ILE:HD11 | 1        | 0.52          |
| (1,1336) | 1:59:A:ASP:HB3  | 1:60:A:ILE:HD12 | 1        | 0.52          |
| (1,1336) | 1:59:A:ASP:HB3  | 1:60:A:ILE:HD13 | 1        | 0.52          |
| (1,1280) | 1:36:A:ALA:HB1  | 1:37:A:ASP:HB3  | 12       | 0.52          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1280) | 1:36:A:ALA:HB2  | 1:37:A:ASP:HB3  | 12       | 0.52          |
| (1,1280) | 1:36:A:ALA:HB3  | 1:37:A:ASP:HB3  | 12       | 0.52          |
| (1,1248) | 1:8:A:VAL:HG11  | 1:43:A:LEU:HD21 | 15       | 0.52          |
| (1,1248) | 1:8:A:VAL:HG11  | 1:43:A:LEU:HD22 | 15       | 0.52          |
| (1,1248) | 1:8:A:VAL:HG11  | 1:43:A:LEU:HD23 | 15       | 0.52          |
| (1,1248) | 1:8:A:VAL:HG12  | 1:43:A:LEU:HD21 | 15       | 0.52          |
| (1,1248) | 1:8:A:VAL:HG12  | 1:43:A:LEU:HD22 | 15       | 0.52          |
| (1,1248) | 1:8:A:VAL:HG12  | 1:43:A:LEU:HD23 | 15       | 0.52          |
| (1,1248) | 1:8:A:VAL:HG13  | 1:43:A:LEU:HD21 | 15       | 0.52          |
| (1,1248) | 1:8:A:VAL:HG13  | 1:43:A:LEU:HD22 | 15       | 0.52          |
| (1,1248) | 1:8:A:VAL:HG13  | 1:43:A:LEU:HD23 | 15       | 0.52          |
| (1,1199) | 1:69:A:LEU:HA   | 1:69:A:LEU:HD21 | 1        | 0.52          |
| (1,1199) | 1:69:A:LEU:HA   | 1:69:A:LEU:HD22 | 1        | 0.52          |
| (1,1199) | 1:69:A:LEU:HA   | 1:69:A:LEU:HD23 | 1        | 0.52          |
| (1,1004) | 1:54:A:ILE:HD11 | 1:58:A:MET:HB3  | 19       | 0.52          |
| (1,1004) | 1:54:A:ILE:HD12 | 1:58:A:MET:HB3  | 19       | 0.52          |
| (1,1004) | 1:54:A:ILE:HD13 | 1:58:A:MET:HB3  | 19       | 0.52          |
| (1,890)  | 1:59:A:ASP:HA   | 1:62:A:LEU:HB3  | 6        | 0.52          |
| (1,868)  | 1:9:A:GLY:H     | 1:75:A:ASN:HB3  | 13       | 0.52          |
| (1,820)  | 1:68:A:LEU:HB2  | 1:71:A:GLU:H    | 2        | 0.52          |
| (1,811)  | 1:7:A:PHE:HE1   | 1:9:A:GLY:HA2   | 6        | 0.52          |
| (1,811)  | 1:7:A:PHE:HE2   | 1:9:A:GLY:HA2   | 6        | 0.52          |
| (1,30)   | 1:32:A:ILE:HG12 | 1:33:A:ARG:H    | 12       | 0.52          |
| (1,1378) | 1:23:A:HIS:HB3  | 1:23:A:HIS:HE1  | 4        | 0.51          |
| (1,1378) | 1:23:A:HIS:HB3  | 1:23:A:HIS:HE1  | 9        | 0.51          |
| (1,1378) | 1:23:A:HIS:HB3  | 1:23:A:HIS:HE1  | 18       | 0.51          |
| (1,1378) | 1:23:A:HIS:HB3  | 1:23:A:HIS:HE1  | 19       | 0.51          |
| (1,1378) | 1:23:A:HIS:HB3  | 1:23:A:HIS:HE1  | 20       | 0.51          |
| (1,1280) | 1:36:A:ALA:HB1  | 1:37:A:ASP:HB3  | 11       | 0.51          |
| (1,1280) | 1:36:A:ALA:HB2  | 1:37:A:ASP:HB3  | 11       | 0.51          |
| (1,1280) | 1:36:A:ALA:HB3  | 1:37:A:ASP:HB3  | 11       | 0.51          |
| (1,1199) | 1:69:A:LEU:HA   | 1:69:A:LEU:HD21 | 16       | 0.51          |
| (1,1199) | 1:69:A:LEU:HA   | 1:69:A:LEU:HD22 | 16       | 0.51          |
| (1,1199) | 1:69:A:LEU:HA   | 1:69:A:LEU:HD23 | 16       | 0.51          |
| (1,1189) | 1:20:A:LEU:HD21 | 1:34:A:LEU:HD11 | 7        | 0.51          |
| (1,1189) | 1:20:A:LEU:HD21 | 1:34:A:LEU:HD12 | 7        | 0.51          |
| (1,1189) | 1:20:A:LEU:HD21 | 1:34:A:LEU:HD13 | 7        | 0.51          |
| (1,1189) | 1:20:A:LEU:HD22 | 1:34:A:LEU:HD11 | 7        | 0.51          |
| (1,1189) | 1:20:A:LEU:HD22 | 1:34:A:LEU:HD12 | 7        | 0.51          |
| (1,1189) | 1:20:A:LEU:HD22 | 1:34:A:LEU:HD13 | 7        | 0.51          |
| (1,1189) | 1:20:A:LEU:HD23 | 1:34:A:LEU:HD11 | 7        | 0.51          |
| (1,1189) | 1:20:A:LEU:HD23 | 1:34:A:LEU:HD12 | 7        | 0.51          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1189) | 1:20:A:LEU:HD23 | 1:34:A:LEU:HD13 | 7        | 0.51          |
| (1,1148) | 1:68:A:LEU:HD21 | 1:71:A:GLU:HA   | 4        | 0.51          |
| (1,1148) | 1:68:A:LEU:HD22 | 1:71:A:GLU:HA   | 4        | 0.51          |
| (1,1148) | 1:68:A:LEU:HD23 | 1:71:A:GLU:HA   | 4        | 0.51          |
| (1,890)  | 1:59:A:ASP:HA   | 1:62:A:LEU:HB3  | 16       | 0.51          |
| (1,868)  | 1:9:A:GLY:H     | 1:75:A:ASN:HB3  | 18       | 0.51          |
| (1,820)  | 1:68:A:LEU:HB2  | 1:71:A:GLU:H    | 18       | 0.51          |
| (1,418)  | 1:80:A:VAL:HG21 | 1:82:A:GLY:H    | 15       | 0.51          |
| (1,418)  | 1:80:A:VAL:HG22 | 1:82:A:GLY:H    | 15       | 0.51          |
| (1,418)  | 1:80:A:VAL:HG23 | 1:82:A:GLY:H    | 15       | 0.51          |
| (1,396)  | 1:55:A:GLN:HE22 | 1:56:A:ARG:HG2  | 1        | 0.51          |
| (1,181)  | 1:68:A:LEU:HB2  | 1:72:A:LYS:H    | 15       | 0.51          |
| (1,1378) | 1:23:A:HIS:HB3  | 1:23:A:HIS:HE1  | 13       | 0.5           |
| (1,1378) | 1:23:A:HIS:HB3  | 1:23:A:HIS:HE1  | 14       | 0.5           |
| (1,1145) | 1:68:A:LEU:HD21 | 1:71:A:GLU:H    | 8        | 0.5           |
| (1,1145) | 1:68:A:LEU:HD22 | 1:71:A:GLU:H    | 8        | 0.5           |
| (1,1145) | 1:68:A:LEU:HD23 | 1:71:A:GLU:H    | 8        | 0.5           |
| (1,1030) | 1:29:A:PRO:HB2  | 1:43:A:LEU:HB2  | 4        | 0.5           |
| (1,890)  | 1:59:A:ASP:HA   | 1:62:A:LEU:HB3  | 11       | 0.5           |
| (1,890)  | 1:59:A:ASP:HA   | 1:62:A:LEU:HB3  | 14       | 0.5           |
| (1,877)  | 1:7:A:PHE:HB3   | 1:79:A:THR:HB   | 9        | 0.5           |
| (1,806)  | 1:68:A:LEU:HA   | 1:69:A:LEU:HB3  | 15       | 0.5           |
| (1,773)  | 1:65:A:HIS:HB3  | 1:75:A:ASN:HA   | 10       | 0.5           |
| (1,744)  | 1:38:A:LYS:HA   | 1:38:A:LYS:HG3  | 20       | 0.5           |
| (1,674)  | 1:68:A:LEU:HB2  | 1:71:A:GLU:HA   | 10       | 0.5           |
| (1,672)  | 1:20:A:LEU:HA   | 1:20:A:LEU:HD21 | 9        | 0.5           |
| (1,672)  | 1:20:A:LEU:HA   | 1:20:A:LEU:HD22 | 9        | 0.5           |
| (1,672)  | 1:20:A:LEU:HA   | 1:20:A:LEU:HD23 | 9        | 0.5           |
| (1,670)  | 1:20:A:LEU:HA   | 1:23:A:HIS:HB3  | 6        | 0.5           |
| (1,489)  | 1:10:A:SER:HB3  | 1:75:A:ASN:HD22 | 14       | 0.5           |
| (1,1199) | 1:69:A:LEU:HA   | 1:69:A:LEU:HD21 | 3        | 0.49          |
| (1,1199) | 1:69:A:LEU:HA   | 1:69:A:LEU:HD22 | 3        | 0.49          |
| (1,1199) | 1:69:A:LEU:HA   | 1:69:A:LEU:HD23 | 3        | 0.49          |
| (1,1199) | 1:69:A:LEU:HA   | 1:69:A:LEU:HD21 | 6        | 0.49          |
| (1,1199) | 1:69:A:LEU:HA   | 1:69:A:LEU:HD22 | 6        | 0.49          |
| (1,1199) | 1:69:A:LEU:HA   | 1:69:A:LEU:HD23 | 6        | 0.49          |
| (1,1148) | 1:68:A:LEU:HD21 | 1:71:A:GLU:HA   | 7        | 0.49          |
| (1,1148) | 1:68:A:LEU:HD22 | 1:71:A:GLU:HA   | 7        | 0.49          |
| (1,1148) | 1:68:A:LEU:HD23 | 1:71:A:GLU:HA   | 7        | 0.49          |
| (1,1145) | 1:68:A:LEU:HD21 | 1:71:A:GLU:H    | 2        | 0.49          |
| (1,1145) | 1:68:A:LEU:HD22 | 1:71:A:GLU:H    | 2        | 0.49          |
| (1,1145) | 1:68:A:LEU:HD23 | 1:71:A:GLU:H    | 2        | 0.49          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1145) | 1:68:A:LEU:HD21 | 1:71:A:GLU:H    | 14       | 0.49          |
| (1,1145) | 1:68:A:LEU:HD22 | 1:71:A:GLU:H    | 14       | 0.49          |
| (1,1145) | 1:68:A:LEU:HD23 | 1:71:A:GLU:H    | 14       | 0.49          |
| (1,1030) | 1:29:A:PRO:HB2  | 1:43:A:LEU:HB2  | 2        | 0.49          |
| (1,901)  | 1:49:A:LYS:HG2  | 1:50:A:ASP:HB2  | 4        | 0.49          |
| (1,901)  | 1:49:A:LYS:HG2  | 1:50:A:ASP:HB3  | 4        | 0.49          |
| (1,868)  | 1:9:A:GLY:H     | 1:75:A:ASN:HB3  | 16       | 0.49          |
| (1,811)  | 1:7:A:PHE:HE1   | 1:9:A:GLY:HA2   | 3        | 0.49          |
| (1,811)  | 1:7:A:PHE:HE2   | 1:9:A:GLY:HA2   | 3        | 0.49          |
| (1,773)  | 1:65:A:HIS:HB3  | 1:75:A:ASN:HA   | 11       | 0.49          |
| (1,721)  | 1:17:A:ALA:HA   | 1:20:A:LEU:HD11 | 6        | 0.49          |
| (1,721)  | 1:17:A:ALA:HA   | 1:20:A:LEU:HD12 | 6        | 0.49          |
| (1,721)  | 1:17:A:ALA:HA   | 1:20:A:LEU:HD13 | 6        | 0.49          |
| (1,644)  | 1:56:A:ARG:HA   | 1:59:A:ASP:HB3  | 4        | 0.49          |
| (1,30)   | 1:32:A:ILE:HG12 | 1:33:A:ARG:H    | 8        | 0.49          |
| (1,1356) | 1:20:A:LEU:HD21 | 1:24:A:PHE:HD1  | 9        | 0.48          |
| (1,1356) | 1:20:A:LEU:HD21 | 1:24:A:PHE:HD2  | 9        | 0.48          |
| (1,1356) | 1:20:A:LEU:HD22 | 1:24:A:PHE:HD1  | 9        | 0.48          |
| (1,1356) | 1:20:A:LEU:HD22 | 1:24:A:PHE:HD2  | 9        | 0.48          |
| (1,1356) | 1:20:A:LEU:HD23 | 1:24:A:PHE:HD1  | 9        | 0.48          |
| (1,1356) | 1:20:A:LEU:HD23 | 1:24:A:PHE:HD2  | 9        | 0.48          |
| (1,1336) | 1:59:A:ASP:HB3  | 1:60:A:ILE:HD11 | 10       | 0.48          |
| (1,1336) | 1:59:A:ASP:HB3  | 1:60:A:ILE:HD12 | 10       | 0.48          |
| (1,1336) | 1:59:A:ASP:HB3  | 1:60:A:ILE:HD13 | 10       | 0.48          |
| (1,1248) | 1:8:A:VAL:HG11  | 1:43:A:LEU:HD21 | 19       | 0.48          |
| (1,1248) | 1:8:A:VAL:HG11  | 1:43:A:LEU:HD22 | 19       | 0.48          |
| (1,1248) | 1:8:A:VAL:HG11  | 1:43:A:LEU:HD23 | 19       | 0.48          |
| (1,1248) | 1:8:A:VAL:HG12  | 1:43:A:LEU:HD21 | 19       | 0.48          |
| (1,1248) | 1:8:A:VAL:HG12  | 1:43:A:LEU:HD22 | 19       | 0.48          |
| (1,1248) | 1:8:A:VAL:HG12  | 1:43:A:LEU:HD23 | 19       | 0.48          |
| (1,1248) | 1:8:A:VAL:HG13  | 1:43:A:LEU:HD21 | 19       | 0.48          |
| (1,1248) | 1:8:A:VAL:HG13  | 1:43:A:LEU:HD22 | 19       | 0.48          |
| (1,1248) | 1:8:A:VAL:HG13  | 1:43:A:LEU:HD23 | 19       | 0.48          |
| (1,1040) | 1:12:A:PRO:HG2  | 1:70:A:LYS:HB3  | 8        | 0.48          |
| (1,1030) | 1:29:A:PRO:HB2  | 1:43:A:LEU:HB2  | 1        | 0.48          |
| (1,1004) | 1:54:A:ILE:HD11 | 1:58:A:MET:HB3  | 10       | 0.48          |
| (1,1004) | 1:54:A:ILE:HD12 | 1:58:A:MET:HB3  | 10       | 0.48          |
| (1,1004) | 1:54:A:ILE:HD13 | 1:58:A:MET:HB3  | 10       | 0.48          |
| (1,674)  | 1:68:A:LEU:HB2  | 1:71:A:GLU:HA   | 19       | 0.48          |
| (1,672)  | 1:20:A:LEU:HA   | 1:20:A:LEU:HD21 | 15       | 0.48          |
| (1,672)  | 1:20:A:LEU:HA   | 1:20:A:LEU:HD22 | 15       | 0.48          |
| (1,672)  | 1:20:A:LEU:HA   | 1:20:A:LEU:HD23 | 15       | 0.48          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,644)  | 1:56:A:ARG:HA   | 1:59:A:ASP:HB3  | 3        | 0.48          |
| (1,309)  | 1:58:A:MET:H    | 1:59:A:ASP:HB3  | 7        | 0.48          |
| (1,309)  | 1:58:A:MET:H    | 1:59:A:ASP:HB3  | 16       | 0.48          |
| (1,1378) | 1:23:A:HIS:HB3  | 1:23:A:HIS:HE1  | 17       | 0.47          |
| (1,1189) | 1:20:A:LEU:HD21 | 1:34:A:LEU:HD11 | 6        | 0.47          |
| (1,1189) | 1:20:A:LEU:HD21 | 1:34:A:LEU:HD12 | 6        | 0.47          |
| (1,1189) | 1:20:A:LEU:HD21 | 1:34:A:LEU:HD13 | 6        | 0.47          |
| (1,1189) | 1:20:A:LEU:HD22 | 1:34:A:LEU:HD11 | 6        | 0.47          |
| (1,1189) | 1:20:A:LEU:HD22 | 1:34:A:LEU:HD12 | 6        | 0.47          |
| (1,1189) | 1:20:A:LEU:HD22 | 1:34:A:LEU:HD13 | 6        | 0.47          |
| (1,1189) | 1:20:A:LEU:HD23 | 1:34:A:LEU:HD11 | 6        | 0.47          |
| (1,1189) | 1:20:A:LEU:HD23 | 1:34:A:LEU:HD12 | 6        | 0.47          |
| (1,1189) | 1:20:A:LEU:HD23 | 1:34:A:LEU:HD13 | 6        | 0.47          |
| (1,1084) | 1:33:A:ARG:H    | 1:33:A:ARG:HG2  | 20       | 0.47          |
| (1,1030) | 1:29:A:PRO:HB2  | 1:43:A:LEU:HB2  | 15       | 0.47          |
| (1,868)  | 1:9:A:GLY:H     | 1:75:A:ASN:HB3  | 1        | 0.47          |
| (1,721)  | 1:17:A:ALA:HA   | 1:20:A:LEU:HD11 | 13       | 0.47          |
| (1,721)  | 1:17:A:ALA:HA   | 1:20:A:LEU:HD12 | 13       | 0.47          |
| (1,721)  | 1:17:A:ALA:HA   | 1:20:A:LEU:HD13 | 13       | 0.47          |
| (1,672)  | 1:20:A:LEU:HA   | 1:20:A:LEU:HD21 | 13       | 0.47          |
| (1,672)  | 1:20:A:LEU:HA   | 1:20:A:LEU:HD22 | 13       | 0.47          |
| (1,672)  | 1:20:A:LEU:HA   | 1:20:A:LEU:HD23 | 13       | 0.47          |
| (1,1356) | 1:20:A:LEU:HD21 | 1:24:A:PHE:HD1  | 7        | 0.46          |
| (1,1356) | 1:20:A:LEU:HD21 | 1:24:A:PHE:HD2  | 7        | 0.46          |
| (1,1356) | 1:20:A:LEU:HD22 | 1:24:A:PHE:HD1  | 7        | 0.46          |
| (1,1356) | 1:20:A:LEU:HD22 | 1:24:A:PHE:HD2  | 7        | 0.46          |
| (1,1356) | 1:20:A:LEU:HD23 | 1:24:A:PHE:HD1  | 7        | 0.46          |
| (1,1356) | 1:20:A:LEU:HD23 | 1:24:A:PHE:HD2  | 7        | 0.46          |
| (1,1199) | 1:69:A:LEU:HA   | 1:69:A:LEU:HD21 | 18       | 0.46          |
| (1,1199) | 1:69:A:LEU:HA   | 1:69:A:LEU:HD22 | 18       | 0.46          |
| (1,1199) | 1:69:A:LEU:HA   | 1:69:A:LEU:HD23 | 18       | 0.46          |
| (1,1199) | 1:69:A:LEU:HA   | 1:69:A:LEU:HD21 | 19       | 0.46          |
| (1,1199) | 1:69:A:LEU:HA   | 1:69:A:LEU:HD22 | 19       | 0.46          |
| (1,1199) | 1:69:A:LEU:HA   | 1:69:A:LEU:HD23 | 19       | 0.46          |
| (1,1134) | 1:69:A:LEU:HD11 | 1:74:A:ILE:HD11 | 9        | 0.46          |
| (1,1134) | 1:69:A:LEU:HD11 | 1:74:A:ILE:HD12 | 9        | 0.46          |
| (1,1134) | 1:69:A:LEU:HD11 | 1:74:A:ILE:HD13 | 9        | 0.46          |
| (1,1134) | 1:69:A:LEU:HD12 | 1:74:A:ILE:HD11 | 9        | 0.46          |
| (1,1134) | 1:69:A:LEU:HD12 | 1:74:A:ILE:HD12 | 9        | 0.46          |
| (1,1134) | 1:69:A:LEU:HD12 | 1:74:A:ILE:HD13 | 9        | 0.46          |
| (1,1134) | 1:69:A:LEU:HD13 | 1:74:A:ILE:HD11 | 9        | 0.46          |
| (1,1134) | 1:69:A:LEU:HD13 | 1:74:A:ILE:HD12 | 9        | 0.46          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1134) | 1:69:A:LEU:HD13 | 1:74:A:ILE:HD13 | 9        | 0.46          |
| (1,1132) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD11 | 1        | 0.46          |
| (1,1132) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD12 | 1        | 0.46          |
| (1,1132) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD13 | 1        | 0.46          |
| (1,1003) | 1:55:A:GLN:HA   | 1:58:A:MET:HB3  | 17       | 0.46          |
| (1,672)  | 1:20:A:LEU:HA   | 1:20:A:LEU:HD21 | 7        | 0.46          |
| (1,672)  | 1:20:A:LEU:HA   | 1:20:A:LEU:HD22 | 7        | 0.46          |
| (1,672)  | 1:20:A:LEU:HA   | 1:20:A:LEU:HD23 | 7        | 0.46          |
| (1,566)  | 1:59:A:ASP:HB2  | 1:60:A:ILE:HA   | 8        | 0.46          |
| (1,325)  | 1:49:A:LYS:H    | 1:49:A:LYS:HG3  | 12       | 0.46          |
| (1,309)  | 1:58:A:MET:H    | 1:59:A:ASP:HB3  | 8        | 0.46          |
| (1,181)  | 1:68:A:LEU:HB2  | 1:72:A:LYS:H    | 16       | 0.46          |
| (1,135)  | 1:32:A:ILE:H    | 1:32:A:ILE:HG12 | 18       | 0.46          |
| (1,53)   | 1:68:A:LEU:HB2  | 1:69:A:LEU:H    | 3        | 0.46          |
| (1,1378) | 1:23:A:HIS:HB3  | 1:23:A:HIS:HE1  | 12       | 0.45          |
| (1,1128) | 1:20:A:LEU:HD11 | 1:34:A:LEU:HB2  | 7        | 0.45          |
| (1,1128) | 1:20:A:LEU:HD12 | 1:34:A:LEU:HB2  | 7        | 0.45          |
| (1,1128) | 1:20:A:LEU:HD13 | 1:34:A:LEU:HB2  | 7        | 0.45          |
| (1,1128) | 1:20:A:LEU:HD11 | 1:34:A:LEU:HB2  | 13       | 0.45          |
| (1,1128) | 1:20:A:LEU:HD12 | 1:34:A:LEU:HB2  | 13       | 0.45          |
| (1,1128) | 1:20:A:LEU:HD13 | 1:34:A:LEU:HB2  | 13       | 0.45          |
| (1,1003) | 1:55:A:GLN:HA   | 1:58:A:MET:HB3  | 2        | 0.45          |
| (1,988)  | 1:23:A:HIS:HD2  | 1:64:A:GLN:HG2  | 14       | 0.45          |
| (1,868)  | 1:9:A:GLY:H     | 1:75:A:ASN:HB3  | 2        | 0.45          |
| (1,820)  | 1:68:A:LEU:HB2  | 1:71:A:GLU:H    | 12       | 0.45          |
| (1,806)  | 1:68:A:LEU:HA   | 1:69:A:LEU:HB3  | 8        | 0.45          |
| (1,744)  | 1:38:A:LYS:HA   | 1:38:A:LYS:HG3  | 4        | 0.45          |
| (1,744)  | 1:38:A:LYS:HA   | 1:38:A:LYS:HG3  | 11       | 0.45          |
| (1,744)  | 1:38:A:LYS:HA   | 1:38:A:LYS:HG3  | 12       | 0.45          |
| (1,672)  | 1:20:A:LEU:HA   | 1:20:A:LEU:HD21 | 6        | 0.45          |
| (1,672)  | 1:20:A:LEU:HA   | 1:20:A:LEU:HD22 | 6        | 0.45          |
| (1,672)  | 1:20:A:LEU:HA   | 1:20:A:LEU:HD23 | 6        | 0.45          |
| (1,670)  | 1:20:A:LEU:HA   | 1:23:A:HIS:HB3  | 1        | 0.45          |
| (1,598)  | 1:12:A:PRO:HA   | 1:72:A:LYS:HG2  | 10       | 0.45          |
| (1,566)  | 1:59:A:ASP:HB2  | 1:60:A:ILE:HA   | 14       | 0.45          |
| (1,197)  | 1:23:A:HIS:H    | 1:23:A:HIS:HB3  | 5        | 0.45          |
| (1,88)   | 1:78:A:LEU:H    | 1:78:A:LEU:HD11 | 5        | 0.45          |
| (1,88)   | 1:78:A:LEU:H    | 1:78:A:LEU:HD12 | 5        | 0.45          |
| (1,88)   | 1:78:A:LEU:H    | 1:78:A:LEU:HD13 | 5        | 0.45          |
| (1,53)   | 1:68:A:LEU:HB2  | 1:69:A:LEU:H    | 11       | 0.45          |
| (1,53)   | 1:68:A:LEU:HB2  | 1:69:A:LEU:H    | 12       | 0.45          |
| (1,53)   | 1:68:A:LEU:HB2  | 1:69:A:LEU:H    | 16       | 0.45          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1359) | 1:23:A:HIS:HD2  | 1:64:A:GLN:HB2  | 10       | 0.44          |
| (1,1356) | 1:20:A:LEU:HD21 | 1:24:A:PHE:HD1  | 6        | 0.44          |
| (1,1356) | 1:20:A:LEU:HD21 | 1:24:A:PHE:HD2  | 6        | 0.44          |
| (1,1356) | 1:20:A:LEU:HD22 | 1:24:A:PHE:HD1  | 6        | 0.44          |
| (1,1356) | 1:20:A:LEU:HD22 | 1:24:A:PHE:HD2  | 6        | 0.44          |
| (1,1356) | 1:20:A:LEU:HD23 | 1:24:A:PHE:HD1  | 6        | 0.44          |
| (1,1356) | 1:20:A:LEU:HD23 | 1:24:A:PHE:HD2  | 6        | 0.44          |
| (1,1224) | 1:8:A:VAL:HG21  | 1:9:A:GLY:H     | 2        | 0.44          |
| (1,1224) | 1:8:A:VAL:HG22  | 1:9:A:GLY:H     | 2        | 0.44          |
| (1,1224) | 1:8:A:VAL:HG23  | 1:9:A:GLY:H     | 2        | 0.44          |
| (1,1199) | 1:69:A:LEU:HA   | 1:69:A:LEU:HD21 | 4        | 0.44          |
| (1,1199) | 1:69:A:LEU:HA   | 1:69:A:LEU:HD22 | 4        | 0.44          |
| (1,1199) | 1:69:A:LEU:HA   | 1:69:A:LEU:HD23 | 4        | 0.44          |
| (1,1040) | 1:12:A:PRO:HG2  | 1:70:A:LYS:HB3  | 7        | 0.44          |
| (1,1003) | 1:55:A:GLN:HA   | 1:58:A:MET:HB3  | 13       | 0.44          |
| (1,1003) | 1:55:A:GLN:HA   | 1:58:A:MET:HB3  | 18       | 0.44          |
| (1,988)  | 1:23:A:HIS:HD2  | 1:64:A:GLN:HG2  | 19       | 0.44          |
| (1,890)  | 1:59:A:ASP:HA   | 1:62:A:LEU:HB3  | 20       | 0.44          |
| (1,867)  | 1:70:A:LYS:HB2  | 1:70:A:LYS:HE2  | 13       | 0.44          |
| (1,867)  | 1:70:A:LYS:HB2  | 1:70:A:LYS:HE3  | 13       | 0.44          |
| (1,744)  | 1:38:A:LYS:HA   | 1:38:A:LYS:HG3  | 2        | 0.44          |
| (1,727)  | 1:37:A:ASP:HA   | 1:37:A:ASP:HB2  | 2        | 0.44          |
| (1,727)  | 1:37:A:ASP:HA   | 1:37:A:ASP:HB2  | 9        | 0.44          |
| (1,727)  | 1:37:A:ASP:HA   | 1:37:A:ASP:HB2  | 10       | 0.44          |
| (1,727)  | 1:37:A:ASP:HA   | 1:37:A:ASP:HB2  | 12       | 0.44          |
| (1,727)  | 1:37:A:ASP:HA   | 1:37:A:ASP:HB2  | 14       | 0.44          |
| (1,727)  | 1:37:A:ASP:HA   | 1:37:A:ASP:HB2  | 16       | 0.44          |
| (1,672)  | 1:20:A:LEU:HA   | 1:20:A:LEU:HD21 | 11       | 0.44          |
| (1,672)  | 1:20:A:LEU:HA   | 1:20:A:LEU:HD22 | 11       | 0.44          |
| (1,672)  | 1:20:A:LEU:HA   | 1:20:A:LEU:HD23 | 11       | 0.44          |
| (1,670)  | 1:20:A:LEU:HA   | 1:23:A:HIS:HB3  | 17       | 0.44          |
| (1,482)  | 1:10:A:SER:HB3  | 1:75:A:ASN:HD21 | 8        | 0.44          |
| (1,418)  | 1:80:A:VAL:HG21 | 1:82:A:GLY:H    | 7        | 0.44          |
| (1,418)  | 1:80:A:VAL:HG22 | 1:82:A:GLY:H    | 7        | 0.44          |
| (1,418)  | 1:80:A:VAL:HG23 | 1:82:A:GLY:H    | 7        | 0.44          |
| (1,325)  | 1:49:A:LYS:H    | 1:49:A:LYS:HG3  | 17       | 0.44          |
| (1,88)   | 1:78:A:LEU:H    | 1:78:A:LEU:HD11 | 17       | 0.44          |
| (1,88)   | 1:78:A:LEU:H    | 1:78:A:LEU:HD12 | 17       | 0.44          |
| (1,88)   | 1:78:A:LEU:H    | 1:78:A:LEU:HD13 | 17       | 0.44          |
| (1,76)   | 1:68:A:LEU:HD11 | 1:73:A:LYS:H    | 18       | 0.44          |
| (1,76)   | 1:68:A:LEU:HD12 | 1:73:A:LYS:H    | 18       | 0.44          |
| (1,76)   | 1:68:A:LEU:HD13 | 1:73:A:LYS:H    | 18       | 0.44          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,53)   | 1:68:A:LEU:HB2  | 1:69:A:LEU:H    | 7        | 0.44          |
| (1,53)   | 1:68:A:LEU:HB2  | 1:69:A:LEU:H    | 8        | 0.44          |
| (1,53)   | 1:68:A:LEU:HB2  | 1:69:A:LEU:H    | 9        | 0.44          |
| (1,53)   | 1:68:A:LEU:HB2  | 1:69:A:LEU:H    | 10       | 0.44          |
| (1,53)   | 1:68:A:LEU:HB2  | 1:69:A:LEU:H    | 13       | 0.44          |
| (1,53)   | 1:68:A:LEU:HB2  | 1:69:A:LEU:H    | 15       | 0.44          |
| (1,53)   | 1:68:A:LEU:HB2  | 1:69:A:LEU:H    | 17       | 0.44          |
| (1,53)   | 1:68:A:LEU:HB2  | 1:69:A:LEU:H    | 18       | 0.44          |
| (1,53)   | 1:68:A:LEU:HB2  | 1:69:A:LEU:H    | 19       | 0.44          |
| (1,1313) | 1:58:A:MET:HB3  | 1:58:A:MET:HE1  | 5        | 0.43          |
| (1,1313) | 1:58:A:MET:HB3  | 1:58:A:MET:HE2  | 5        | 0.43          |
| (1,1313) | 1:58:A:MET:HB3  | 1:58:A:MET:HE3  | 5        | 0.43          |
| (1,1309) | 1:55:A:GLN:HE21 | 1:58:A:MET:HE1  | 11       | 0.43          |
| (1,1309) | 1:55:A:GLN:HE21 | 1:58:A:MET:HE2  | 11       | 0.43          |
| (1,1309) | 1:55:A:GLN:HE21 | 1:58:A:MET:HE3  | 11       | 0.43          |
| (1,1201) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD21 | 4        | 0.43          |
| (1,1201) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD22 | 4        | 0.43          |
| (1,1201) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD23 | 4        | 0.43          |
| (1,1134) | 1:69:A:LEU:HD11 | 1:74:A:ILE:HD11 | 18       | 0.43          |
| (1,1134) | 1:69:A:LEU:HD11 | 1:74:A:ILE:HD12 | 18       | 0.43          |
| (1,1134) | 1:69:A:LEU:HD11 | 1:74:A:ILE:HD13 | 18       | 0.43          |
| (1,1134) | 1:69:A:LEU:HD12 | 1:74:A:ILE:HD11 | 18       | 0.43          |
| (1,1134) | 1:69:A:LEU:HD12 | 1:74:A:ILE:HD12 | 18       | 0.43          |
| (1,1134) | 1:69:A:LEU:HD12 | 1:74:A:ILE:HD13 | 18       | 0.43          |
| (1,1134) | 1:69:A:LEU:HD13 | 1:74:A:ILE:HD11 | 18       | 0.43          |
| (1,1134) | 1:69:A:LEU:HD13 | 1:74:A:ILE:HD12 | 18       | 0.43          |
| (1,1134) | 1:69:A:LEU:HD13 | 1:74:A:ILE:HD13 | 18       | 0.43          |
| (1,1026) | 1:29:A:PRO:HB3  | 1:32:A:ILE:HD11 | 2        | 0.43          |
| (1,1026) | 1:29:A:PRO:HB3  | 1:32:A:ILE:HD12 | 2        | 0.43          |
| (1,1026) | 1:29:A:PRO:HB3  | 1:32:A:ILE:HD13 | 2        | 0.43          |
| (1,1004) | 1:54:A:ILE:HD11 | 1:58:A:MET:HB3  | 5        | 0.43          |
| (1,1004) | 1:54:A:ILE:HD12 | 1:58:A:MET:HB3  | 5        | 0.43          |
| (1,1004) | 1:54:A:ILE:HD13 | 1:58:A:MET:HB3  | 5        | 0.43          |
| (1,1004) | 1:54:A:ILE:HD11 | 1:58:A:MET:HB3  | 16       | 0.43          |
| (1,1004) | 1:54:A:ILE:HD12 | 1:58:A:MET:HB3  | 16       | 0.43          |
| (1,1004) | 1:54:A:ILE:HD13 | 1:58:A:MET:HB3  | 16       | 0.43          |
| (1,949)  | 1:7:A:PHE:HB2   | 1:77:A:GLU:HG3  | 8        | 0.43          |
| (1,868)  | 1:9:A:GLY:H     | 1:75:A:ASN:HB3  | 5        | 0.43          |
| (1,868)  | 1:9:A:GLY:H     | 1:75:A:ASN:HB3  | 11       | 0.43          |
| (1,867)  | 1:70:A:LYS:HB2  | 1:70:A:LYS:HE2  | 6        | 0.43          |
| (1,867)  | 1:70:A:LYS:HB2  | 1:70:A:LYS:HE3  | 6        | 0.43          |
| (1,727)  | 1:37:A:ASP:HA   | 1:37:A:ASP:HB2  | 1        | 0.43          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,727)  | 1:37:A:ASP:HA  | 1:37:A:ASP:HB2  | 3        | 0.43          |
| (1,727)  | 1:37:A:ASP:HA  | 1:37:A:ASP:HB2  | 4        | 0.43          |
| (1,727)  | 1:37:A:ASP:HA  | 1:37:A:ASP:HB2  | 11       | 0.43          |
| (1,566)  | 1:59:A:ASP:HB2 | 1:60:A:ILE:HA   | 2        | 0.43          |
| (1,343)  | 1:68:A:LEU:H   | 1:68:A:LEU:HB3  | 8        | 0.43          |
| (1,325)  | 1:49:A:LYS:H   | 1:49:A:LYS:HG3  | 1        | 0.43          |
| (1,197)  | 1:23:A:HIS:H   | 1:23:A:HIS:HB3  | 13       | 0.43          |
| (1,88)   | 1:78:A:LEU:H   | 1:78:A:LEU:HD11 | 13       | 0.43          |
| (1,88)   | 1:78:A:LEU:H   | 1:78:A:LEU:HD12 | 13       | 0.43          |
| (1,88)   | 1:78:A:LEU:H   | 1:78:A:LEU:HD13 | 13       | 0.43          |
| (1,53)   | 1:68:A:LEU:HB2 | 1:69:A:LEU:H    | 4        | 0.43          |
| (1,53)   | 1:68:A:LEU:HB2 | 1:69:A:LEU:H    | 14       | 0.43          |
| (1,1313) | 1:58:A:MET:HB3 | 1:58:A:MET:HE1  | 16       | 0.42          |
| (1,1313) | 1:58:A:MET:HB3 | 1:58:A:MET:HE2  | 16       | 0.42          |
| (1,1313) | 1:58:A:MET:HB3 | 1:58:A:MET:HE3  | 16       | 0.42          |
| (1,1163) | 1:4:A:PHE:HB2  | 1:78:A:LEU:HD21 | 10       | 0.42          |
| (1,1163) | 1:4:A:PHE:HB2  | 1:78:A:LEU:HD22 | 10       | 0.42          |
| (1,1163) | 1:4:A:PHE:HB2  | 1:78:A:LEU:HD23 | 10       | 0.42          |
| (1,1163) | 1:4:A:PHE:HB3  | 1:78:A:LEU:HD21 | 10       | 0.42          |
| (1,1163) | 1:4:A:PHE:HB3  | 1:78:A:LEU:HD22 | 10       | 0.42          |
| (1,1163) | 1:4:A:PHE:HB3  | 1:78:A:LEU:HD23 | 10       | 0.42          |
| (1,1161) | 1:4:A:PHE:HD1  | 1:78:A:LEU:HD21 | 6        | 0.42          |
| (1,1161) | 1:4:A:PHE:HD1  | 1:78:A:LEU:HD22 | 6        | 0.42          |
| (1,1161) | 1:4:A:PHE:HD1  | 1:78:A:LEU:HD23 | 6        | 0.42          |
| (1,1161) | 1:4:A:PHE:HD2  | 1:78:A:LEU:HD21 | 6        | 0.42          |
| (1,1161) | 1:4:A:PHE:HD2  | 1:78:A:LEU:HD22 | 6        | 0.42          |
| (1,1161) | 1:4:A:PHE:HD2  | 1:78:A:LEU:HD23 | 6        | 0.42          |
| (1,1161) | 1:4:A:PHE:HD1  | 1:78:A:LEU:HD21 | 8        | 0.42          |
| (1,1161) | 1:4:A:PHE:HD1  | 1:78:A:LEU:HD22 | 8        | 0.42          |
| (1,1161) | 1:4:A:PHE:HD1  | 1:78:A:LEU:HD23 | 8        | 0.42          |
| (1,1161) | 1:4:A:PHE:HD2  | 1:78:A:LEU:HD21 | 8        | 0.42          |
| (1,1161) | 1:4:A:PHE:HD2  | 1:78:A:LEU:HD22 | 8        | 0.42          |
| (1,1161) | 1:4:A:PHE:HD2  | 1:78:A:LEU:HD23 | 8        | 0.42          |
| (1,1011) | 1:65:A:HIS:HB3 | 1:76:A:VAL:HB   | 2        | 0.42          |
| (1,1011) | 1:65:A:HIS:HB3 | 1:76:A:VAL:HB   | 5        | 0.42          |
| (1,1011) | 1:65:A:HIS:HB3 | 1:76:A:VAL:HB   | 6        | 0.42          |
| (1,1011) | 1:65:A:HIS:HB3 | 1:76:A:VAL:HB   | 17       | 0.42          |
| (1,1003) | 1:55:A:GLN:HA  | 1:58:A:MET:HB3  | 14       | 0.42          |
| (1,1003) | 1:55:A:GLN:HA  | 1:58:A:MET:HB3  | 15       | 0.42          |
| (1,877)  | 1:7:A:PHE:HB3  | 1:79:A:THR:HB   | 12       | 0.42          |
| (1,868)  | 1:9:A:GLY:H    | 1:75:A:ASN:HB3  | 7        | 0.42          |
| (1,727)  | 1:37:A:ASP:HA  | 1:37:A:ASP:HB2  | 5        | 0.42          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,727)  | 1:37:A:ASP:HA   | 1:37:A:ASP:HB2  | 6        | 0.42          |
| (1,727)  | 1:37:A:ASP:HA   | 1:37:A:ASP:HB2  | 7        | 0.42          |
| (1,727)  | 1:37:A:ASP:HA   | 1:37:A:ASP:HB2  | 8        | 0.42          |
| (1,727)  | 1:37:A:ASP:HA   | 1:37:A:ASP:HB2  | 15       | 0.42          |
| (1,727)  | 1:37:A:ASP:HA   | 1:37:A:ASP:HB2  | 17       | 0.42          |
| (1,727)  | 1:37:A:ASP:HA   | 1:37:A:ASP:HB2  | 18       | 0.42          |
| (1,727)  | 1:37:A:ASP:HA   | 1:37:A:ASP:HB2  | 19       | 0.42          |
| (1,727)  | 1:37:A:ASP:HA   | 1:37:A:ASP:HB2  | 20       | 0.42          |
| (1,580)  | 1:10:A:SER:HB2  | 1:74:A:ILE:HB   | 1        | 0.42          |
| (1,580)  | 1:10:A:SER:HB2  | 1:74:A:ILE:HB   | 4        | 0.42          |
| (1,580)  | 1:10:A:SER:HB2  | 1:74:A:ILE:HB   | 8        | 0.42          |
| (1,580)  | 1:10:A:SER:HB2  | 1:74:A:ILE:HB   | 12       | 0.42          |
| (1,343)  | 1:68:A:LEU:H    | 1:68:A:LEU:HB3  | 14       | 0.42          |
| (1,343)  | 1:68:A:LEU:H    | 1:68:A:LEU:HB3  | 17       | 0.42          |
| (1,325)  | 1:49:A:LYS:H    | 1:49:A:LYS:HG3  | 2        | 0.42          |
| (1,212)  | 1:8:A:VAL:HG21  | 1:75:A:ASN:H    | 15       | 0.42          |
| (1,212)  | 1:8:A:VAL:HG22  | 1:75:A:ASN:H    | 15       | 0.42          |
| (1,212)  | 1:8:A:VAL:HG23  | 1:75:A:ASN:H    | 15       | 0.42          |
| (1,53)   | 1:68:A:LEU:HB2  | 1:69:A:LEU:H    | 2        | 0.42          |
| (1,1161) | 1:4:A:PHE:HD1   | 1:78:A:LEU:HD21 | 4        | 0.41          |
| (1,1161) | 1:4:A:PHE:HD1   | 1:78:A:LEU:HD22 | 4        | 0.41          |
| (1,1161) | 1:4:A:PHE:HD1   | 1:78:A:LEU:HD23 | 4        | 0.41          |
| (1,1161) | 1:4:A:PHE:HD2   | 1:78:A:LEU:HD21 | 4        | 0.41          |
| (1,1161) | 1:4:A:PHE:HD2   | 1:78:A:LEU:HD22 | 4        | 0.41          |
| (1,1161) | 1:4:A:PHE:HD2   | 1:78:A:LEU:HD23 | 4        | 0.41          |
| (1,1160) | 1:78:A:LEU:HD21 | 1:79:A:THR:H    | 20       | 0.41          |
| (1,1160) | 1:78:A:LEU:HD22 | 1:79:A:THR:H    | 20       | 0.41          |
| (1,1160) | 1:78:A:LEU:HD23 | 1:79:A:THR:H    | 20       | 0.41          |
| (1,1127) | 1:20:A:LEU:HD11 | 1:34:A:LEU:HG   | 9        | 0.41          |
| (1,1127) | 1:20:A:LEU:HD12 | 1:34:A:LEU:HG   | 9        | 0.41          |
| (1,1127) | 1:20:A:LEU:HD13 | 1:34:A:LEU:HG   | 9        | 0.41          |
| (1,1084) | 1:33:A:ARG:H    | 1:33:A:ARG:HG2  | 12       | 0.41          |
| (1,1003) | 1:55:A:GLN:HA   | 1:58:A:MET:HB3  | 3        | 0.41          |
| (1,987)  | 1:24:A:PHE:HD1  | 1:64:A:GLN:HG2  | 10       | 0.41          |
| (1,987)  | 1:24:A:PHE:HD2  | 1:64:A:GLN:HG2  | 10       | 0.41          |
| (1,868)  | 1:9:A:GLY:H     | 1:75:A:ASN:HB3  | 6        | 0.41          |
| (1,868)  | 1:9:A:GLY:H     | 1:75:A:ASN:HB3  | 15       | 0.41          |
| (1,820)  | 1:68:A:LEU:HB2  | 1:71:A:GLU:H    | 14       | 0.41          |
| (1,674)  | 1:68:A:LEU:HB2  | 1:71:A:GLU:HA   | 15       | 0.41          |
| (1,580)  | 1:10:A:SER:HB2  | 1:74:A:ILE:HB   | 6        | 0.41          |
| (1,580)  | 1:10:A:SER:HB2  | 1:74:A:ILE:HB   | 15       | 0.41          |
| (1,580)  | 1:10:A:SER:HB2  | 1:74:A:ILE:HB   | 16       | 0.41          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,580)  | 1:10:A:SER:HB2  | 1:74:A:ILE:HB   | 17       | 0.41          |
| (1,418)  | 1:80:A:VAL:HG21 | 1:82:A:GLY:H    | 8        | 0.41          |
| (1,418)  | 1:80:A:VAL:HG22 | 1:82:A:GLY:H    | 8        | 0.41          |
| (1,418)  | 1:80:A:VAL:HG23 | 1:82:A:GLY:H    | 8        | 0.41          |
| (1,325)  | 1:49:A:LYS:H    | 1:49:A:LYS:HG3  | 5        | 0.41          |
| (1,309)  | 1:58:A:MET:H    | 1:59:A:ASP:HB3  | 2        | 0.41          |
| (1,290)  | 1:27:A:SER:HB2  | 1:60:A:ILE:H    | 9        | 0.41          |
| (1,180)  | 1:72:A:LYS:H    | 1:72:A:LYS:HG3  | 14       | 0.41          |
| (1,1248) | 1:8:A:VAL:HG11  | 1:43:A:LEU:HD21 | 3        | 0.4           |
| (1,1248) | 1:8:A:VAL:HG11  | 1:43:A:LEU:HD22 | 3        | 0.4           |
| (1,1248) | 1:8:A:VAL:HG11  | 1:43:A:LEU:HD23 | 3        | 0.4           |
| (1,1248) | 1:8:A:VAL:HG12  | 1:43:A:LEU:HD21 | 3        | 0.4           |
| (1,1248) | 1:8:A:VAL:HG12  | 1:43:A:LEU:HD22 | 3        | 0.4           |
| (1,1248) | 1:8:A:VAL:HG12  | 1:43:A:LEU:HD23 | 3        | 0.4           |
| (1,1248) | 1:8:A:VAL:HG13  | 1:43:A:LEU:HD21 | 3        | 0.4           |
| (1,1248) | 1:8:A:VAL:HG13  | 1:43:A:LEU:HD22 | 3        | 0.4           |
| (1,1248) | 1:8:A:VAL:HG13  | 1:43:A:LEU:HD23 | 3        | 0.4           |
| (1,1030) | 1:29:A:PRO:HB2  | 1:43:A:LEU:HB2  | 8        | 0.4           |
| (1,1012) | 1:65:A:HIS:HB3  | 1:76:A:VAL:HG21 | 2        | 0.4           |
| (1,1012) | 1:65:A:HIS:HB3  | 1:76:A:VAL:HG22 | 2        | 0.4           |
| (1,1012) | 1:65:A:HIS:HB3  | 1:76:A:VAL:HG23 | 2        | 0.4           |
| (1,1011) | 1:65:A:HIS:HB3  | 1:76:A:VAL:HB   | 9        | 0.4           |
| (1,987)  | 1:24:A:PHE:HD1  | 1:64:A:GLN:HG2  | 15       | 0.4           |
| (1,987)  | 1:24:A:PHE:HD2  | 1:64:A:GLN:HG2  | 15       | 0.4           |
| (1,890)  | 1:59:A:ASP:HA   | 1:62:A:LEU:HB3  | 1        | 0.4           |
| (1,890)  | 1:59:A:ASP:HA   | 1:62:A:LEU:HB3  | 5        | 0.4           |
| (1,890)  | 1:59:A:ASP:HA   | 1:62:A:LEU:HB3  | 10       | 0.4           |
| (1,868)  | 1:9:A:GLY:H     | 1:75:A:ASN:HB3  | 19       | 0.4           |
| (1,820)  | 1:68:A:LEU:HB2  | 1:71:A:GLU:H    | 20       | 0.4           |
| (1,789)  | 1:11:A:LEU:HB3  | 1:39:A:GLY:HA2  | 11       | 0.4           |
| (1,744)  | 1:38:A:LYS:HA   | 1:38:A:LYS:HG3  | 1        | 0.4           |
| (1,580)  | 1:10:A:SER:HB2  | 1:74:A:ILE:HB   | 13       | 0.4           |
| (1,580)  | 1:10:A:SER:HB2  | 1:74:A:ILE:HB   | 20       | 0.4           |
| (1,343)  | 1:68:A:LEU:H    | 1:68:A:LEU:HB3  | 2        | 0.4           |
| (1,343)  | 1:68:A:LEU:H    | 1:68:A:LEU:HB3  | 7        | 0.4           |
| (1,343)  | 1:68:A:LEU:H    | 1:68:A:LEU:HB3  | 15       | 0.4           |
| (1,328)  | 1:62:A:LEU:H    | 1:62:A:LEU:HB3  | 7        | 0.4           |
| (1,197)  | 1:23:A:HIS:H    | 1:23:A:HIS:HB3  | 10       | 0.4           |
| (1,197)  | 1:23:A:HIS:H    | 1:23:A:HIS:HB3  | 20       | 0.4           |
| (1,180)  | 1:72:A:LYS:H    | 1:72:A:LYS:HG3  | 5        | 0.4           |
| (1,88)   | 1:78:A:LEU:H    | 1:78:A:LEU:HD11 | 10       | 0.4           |
| (1,88)   | 1:78:A:LEU:H    | 1:78:A:LEU:HD12 | 10       | 0.4           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,88)   | 1:78:A:LEU:H    | 1:78:A:LEU:HD13 | 10       | 0.4           |
| (1,1248) | 1:8:A:VAL:HG11  | 1:43:A:LEU:HD21 | 1        | 0.39          |
| (1,1248) | 1:8:A:VAL:HG11  | 1:43:A:LEU:HD22 | 1        | 0.39          |
| (1,1248) | 1:8:A:VAL:HG11  | 1:43:A:LEU:HD23 | 1        | 0.39          |
| (1,1248) | 1:8:A:VAL:HG12  | 1:43:A:LEU:HD21 | 1        | 0.39          |
| (1,1248) | 1:8:A:VAL:HG12  | 1:43:A:LEU:HD22 | 1        | 0.39          |
| (1,1248) | 1:8:A:VAL:HG12  | 1:43:A:LEU:HD23 | 1        | 0.39          |
| (1,1248) | 1:8:A:VAL:HG13  | 1:43:A:LEU:HD21 | 1        | 0.39          |
| (1,1248) | 1:8:A:VAL:HG13  | 1:43:A:LEU:HD22 | 1        | 0.39          |
| (1,1248) | 1:8:A:VAL:HG13  | 1:43:A:LEU:HD23 | 1        | 0.39          |
| (1,1132) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD11 | 9        | 0.39          |
| (1,1132) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD12 | 9        | 0.39          |
| (1,1132) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD13 | 9        | 0.39          |
| (1,1084) | 1:33:A:ARG:H    | 1:33:A:ARG:HG2  | 8        | 0.39          |
| (1,1084) | 1:33:A:ARG:H    | 1:33:A:ARG:HG2  | 19       | 0.39          |
| (1,925)  | 1:37:A:ASP:HB2  | 1:38:A:LYS:HG3  | 13       | 0.39          |
| (1,744)  | 1:38:A:LYS:HA   | 1:38:A:LYS:HG3  | 13       | 0.39          |
| (1,744)  | 1:38:A:LYS:HA   | 1:38:A:LYS:HG3  | 17       | 0.39          |
| (1,580)  | 1:10:A:SER:HB2  | 1:74:A:ILE:HB   | 11       | 0.39          |
| (1,580)  | 1:10:A:SER:HB2  | 1:74:A:ILE:HB   | 14       | 0.39          |
| (1,566)  | 1:59:A:ASP:HB2  | 1:60:A:ILE:HA   | 16       | 0.39          |
| (1,396)  | 1:55:A:GLN:HE22 | 1:56:A:ARG:HG2  | 2        | 0.39          |
| (1,328)  | 1:62:A:LEU:H    | 1:62:A:LEU:HB3  | 12       | 0.39          |
| (1,76)   | 1:68:A:LEU:HD11 | 1:73:A:LYS:H    | 15       | 0.39          |
| (1,76)   | 1:68:A:LEU:HD12 | 1:73:A:LYS:H    | 15       | 0.39          |
| (1,76)   | 1:68:A:LEU:HD13 | 1:73:A:LYS:H    | 15       | 0.39          |
| (1,1356) | 1:20:A:LEU:HD21 | 1:24:A:PHE:HD1  | 11       | 0.38          |
| (1,1356) | 1:20:A:LEU:HD21 | 1:24:A:PHE:HD2  | 11       | 0.38          |
| (1,1356) | 1:20:A:LEU:HD22 | 1:24:A:PHE:HD1  | 11       | 0.38          |
| (1,1356) | 1:20:A:LEU:HD22 | 1:24:A:PHE:HD2  | 11       | 0.38          |
| (1,1356) | 1:20:A:LEU:HD23 | 1:24:A:PHE:HD1  | 11       | 0.38          |
| (1,1356) | 1:20:A:LEU:HD23 | 1:24:A:PHE:HD2  | 11       | 0.38          |
| (1,1248) | 1:8:A:VAL:HG11  | 1:43:A:LEU:HD21 | 11       | 0.38          |
| (1,1248) | 1:8:A:VAL:HG11  | 1:43:A:LEU:HD22 | 11       | 0.38          |
| (1,1248) | 1:8:A:VAL:HG11  | 1:43:A:LEU:HD23 | 11       | 0.38          |
| (1,1248) | 1:8:A:VAL:HG12  | 1:43:A:LEU:HD21 | 11       | 0.38          |
| (1,1248) | 1:8:A:VAL:HG12  | 1:43:A:LEU:HD22 | 11       | 0.38          |
| (1,1248) | 1:8:A:VAL:HG12  | 1:43:A:LEU:HD23 | 11       | 0.38          |
| (1,1248) | 1:8:A:VAL:HG13  | 1:43:A:LEU:HD21 | 11       | 0.38          |
| (1,1248) | 1:8:A:VAL:HG13  | 1:43:A:LEU:HD22 | 11       | 0.38          |
| (1,1248) | 1:8:A:VAL:HG13  | 1:43:A:LEU:HD23 | 11       | 0.38          |
| (1,1132) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD11 | 18       | 0.38          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1132) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD12 | 18       | 0.38          |
| (1,1132) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD13 | 18       | 0.38          |
| (1,1011) | 1:65:A:HIS:HB3  | 1:76:A:VAL:HB   | 10       | 0.38          |
| (1,1011) | 1:65:A:HIS:HB3  | 1:76:A:VAL:HB   | 16       | 0.38          |
| (1,1003) | 1:55:A:GLN:HA   | 1:58:A:MET:HB3  | 12       | 0.38          |
| (1,901)  | 1:49:A:LYS:HG2  | 1:50:A:ASP:HB2  | 1        | 0.38          |
| (1,901)  | 1:49:A:LYS:HG2  | 1:50:A:ASP:HB3  | 1        | 0.38          |
| (1,811)  | 1:7:A:PHE:HE1   | 1:9:A:GLY:HA2   | 10       | 0.38          |
| (1,811)  | 1:7:A:PHE:HE2   | 1:9:A:GLY:HA2   | 10       | 0.38          |
| (1,789)  | 1:11:A:LEU:HB3  | 1:39:A:GLY:HA2  | 15       | 0.38          |
| (1,721)  | 1:17:A:ALA:HA   | 1:20:A:LEU:HD11 | 15       | 0.38          |
| (1,721)  | 1:17:A:ALA:HA   | 1:20:A:LEU:HD12 | 15       | 0.38          |
| (1,721)  | 1:17:A:ALA:HA   | 1:20:A:LEU:HD13 | 15       | 0.38          |
| (1,418)  | 1:80:A:VAL:HG21 | 1:82:A:GLY:H    | 9        | 0.38          |
| (1,418)  | 1:80:A:VAL:HG22 | 1:82:A:GLY:H    | 9        | 0.38          |
| (1,418)  | 1:80:A:VAL:HG23 | 1:82:A:GLY:H    | 9        | 0.38          |
| (1,343)  | 1:68:A:LEU:H    | 1:68:A:LEU:HB3  | 4        | 0.38          |
| (1,343)  | 1:68:A:LEU:H    | 1:68:A:LEU:HB3  | 5        | 0.38          |
| (1,328)  | 1:62:A:LEU:H    | 1:62:A:LEU:HB3  | 2        | 0.38          |
| (1,328)  | 1:62:A:LEU:H    | 1:62:A:LEU:HB3  | 10       | 0.38          |
| (1,325)  | 1:49:A:LYS:H    | 1:49:A:LYS:HG3  | 20       | 0.38          |
| (1,197)  | 1:23:A:HIS:H    | 1:23:A:HIS:HB3  | 15       | 0.38          |
| (1,88)   | 1:78:A:LEU:H    | 1:78:A:LEU:HD11 | 9        | 0.38          |
| (1,88)   | 1:78:A:LEU:H    | 1:78:A:LEU:HD12 | 9        | 0.38          |
| (1,88)   | 1:78:A:LEU:H    | 1:78:A:LEU:HD13 | 9        | 0.38          |
| (1,1336) | 1:59:A:ASP:HB3  | 1:60:A:ILE:HD11 | 18       | 0.37          |
| (1,1336) | 1:59:A:ASP:HB3  | 1:60:A:ILE:HD12 | 18       | 0.37          |
| (1,1336) | 1:59:A:ASP:HB3  | 1:60:A:ILE:HD13 | 18       | 0.37          |
| (1,1313) | 1:58:A:MET:HB3  | 1:58:A:MET:HE1  | 4        | 0.37          |
| (1,1313) | 1:58:A:MET:HB3  | 1:58:A:MET:HE2  | 4        | 0.37          |
| (1,1313) | 1:58:A:MET:HB3  | 1:58:A:MET:HE3  | 4        | 0.37          |
| (1,1309) | 1:55:A:GLN:HE21 | 1:58:A:MET:HE1  | 2        | 0.37          |
| (1,1309) | 1:55:A:GLN:HE21 | 1:58:A:MET:HE2  | 2        | 0.37          |
| (1,1309) | 1:55:A:GLN:HE21 | 1:58:A:MET:HE3  | 2        | 0.37          |
| (1,1145) | 1:68:A:LEU:HD21 | 1:71:A:GLU:H    | 4        | 0.37          |
| (1,1145) | 1:68:A:LEU:HD22 | 1:71:A:GLU:H    | 4        | 0.37          |
| (1,1145) | 1:68:A:LEU:HD23 | 1:71:A:GLU:H    | 4        | 0.37          |
| (1,901)  | 1:49:A:LYS:HG2  | 1:50:A:ASP:HB2  | 20       | 0.37          |
| (1,901)  | 1:49:A:LYS:HG2  | 1:50:A:ASP:HB3  | 20       | 0.37          |
| (1,343)  | 1:68:A:LEU:H    | 1:68:A:LEU:HB3  | 11       | 0.37          |
| (1,343)  | 1:68:A:LEU:H    | 1:68:A:LEU:HB3  | 12       | 0.37          |
| (1,343)  | 1:68:A:LEU:H    | 1:68:A:LEU:HB3  | 16       | 0.37          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,343)  | 1:68:A:LEU:H    | 1:68:A:LEU:HB3  | 18       | 0.37          |
| (1,343)  | 1:68:A:LEU:H    | 1:68:A:LEU:HB3  | 20       | 0.37          |
| (1,328)  | 1:62:A:LEU:H    | 1:62:A:LEU:HB3  | 6        | 0.37          |
| (1,328)  | 1:62:A:LEU:H    | 1:62:A:LEU:HB3  | 18       | 0.37          |
| (1,197)  | 1:23:A:HIS:H    | 1:23:A:HIS:HB3  | 2        | 0.37          |
| (1,88)   | 1:78:A:LEU:H    | 1:78:A:LEU:HD11 | 2        | 0.37          |
| (1,88)   | 1:78:A:LEU:H    | 1:78:A:LEU:HD12 | 2        | 0.37          |
| (1,88)   | 1:78:A:LEU:H    | 1:78:A:LEU:HD13 | 2        | 0.37          |
| (1,88)   | 1:78:A:LEU:H    | 1:78:A:LEU:HD11 | 6        | 0.37          |
| (1,88)   | 1:78:A:LEU:H    | 1:78:A:LEU:HD12 | 6        | 0.37          |
| (1,88)   | 1:78:A:LEU:H    | 1:78:A:LEU:HD13 | 6        | 0.37          |
| (1,15)   | 1:6:A:VAL:H     | 1:43:A:LEU:HB3  | 14       | 0.37          |
| (1,1356) | 1:20:A:LEU:HD21 | 1:24:A:PHE:HD1  | 13       | 0.36          |
| (1,1356) | 1:20:A:LEU:HD21 | 1:24:A:PHE:HD2  | 13       | 0.36          |
| (1,1356) | 1:20:A:LEU:HD22 | 1:24:A:PHE:HD1  | 13       | 0.36          |
| (1,1356) | 1:20:A:LEU:HD22 | 1:24:A:PHE:HD2  | 13       | 0.36          |
| (1,1356) | 1:20:A:LEU:HD23 | 1:24:A:PHE:HD1  | 13       | 0.36          |
| (1,1356) | 1:20:A:LEU:HD23 | 1:24:A:PHE:HD2  | 13       | 0.36          |
| (1,1309) | 1:55:A:GLN:HE21 | 1:58:A:MET:HE1  | 8        | 0.36          |
| (1,1309) | 1:55:A:GLN:HE21 | 1:58:A:MET:HE2  | 8        | 0.36          |
| (1,1309) | 1:55:A:GLN:HE21 | 1:58:A:MET:HE3  | 8        | 0.36          |
| (1,1258) | 1:79:A:THR:HG21 | 1:80:A:VAL:HG11 | 8        | 0.36          |
| (1,1258) | 1:79:A:THR:HG21 | 1:80:A:VAL:HG12 | 8        | 0.36          |
| (1,1258) | 1:79:A:THR:HG21 | 1:80:A:VAL:HG13 | 8        | 0.36          |
| (1,1258) | 1:79:A:THR:HG22 | 1:80:A:VAL:HG11 | 8        | 0.36          |
| (1,1258) | 1:79:A:THR:HG22 | 1:80:A:VAL:HG12 | 8        | 0.36          |
| (1,1258) | 1:79:A:THR:HG22 | 1:80:A:VAL:HG13 | 8        | 0.36          |
| (1,1258) | 1:79:A:THR:HG23 | 1:80:A:VAL:HG11 | 8        | 0.36          |
| (1,1258) | 1:79:A:THR:HG23 | 1:80:A:VAL:HG12 | 8        | 0.36          |
| (1,1258) | 1:79:A:THR:HG23 | 1:80:A:VAL:HG13 | 8        | 0.36          |
| (1,1148) | 1:68:A:LEU:HD21 | 1:71:A:GLU:HA   | 18       | 0.36          |
| (1,1148) | 1:68:A:LEU:HD22 | 1:71:A:GLU:HA   | 18       | 0.36          |
| (1,1148) | 1:68:A:LEU:HD23 | 1:71:A:GLU:HA   | 18       | 0.36          |
| (1,1145) | 1:68:A:LEU:HD21 | 1:71:A:GLU:H    | 1        | 0.36          |
| (1,1145) | 1:68:A:LEU:HD22 | 1:71:A:GLU:H    | 1        | 0.36          |
| (1,1145) | 1:68:A:LEU:HD23 | 1:71:A:GLU:H    | 1        | 0.36          |
| (1,1145) | 1:68:A:LEU:HD21 | 1:71:A:GLU:H    | 18       | 0.36          |
| (1,1145) | 1:68:A:LEU:HD22 | 1:71:A:GLU:H    | 18       | 0.36          |
| (1,1145) | 1:68:A:LEU:HD23 | 1:71:A:GLU:H    | 18       | 0.36          |
| (1,1011) | 1:65:A:HIS:HB3  | 1:76:A:VAL:HB   | 8        | 0.36          |
| (1,820)  | 1:68:A:LEU:HB2  | 1:71:A:GLU:H    | 11       | 0.36          |
| (1,744)  | 1:38:A:LYS:HA   | 1:38:A:LYS:HG3  | 6        | 0.36          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,343)  | 1:68:A:LEU:H    | 1:68:A:LEU:HB3  | 9        | 0.36          |
| (1,328)  | 1:62:A:LEU:H    | 1:62:A:LEU:HB3  | 11       | 0.36          |
| (1,328)  | 1:62:A:LEU:H    | 1:62:A:LEU:HB3  | 13       | 0.36          |
| (1,53)   | 1:68:A:LEU:HB2  | 1:69:A:LEU:H    | 6        | 0.36          |
| (1,1226) | 1:8:A:VAL:HG21  | 1:11:A:LEU:HD21 | 1        | 0.35          |
| (1,1226) | 1:8:A:VAL:HG21  | 1:11:A:LEU:HD22 | 1        | 0.35          |
| (1,1226) | 1:8:A:VAL:HG21  | 1:11:A:LEU:HD23 | 1        | 0.35          |
| (1,1226) | 1:8:A:VAL:HG22  | 1:11:A:LEU:HD21 | 1        | 0.35          |
| (1,1226) | 1:8:A:VAL:HG22  | 1:11:A:LEU:HD22 | 1        | 0.35          |
| (1,1226) | 1:8:A:VAL:HG22  | 1:11:A:LEU:HD23 | 1        | 0.35          |
| (1,1226) | 1:8:A:VAL:HG23  | 1:11:A:LEU:HD21 | 1        | 0.35          |
| (1,1226) | 1:8:A:VAL:HG23  | 1:11:A:LEU:HD22 | 1        | 0.35          |
| (1,1226) | 1:8:A:VAL:HG23  | 1:11:A:LEU:HD23 | 1        | 0.35          |
| (1,1215) | 1:23:A:HIS:H    | 1:69:A:LEU:HD21 | 13       | 0.35          |
| (1,1215) | 1:23:A:HIS:H    | 1:69:A:LEU:HD22 | 13       | 0.35          |
| (1,1215) | 1:23:A:HIS:H    | 1:69:A:LEU:HD23 | 13       | 0.35          |
| (1,1121) | 1:40:A:ILE:HG12 | 1:42:A:PHE:HE1  | 16       | 0.35          |
| (1,1121) | 1:40:A:ILE:HG12 | 1:42:A:PHE:HE2  | 16       | 0.35          |
| (1,890)  | 1:59:A:ASP:HA   | 1:62:A:LEU:HB3  | 17       | 0.35          |
| (1,789)  | 1:11:A:LEU:HB3  | 1:39:A:GLY:HA2  | 3        | 0.35          |
| (1,789)  | 1:11:A:LEU:HB3  | 1:39:A:GLY:HA2  | 17       | 0.35          |
| (1,789)  | 1:11:A:LEU:HB3  | 1:39:A:GLY:HA2  | 18       | 0.35          |
| (1,744)  | 1:38:A:LYS:HA   | 1:38:A:LYS:HG3  | 19       | 0.35          |
| (1,732)  | 1:31:A:GLN:HA   | 1:31:A:GLN:HG2  | 11       | 0.35          |
| (1,732)  | 1:31:A:GLN:HA   | 1:31:A:GLN:HG2  | 17       | 0.35          |
| (1,566)  | 1:59:A:ASP:HB2  | 1:60:A:ILE:HA   | 7        | 0.35          |
| (1,468)  | 1:64:A:GLN:H    | 1:65:A:HIS:HB3  | 20       | 0.35          |
| (1,343)  | 1:68:A:LEU:H    | 1:68:A:LEU:HB3  | 10       | 0.35          |
| (1,343)  | 1:68:A:LEU:H    | 1:68:A:LEU:HB3  | 13       | 0.35          |
| (1,328)  | 1:62:A:LEU:H    | 1:62:A:LEU:HB3  | 1        | 0.35          |
| (1,328)  | 1:62:A:LEU:H    | 1:62:A:LEU:HB3  | 3        | 0.35          |
| (1,328)  | 1:62:A:LEU:H    | 1:62:A:LEU:HB3  | 16       | 0.35          |
| (1,53)   | 1:68:A:LEU:HB2  | 1:69:A:LEU:H    | 20       | 0.35          |
| (1,15)   | 1:6:A:VAL:H     | 1:43:A:LEU:HB3  | 8        | 0.35          |
| (1,1356) | 1:20:A:LEU:HD21 | 1:24:A:PHE:HD1  | 15       | 0.34          |
| (1,1356) | 1:20:A:LEU:HD21 | 1:24:A:PHE:HD2  | 15       | 0.34          |
| (1,1356) | 1:20:A:LEU:HD22 | 1:24:A:PHE:HD1  | 15       | 0.34          |
| (1,1356) | 1:20:A:LEU:HD22 | 1:24:A:PHE:HD2  | 15       | 0.34          |
| (1,1356) | 1:20:A:LEU:HD23 | 1:24:A:PHE:HD1  | 15       | 0.34          |
| (1,1356) | 1:20:A:LEU:HD23 | 1:24:A:PHE:HD2  | 15       | 0.34          |
| (1,1353) | 1:23:A:HIS:HB2  | 1:24:A:PHE:HD1  | 18       | 0.34          |
| (1,1353) | 1:23:A:HIS:HB2  | 1:24:A:PHE:HD2  | 18       | 0.34          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1232) | 1:6:A:VAL:HG11  | 1:7:A:PHE:HB2   | 17       | 0.34          |
| (1,1232) | 1:6:A:VAL:HG12  | 1:7:A:PHE:HB2   | 17       | 0.34          |
| (1,1232) | 1:6:A:VAL:HG13  | 1:7:A:PHE:HB2   | 17       | 0.34          |
| (1,1201) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD21 | 18       | 0.34          |
| (1,1201) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD22 | 18       | 0.34          |
| (1,1201) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD23 | 18       | 0.34          |
| (1,1161) | 1:4:A:PHE:HD1   | 1:78:A:LEU:HD21 | 2        | 0.34          |
| (1,1161) | 1:4:A:PHE:HD1   | 1:78:A:LEU:HD22 | 2        | 0.34          |
| (1,1161) | 1:4:A:PHE:HD1   | 1:78:A:LEU:HD23 | 2        | 0.34          |
| (1,1161) | 1:4:A:PHE:HD2   | 1:78:A:LEU:HD21 | 2        | 0.34          |
| (1,1161) | 1:4:A:PHE:HD2   | 1:78:A:LEU:HD22 | 2        | 0.34          |
| (1,1161) | 1:4:A:PHE:HD2   | 1:78:A:LEU:HD23 | 2        | 0.34          |
| (1,1134) | 1:69:A:LEU:HD11 | 1:74:A:ILE:HD11 | 6        | 0.34          |
| (1,1134) | 1:69:A:LEU:HD11 | 1:74:A:ILE:HD12 | 6        | 0.34          |
| (1,1134) | 1:69:A:LEU:HD11 | 1:74:A:ILE:HD13 | 6        | 0.34          |
| (1,1134) | 1:69:A:LEU:HD12 | 1:74:A:ILE:HD11 | 6        | 0.34          |
| (1,1134) | 1:69:A:LEU:HD12 | 1:74:A:ILE:HD12 | 6        | 0.34          |
| (1,1134) | 1:69:A:LEU:HD12 | 1:74:A:ILE:HD13 | 6        | 0.34          |
| (1,1134) | 1:69:A:LEU:HD13 | 1:74:A:ILE:HD11 | 6        | 0.34          |
| (1,1134) | 1:69:A:LEU:HD13 | 1:74:A:ILE:HD12 | 6        | 0.34          |
| (1,1134) | 1:69:A:LEU:HD13 | 1:74:A:ILE:HD13 | 6        | 0.34          |
| (1,1024) | 1:29:A:PRO:HB3  | 1:44:A:GLU:H    | 5        | 0.34          |
| (1,1011) | 1:65:A:HIS:HB3  | 1:76:A:VAL:HB   | 3        | 0.34          |
| (1,1011) | 1:65:A:HIS:HB3  | 1:76:A:VAL:HB   | 18       | 0.34          |
| (1,1004) | 1:54:A:ILE:HD11 | 1:58:A:MET:HB3  | 1        | 0.34          |
| (1,1004) | 1:54:A:ILE:HD12 | 1:58:A:MET:HB3  | 1        | 0.34          |
| (1,1004) | 1:54:A:ILE:HD13 | 1:58:A:MET:HB3  | 1        | 0.34          |
| (1,892)  | 1:62:A:LEU:HB2  | 1:63:A:LEU:HA   | 19       | 0.34          |
| (1,744)  | 1:38:A:LYS:HA   | 1:38:A:LYS:HG3  | 8        | 0.34          |
| (1,328)  | 1:62:A:LEU:H    | 1:62:A:LEU:HB3  | 4        | 0.34          |
| (1,328)  | 1:62:A:LEU:H    | 1:62:A:LEU:HB3  | 15       | 0.34          |
| (1,197)  | 1:23:A:HIS:H    | 1:23:A:HIS:HB3  | 4        | 0.34          |
| (1,101)  | 1:17:A:ALA:H    | 1:20:A:LEU:HD11 | 11       | 0.34          |
| (1,101)  | 1:17:A:ALA:H    | 1:20:A:LEU:HD12 | 11       | 0.34          |
| (1,101)  | 1:17:A:ALA:H    | 1:20:A:LEU:HD13 | 11       | 0.34          |
| (1,88)   | 1:78:A:LEU:H    | 1:78:A:LEU:HD11 | 12       | 0.34          |
| (1,88)   | 1:78:A:LEU:H    | 1:78:A:LEU:HD12 | 12       | 0.34          |
| (1,88)   | 1:78:A:LEU:H    | 1:78:A:LEU:HD13 | 12       | 0.34          |
| (1,76)   | 1:68:A:LEU:HD11 | 1:73:A:LYS:H    | 2        | 0.34          |
| (1,76)   | 1:68:A:LEU:HD12 | 1:73:A:LYS:H    | 2        | 0.34          |
| (1,76)   | 1:68:A:LEU:HD13 | 1:73:A:LYS:H    | 2        | 0.34          |
| (1,76)   | 1:68:A:LEU:HD11 | 1:73:A:LYS:H    | 5        | 0.34          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,76)   | 1:68:A:LEU:HD12 | 1:73:A:LYS:H    | 5        | 0.34          |
| (1,76)   | 1:68:A:LEU:HD13 | 1:73:A:LYS:H    | 5        | 0.34          |
| (1,55)   | 1:68:A:LEU:HD11 | 1:69:A:LEU:H    | 1        | 0.34          |
| (1,55)   | 1:68:A:LEU:HD12 | 1:69:A:LEU:H    | 1        | 0.34          |
| (1,55)   | 1:68:A:LEU:HD13 | 1:69:A:LEU:H    | 1        | 0.34          |
| (1,53)   | 1:68:A:LEU:HB2  | 1:69:A:LEU:H    | 5        | 0.34          |
| (2,2)    | 1:76:A:VAL:N    | 1:65:A:HIS:HD2  | 17       | 0.33          |
| (1,1255) | 1:18:A:VAL:HG11 | 1:22:A:ASN:HB2  | 12       | 0.33          |
| (1,1255) | 1:18:A:VAL:HG11 | 1:22:A:ASN:HB3  | 12       | 0.33          |
| (1,1255) | 1:18:A:VAL:HG12 | 1:22:A:ASN:HB2  | 12       | 0.33          |
| (1,1255) | 1:18:A:VAL:HG12 | 1:22:A:ASN:HB3  | 12       | 0.33          |
| (1,1255) | 1:18:A:VAL:HG13 | 1:22:A:ASN:HB2  | 12       | 0.33          |
| (1,1255) | 1:18:A:VAL:HG13 | 1:22:A:ASN:HB3  | 12       | 0.33          |
| (1,1226) | 1:8:A:VAL:HG21  | 1:11:A:LEU:HD21 | 8        | 0.33          |
| (1,1226) | 1:8:A:VAL:HG21  | 1:11:A:LEU:HD22 | 8        | 0.33          |
| (1,1226) | 1:8:A:VAL:HG21  | 1:11:A:LEU:HD23 | 8        | 0.33          |
| (1,1226) | 1:8:A:VAL:HG22  | 1:11:A:LEU:HD21 | 8        | 0.33          |
| (1,1226) | 1:8:A:VAL:HG22  | 1:11:A:LEU:HD22 | 8        | 0.33          |
| (1,1226) | 1:8:A:VAL:HG22  | 1:11:A:LEU:HD23 | 8        | 0.33          |
| (1,1226) | 1:8:A:VAL:HG23  | 1:11:A:LEU:HD21 | 8        | 0.33          |
| (1,1226) | 1:8:A:VAL:HG23  | 1:11:A:LEU:HD22 | 8        | 0.33          |
| (1,1226) | 1:8:A:VAL:HG23  | 1:11:A:LEU:HD23 | 8        | 0.33          |
| (1,1145) | 1:68:A:LEU:HD21 | 1:71:A:GLU:H    | 20       | 0.33          |
| (1,1145) | 1:68:A:LEU:HD22 | 1:71:A:GLU:H    | 20       | 0.33          |
| (1,1145) | 1:68:A:LEU:HD23 | 1:71:A:GLU:H    | 20       | 0.33          |
| (1,1071) | 1:24:A:PHE:HE1  | 1:64:A:GLN:HB3  | 17       | 0.33          |
| (1,1071) | 1:24:A:PHE:HE2  | 1:64:A:GLN:HB3  | 17       | 0.33          |
| (1,1024) | 1:29:A:PRO:HB3  | 1:44:A:GLU:H    | 1        | 0.33          |
| (1,1011) | 1:65:A:HIS:HB3  | 1:76:A:VAL:HB   | 4        | 0.33          |
| (1,1011) | 1:65:A:HIS:HB3  | 1:76:A:VAL:HB   | 15       | 0.33          |
| (1,1004) | 1:54:A:ILE:HD11 | 1:58:A:MET:HB3  | 15       | 0.33          |
| (1,1004) | 1:54:A:ILE:HD12 | 1:58:A:MET:HB3  | 15       | 0.33          |
| (1,1004) | 1:54:A:ILE:HD13 | 1:58:A:MET:HB3  | 15       | 0.33          |
| (1,809)  | 1:7:A:PHE:HZ    | 1:9:A:GLY:HA2   | 20       | 0.33          |
| (1,343)  | 1:68:A:LEU:H    | 1:68:A:LEU:HB3  | 19       | 0.33          |
| (1,328)  | 1:62:A:LEU:H    | 1:62:A:LEU:HB3  | 5        | 0.33          |
| (1,325)  | 1:49:A:LYS:H    | 1:49:A:LYS:HG3  | 14       | 0.33          |
| (1,88)   | 1:78:A:LEU:H    | 1:78:A:LEU:HD11 | 4        | 0.33          |
| (1,88)   | 1:78:A:LEU:H    | 1:78:A:LEU:HD12 | 4        | 0.33          |
| (1,88)   | 1:78:A:LEU:H    | 1:78:A:LEU:HD13 | 4        | 0.33          |
| (1,88)   | 1:78:A:LEU:H    | 1:78:A:LEU:HD11 | 8        | 0.33          |
| (1,88)   | 1:78:A:LEU:H    | 1:78:A:LEU:HD12 | 8        | 0.33          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,88)   | 1:78:A:LEU:H    | 1:78:A:LEU:HD13 | 8        | 0.33          |
| (1,88)   | 1:78:A:LEU:H    | 1:78:A:LEU:HD11 | 15       | 0.33          |
| (1,88)   | 1:78:A:LEU:H    | 1:78:A:LEU:HD12 | 15       | 0.33          |
| (1,88)   | 1:78:A:LEU:H    | 1:78:A:LEU:HD13 | 15       | 0.33          |
| (1,88)   | 1:78:A:LEU:H    | 1:78:A:LEU:HD11 | 16       | 0.33          |
| (1,88)   | 1:78:A:LEU:H    | 1:78:A:LEU:HD12 | 16       | 0.33          |
| (1,88)   | 1:78:A:LEU:H    | 1:78:A:LEU:HD13 | 16       | 0.33          |
| (1,1353) | 1:23:A:HIS:HB2  | 1:24:A:PHE:HD1  | 16       | 0.32          |
| (1,1353) | 1:23:A:HIS:HB2  | 1:24:A:PHE:HD2  | 16       | 0.32          |
| (1,1336) | 1:59:A:ASP:HB3  | 1:60:A:ILE:HD11 | 19       | 0.32          |
| (1,1336) | 1:59:A:ASP:HB3  | 1:60:A:ILE:HD12 | 19       | 0.32          |
| (1,1336) | 1:59:A:ASP:HB3  | 1:60:A:ILE:HD13 | 19       | 0.32          |
| (1,1313) | 1:58:A:MET:HB3  | 1:58:A:MET:HE1  | 1        | 0.32          |
| (1,1313) | 1:58:A:MET:HB3  | 1:58:A:MET:HE2  | 1        | 0.32          |
| (1,1313) | 1:58:A:MET:HB3  | 1:58:A:MET:HE3  | 1        | 0.32          |
| (1,1309) | 1:55:A:GLN:HE21 | 1:58:A:MET:HE1  | 15       | 0.32          |
| (1,1309) | 1:55:A:GLN:HE21 | 1:58:A:MET:HE2  | 15       | 0.32          |
| (1,1309) | 1:55:A:GLN:HE21 | 1:58:A:MET:HE3  | 15       | 0.32          |
| (1,1232) | 1:6:A:VAL:HG11  | 1:7:A:PHE:HB2   | 5        | 0.32          |
| (1,1232) | 1:6:A:VAL:HG12  | 1:7:A:PHE:HB2   | 5        | 0.32          |
| (1,1232) | 1:6:A:VAL:HG13  | 1:7:A:PHE:HB2   | 5        | 0.32          |
| (1,1226) | 1:8:A:VAL:HG21  | 1:11:A:LEU:HD21 | 7        | 0.32          |
| (1,1226) | 1:8:A:VAL:HG21  | 1:11:A:LEU:HD22 | 7        | 0.32          |
| (1,1226) | 1:8:A:VAL:HG21  | 1:11:A:LEU:HD23 | 7        | 0.32          |
| (1,1226) | 1:8:A:VAL:HG22  | 1:11:A:LEU:HD21 | 7        | 0.32          |
| (1,1226) | 1:8:A:VAL:HG22  | 1:11:A:LEU:HD22 | 7        | 0.32          |
| (1,1226) | 1:8:A:VAL:HG22  | 1:11:A:LEU:HD23 | 7        | 0.32          |
| (1,1226) | 1:8:A:VAL:HG23  | 1:11:A:LEU:HD21 | 7        | 0.32          |
| (1,1226) | 1:8:A:VAL:HG23  | 1:11:A:LEU:HD22 | 7        | 0.32          |
| (1,1226) | 1:8:A:VAL:HG23  | 1:11:A:LEU:HD23 | 7        | 0.32          |
| (1,1226) | 1:8:A:VAL:HG21  | 1:11:A:LEU:HD21 | 12       | 0.32          |
| (1,1226) | 1:8:A:VAL:HG21  | 1:11:A:LEU:HD22 | 12       | 0.32          |
| (1,1226) | 1:8:A:VAL:HG21  | 1:11:A:LEU:HD23 | 12       | 0.32          |
| (1,1226) | 1:8:A:VAL:HG22  | 1:11:A:LEU:HD21 | 12       | 0.32          |
| (1,1226) | 1:8:A:VAL:HG22  | 1:11:A:LEU:HD22 | 12       | 0.32          |
| (1,1226) | 1:8:A:VAL:HG22  | 1:11:A:LEU:HD23 | 12       | 0.32          |
| (1,1226) | 1:8:A:VAL:HG23  | 1:11:A:LEU:HD21 | 12       | 0.32          |
| (1,1226) | 1:8:A:VAL:HG23  | 1:11:A:LEU:HD22 | 12       | 0.32          |
| (1,1226) | 1:8:A:VAL:HG23  | 1:11:A:LEU:HD23 | 12       | 0.32          |
| (1,1215) | 1:23:A:HIS:H    | 1:69:A:LEU:HD21 | 7        | 0.32          |
| (1,1215) | 1:23:A:HIS:H    | 1:69:A:LEU:HD22 | 7        | 0.32          |
| (1,1215) | 1:23:A:HIS:H    | 1:69:A:LEU:HD23 | 7        | 0.32          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1084) | 1:33:A:ARG:H    | 1:33:A:ARG:HG2  | 9        | 0.32          |
| (1,1024) | 1:29:A:PRO:HB3  | 1:44:A:GLU:H    | 7        | 0.32          |
| (1,1024) | 1:29:A:PRO:HB3  | 1:44:A:GLU:H    | 9        | 0.32          |
| (1,1024) | 1:29:A:PRO:HB3  | 1:44:A:GLU:H    | 10       | 0.32          |
| (1,1024) | 1:29:A:PRO:HB3  | 1:44:A:GLU:H    | 16       | 0.32          |
| (1,1024) | 1:29:A:PRO:HB3  | 1:44:A:GLU:H    | 17       | 0.32          |
| (1,1012) | 1:65:A:HIS:HB3  | 1:76:A:VAL:HG21 | 6        | 0.32          |
| (1,1012) | 1:65:A:HIS:HB3  | 1:76:A:VAL:HG22 | 6        | 0.32          |
| (1,1012) | 1:65:A:HIS:HB3  | 1:76:A:VAL:HG23 | 6        | 0.32          |
| (1,1011) | 1:65:A:HIS:HB3  | 1:76:A:VAL:HB   | 13       | 0.32          |
| (1,1003) | 1:55:A:GLN:HA   | 1:58:A:MET:HB3  | 6        | 0.32          |
| (1,868)  | 1:9:A:GLY:H     | 1:75:A:ASN:HB3  | 12       | 0.32          |
| (1,824)  | 1:56:A:ARG:HB2  | 1:56:A:ARG:HD2  | 18       | 0.32          |
| (1,824)  | 1:56:A:ARG:HB3  | 1:56:A:ARG:HD2  | 18       | 0.32          |
| (1,820)  | 1:68:A:LEU:HB2  | 1:71:A:GLU:H    | 16       | 0.32          |
| (1,811)  | 1:7:A:PHE:HE1   | 1:9:A:GLY:HA2   | 16       | 0.32          |
| (1,811)  | 1:7:A:PHE:HE2   | 1:9:A:GLY:HA2   | 16       | 0.32          |
| (1,811)  | 1:7:A:PHE:HE1   | 1:9:A:GLY:HA2   | 20       | 0.32          |
| (1,811)  | 1:7:A:PHE:HE2   | 1:9:A:GLY:HA2   | 20       | 0.32          |
| (1,670)  | 1:20:A:LEU:HA   | 1:23:A:HIS:HB3  | 3        | 0.32          |
| (1,461)  | 1:29:A:PRO:HB3  | 1:31:A:GLN:H    | 6        | 0.32          |
| (1,328)  | 1:62:A:LEU:H    | 1:62:A:LEU:HB3  | 14       | 0.32          |
| (1,328)  | 1:62:A:LEU:H    | 1:62:A:LEU:HB3  | 17       | 0.32          |
| (1,88)   | 1:78:A:LEU:H    | 1:78:A:LEU:HD11 | 18       | 0.32          |
| (1,88)   | 1:78:A:LEU:H    | 1:78:A:LEU:HD12 | 18       | 0.32          |
| (1,88)   | 1:78:A:LEU:H    | 1:78:A:LEU:HD13 | 18       | 0.32          |
| (1,15)   | 1:6:A:VAL:H     | 1:43:A:LEU:HB3  | 3        | 0.32          |
| (1,15)   | 1:6:A:VAL:H     | 1:43:A:LEU:HB3  | 15       | 0.32          |
| (1,1226) | 1:8:A:VAL:HG21  | 1:11:A:LEU:HD21 | 17       | 0.31          |
| (1,1226) | 1:8:A:VAL:HG21  | 1:11:A:LEU:HD22 | 17       | 0.31          |
| (1,1226) | 1:8:A:VAL:HG21  | 1:11:A:LEU:HD23 | 17       | 0.31          |
| (1,1226) | 1:8:A:VAL:HG22  | 1:11:A:LEU:HD21 | 17       | 0.31          |
| (1,1226) | 1:8:A:VAL:HG22  | 1:11:A:LEU:HD22 | 17       | 0.31          |
| (1,1226) | 1:8:A:VAL:HG22  | 1:11:A:LEU:HD23 | 17       | 0.31          |
| (1,1226) | 1:8:A:VAL:HG23  | 1:11:A:LEU:HD21 | 17       | 0.31          |
| (1,1226) | 1:8:A:VAL:HG23  | 1:11:A:LEU:HD22 | 17       | 0.31          |
| (1,1226) | 1:8:A:VAL:HG23  | 1:11:A:LEU:HD23 | 17       | 0.31          |
| (1,1202) | 1:69:A:LEU:HD21 | 1:70:A:LYS:HG2  | 18       | 0.31          |
| (1,1202) | 1:69:A:LEU:HD21 | 1:70:A:LYS:HG3  | 18       | 0.31          |
| (1,1202) | 1:69:A:LEU:HD22 | 1:70:A:LYS:HG2  | 18       | 0.31          |
| (1,1202) | 1:69:A:LEU:HD22 | 1:70:A:LYS:HG3  | 18       | 0.31          |
| (1,1202) | 1:69:A:LEU:HD23 | 1:70:A:LYS:HG2  | 18       | 0.31          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1202) | 1:69:A:LEU:HD23 | 1:70:A:LYS:HG3  | 18       | 0.31          |
| (1,1024) | 1:29:A:PRO:HB3  | 1:44:A:GLU:H    | 3        | 0.31          |
| (1,1024) | 1:29:A:PRO:HB3  | 1:44:A:GLU:H    | 6        | 0.31          |
| (1,1024) | 1:29:A:PRO:HB3  | 1:44:A:GLU:H    | 13       | 0.31          |
| (1,1024) | 1:29:A:PRO:HB3  | 1:44:A:GLU:H    | 19       | 0.31          |
| (1,1012) | 1:65:A:HIS:HB3  | 1:76:A:VAL:HG21 | 1        | 0.31          |
| (1,1012) | 1:65:A:HIS:HB3  | 1:76:A:VAL:HG22 | 1        | 0.31          |
| (1,1012) | 1:65:A:HIS:HB3  | 1:76:A:VAL:HG23 | 1        | 0.31          |
| (1,1011) | 1:65:A:HIS:HB3  | 1:76:A:VAL:HB   | 12       | 0.31          |
| (1,1011) | 1:65:A:HIS:HB3  | 1:76:A:VAL:HB   | 20       | 0.31          |
| (1,890)  | 1:59:A:ASP:HA   | 1:62:A:LEU:HB3  | 4        | 0.31          |
| (1,787)  | 1:11:A:LEU:HB2  | 1:12:A:PRO:HD2  | 13       | 0.31          |
| (1,744)  | 1:38:A:LYS:HA   | 1:38:A:LYS:HG3  | 14       | 0.31          |
| (1,732)  | 1:31:A:GLN:HA   | 1:31:A:GLN:HG2  | 5        | 0.31          |
| (1,592)  | 1:10:A:SER:H    | 1:10:A:SER:HB3  | 3        | 0.31          |
| (1,592)  | 1:10:A:SER:H    | 1:10:A:SER:HB3  | 9        | 0.31          |
| (1,592)  | 1:10:A:SER:H    | 1:10:A:SER:HB3  | 10       | 0.31          |
| (1,566)  | 1:59:A:ASP:HB2  | 1:60:A:ILE:HA   | 5        | 0.31          |
| (1,468)  | 1:64:A:GLN:H    | 1:65:A:HIS:HB3  | 11       | 0.31          |
| (1,328)  | 1:62:A:LEU:H    | 1:62:A:LEU:HB3  | 9        | 0.31          |
| (1,328)  | 1:62:A:LEU:H    | 1:62:A:LEU:HB3  | 19       | 0.31          |
| (1,325)  | 1:49:A:LYS:H    | 1:49:A:LYS:HG3  | 4        | 0.31          |
| (1,304)  | 1:56:A:ARG:H    | 1:59:A:ASP:HB3  | 17       | 0.31          |
| (1,197)  | 1:23:A:HIS:H    | 1:23:A:HIS:HB3  | 18       | 0.31          |
| (1,180)  | 1:72:A:LYS:H    | 1:72:A:LYS:HG3  | 6        | 0.31          |
| (1,149)  | 1:23:A:HIS:HB2  | 1:25:A:LYS:H    | 3        | 0.31          |
| (1,1336) | 1:59:A:ASP:HB3  | 1:60:A:ILE:HD11 | 15       | 0.3           |
| (1,1336) | 1:59:A:ASP:HB3  | 1:60:A:ILE:HD12 | 15       | 0.3           |
| (1,1336) | 1:59:A:ASP:HB3  | 1:60:A:ILE:HD13 | 15       | 0.3           |
| (1,1313) | 1:58:A:MET:HB3  | 1:58:A:MET:HE1  | 7        | 0.3           |
| (1,1313) | 1:58:A:MET:HB3  | 1:58:A:MET:HE2  | 7        | 0.3           |
| (1,1313) | 1:58:A:MET:HB3  | 1:58:A:MET:HE3  | 7        | 0.3           |
| (1,1145) | 1:68:A:LEU:HD21 | 1:71:A:GLU:H    | 7        | 0.3           |
| (1,1145) | 1:68:A:LEU:HD22 | 1:71:A:GLU:H    | 7        | 0.3           |
| (1,1145) | 1:68:A:LEU:HD23 | 1:71:A:GLU:H    | 7        | 0.3           |
| (1,1030) | 1:29:A:PRO:HB2  | 1:43:A:LEU:HB2  | 3        | 0.3           |
| (1,1030) | 1:29:A:PRO:HB2  | 1:43:A:LEU:HB2  | 6        | 0.3           |
| (1,1030) | 1:29:A:PRO:HB2  | 1:43:A:LEU:HB2  | 17       | 0.3           |
| (1,1024) | 1:29:A:PRO:HB3  | 1:44:A:GLU:H    | 14       | 0.3           |
| (1,1012) | 1:65:A:HIS:HB3  | 1:76:A:VAL:HG21 | 3        | 0.3           |
| (1,1012) | 1:65:A:HIS:HB3  | 1:76:A:VAL:HG22 | 3        | 0.3           |
| (1,1012) | 1:65:A:HIS:HB3  | 1:76:A:VAL:HG23 | 3        | 0.3           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1012) | 1:65:A:HIS:HB3  | 1:76:A:VAL:HG21 | 19       | 0.3           |
| (1,1012) | 1:65:A:HIS:HB3  | 1:76:A:VAL:HG22 | 19       | 0.3           |
| (1,1012) | 1:65:A:HIS:HB3  | 1:76:A:VAL:HG23 | 19       | 0.3           |
| (1,957)  | 1:6:A:VAL:HB    | 1:43:A:LEU:HB3  | 2        | 0.3           |
| (1,957)  | 1:6:A:VAL:HB    | 1:43:A:LEU:HB3  | 18       | 0.3           |
| (1,820)  | 1:68:A:LEU:HB2  | 1:71:A:GLU:H    | 17       | 0.3           |
| (1,808)  | 1:9:A:GLY:HA2   | 1:40:A:ILE:HG13 | 8        | 0.3           |
| (1,808)  | 1:9:A:GLY:HA2   | 1:40:A:ILE:HG13 | 10       | 0.3           |
| (1,592)  | 1:10:A:SER:H    | 1:10:A:SER:HB3  | 2        | 0.3           |
| (1,440)  | 1:25:A:LYS:HB2  | 1:27:A:SER:H    | 4        | 0.3           |
| (1,440)  | 1:25:A:LYS:HB2  | 1:27:A:SER:H    | 5        | 0.3           |
| (1,328)  | 1:62:A:LEU:H    | 1:62:A:LEU:HB3  | 8        | 0.3           |
| (1,328)  | 1:62:A:LEU:H    | 1:62:A:LEU:HB3  | 20       | 0.3           |
| (1,312)  | 1:58:A:MET:H    | 1:58:A:MET:HB3  | 15       | 0.3           |
| (1,290)  | 1:27:A:SER:HB2  | 1:60:A:ILE:H    | 10       | 0.3           |
| (1,197)  | 1:23:A:HIS:H    | 1:23:A:HIS:HB3  | 14       | 0.3           |
| (1,149)  | 1:23:A:HIS:HB2  | 1:25:A:LYS:H    | 17       | 0.3           |
| (1,88)   | 1:78:A:LEU:H    | 1:78:A:LEU:HD11 | 20       | 0.3           |
| (1,88)   | 1:78:A:LEU:H    | 1:78:A:LEU:HD12 | 20       | 0.3           |
| (1,88)   | 1:78:A:LEU:H    | 1:78:A:LEU:HD13 | 20       | 0.3           |
| (1,1226) | 1:8:A:VAL:HG21  | 1:11:A:LEU:HD21 | 19       | 0.29          |
| (1,1226) | 1:8:A:VAL:HG21  | 1:11:A:LEU:HD22 | 19       | 0.29          |
| (1,1226) | 1:8:A:VAL:HG21  | 1:11:A:LEU:HD23 | 19       | 0.29          |
| (1,1226) | 1:8:A:VAL:HG22  | 1:11:A:LEU:HD21 | 19       | 0.29          |
| (1,1226) | 1:8:A:VAL:HG22  | 1:11:A:LEU:HD22 | 19       | 0.29          |
| (1,1226) | 1:8:A:VAL:HG22  | 1:11:A:LEU:HD23 | 19       | 0.29          |
| (1,1226) | 1:8:A:VAL:HG23  | 1:11:A:LEU:HD21 | 19       | 0.29          |
| (1,1226) | 1:8:A:VAL:HG23  | 1:11:A:LEU:HD22 | 19       | 0.29          |
| (1,1226) | 1:8:A:VAL:HG23  | 1:11:A:LEU:HD23 | 19       | 0.29          |
| (1,1148) | 1:68:A:LEU:HD21 | 1:71:A:GLU:HA   | 20       | 0.29          |
| (1,1148) | 1:68:A:LEU:HD22 | 1:71:A:GLU:HA   | 20       | 0.29          |
| (1,1148) | 1:68:A:LEU:HD23 | 1:71:A:GLU:HA   | 20       | 0.29          |
| (1,1132) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD11 | 7        | 0.29          |
| (1,1132) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD12 | 7        | 0.29          |
| (1,1132) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD13 | 7        | 0.29          |
| (1,1084) | 1:33:A:ARG:H    | 1:33:A:ARG:HG2  | 14       | 0.29          |
| (1,1053) | 1:12:A:PRO:HG2  | 1:70:A:LYS:HD2  | 1        | 0.29          |
| (1,1053) | 1:12:A:PRO:HG2  | 1:70:A:LYS:HD3  | 1        | 0.29          |
| (1,1053) | 1:12:A:PRO:HG2  | 1:70:A:LYS:HD2  | 19       | 0.29          |
| (1,1053) | 1:12:A:PRO:HG2  | 1:70:A:LYS:HD3  | 19       | 0.29          |
| (1,1012) | 1:65:A:HIS:HB3  | 1:76:A:VAL:HG21 | 8        | 0.29          |
| (1,1012) | 1:65:A:HIS:HB3  | 1:76:A:VAL:HG22 | 8        | 0.29          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1012) | 1:65:A:HIS:HB3  | 1:76:A:VAL:HG23 | 8        | 0.29          |
| (1,1011) | 1:65:A:HIS:HB3  | 1:76:A:VAL:HB   | 11       | 0.29          |
| (1,1011) | 1:65:A:HIS:HB3  | 1:76:A:VAL:HB   | 14       | 0.29          |
| (1,957)  | 1:6:A:VAL:HB    | 1:43:A:LEU:HB3  | 4        | 0.29          |
| (1,892)  | 1:62:A:LEU:HB2  | 1:63:A:LEU:HA   | 9        | 0.29          |
| (1,890)  | 1:59:A:ASP:HA   | 1:62:A:LEU:HB3  | 3        | 0.29          |
| (1,670)  | 1:20:A:LEU:HA   | 1:23:A:HIS:HB3  | 12       | 0.29          |
| (1,592)  | 1:10:A:SER:H    | 1:10:A:SER:HB3  | 5        | 0.29          |
| (1,592)  | 1:10:A:SER:H    | 1:10:A:SER:HB3  | 7        | 0.29          |
| (1,592)  | 1:10:A:SER:H    | 1:10:A:SER:HB3  | 19       | 0.29          |
| (1,149)  | 1:23:A:HIS:HB2  | 1:25:A:LYS:H    | 8        | 0.29          |
| (1,15)   | 1:6:A:VAL:H     | 1:43:A:LEU:HB3  | 2        | 0.29          |
| (1,15)   | 1:6:A:VAL:H     | 1:43:A:LEU:HB3  | 7        | 0.29          |
| (2,2)    | 1:76:A:VAL:N    | 1:65:A:HIS:HD2  | 16       | 0.28          |
| (1,1226) | 1:8:A:VAL:HG21  | 1:11:A:LEU:HD21 | 16       | 0.28          |
| (1,1226) | 1:8:A:VAL:HG21  | 1:11:A:LEU:HD22 | 16       | 0.28          |
| (1,1226) | 1:8:A:VAL:HG21  | 1:11:A:LEU:HD23 | 16       | 0.28          |
| (1,1226) | 1:8:A:VAL:HG22  | 1:11:A:LEU:HD21 | 16       | 0.28          |
| (1,1226) | 1:8:A:VAL:HG22  | 1:11:A:LEU:HD22 | 16       | 0.28          |
| (1,1226) | 1:8:A:VAL:HG22  | 1:11:A:LEU:HD23 | 16       | 0.28          |
| (1,1226) | 1:8:A:VAL:HG23  | 1:11:A:LEU:HD21 | 16       | 0.28          |
| (1,1226) | 1:8:A:VAL:HG23  | 1:11:A:LEU:HD22 | 16       | 0.28          |
| (1,1226) | 1:8:A:VAL:HG23  | 1:11:A:LEU:HD23 | 16       | 0.28          |
| (1,1160) | 1:78:A:LEU:HD21 | 1:79:A:THR:H    | 4        | 0.28          |
| (1,1160) | 1:78:A:LEU:HD22 | 1:79:A:THR:H    | 4        | 0.28          |
| (1,1160) | 1:78:A:LEU:HD23 | 1:79:A:THR:H    | 4        | 0.28          |
| (1,1145) | 1:68:A:LEU:HD21 | 1:71:A:GLU:H    | 5        | 0.28          |
| (1,1145) | 1:68:A:LEU:HD22 | 1:71:A:GLU:H    | 5        | 0.28          |
| (1,1145) | 1:68:A:LEU:HD23 | 1:71:A:GLU:H    | 5        | 0.28          |
| (1,1121) | 1:40:A:ILE:HG12 | 1:42:A:PHE:HE1  | 3        | 0.28          |
| (1,1121) | 1:40:A:ILE:HG12 | 1:42:A:PHE:HE2  | 3        | 0.28          |
| (1,1071) | 1:24:A:PHE:HE1  | 1:64:A:GLN:HB3  | 12       | 0.28          |
| (1,1071) | 1:24:A:PHE:HE2  | 1:64:A:GLN:HB3  | 12       | 0.28          |
| (1,1040) | 1:12:A:PRO:HG2  | 1:70:A:LYS:HB3  | 6        | 0.28          |
| (1,1030) | 1:29:A:PRO:HB2  | 1:43:A:LEU:HB2  | 18       | 0.28          |
| (1,1024) | 1:29:A:PRO:HB3  | 1:44:A:GLU:H    | 15       | 0.28          |
| (1,1024) | 1:29:A:PRO:HB3  | 1:44:A:GLU:H    | 18       | 0.28          |
| (1,1011) | 1:65:A:HIS:HB3  | 1:76:A:VAL:HB   | 1        | 0.28          |
| (1,957)  | 1:6:A:VAL:HB    | 1:43:A:LEU:HB3  | 6        | 0.28          |
| (1,957)  | 1:6:A:VAL:HB    | 1:43:A:LEU:HB3  | 13       | 0.28          |
| (1,924)  | 1:37:A:ASP:HB2  | 1:38:A:LYS:HA   | 19       | 0.28          |
| (1,789)  | 1:11:A:LEU:HB3  | 1:39:A:GLY:HA2  | 9        | 0.28          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,787)  | 1:11:A:LEU:HB2  | 1:12:A:PRO:HD2  | 15       | 0.28          |
| (1,644)  | 1:56:A:ARG:HA   | 1:59:A:ASP:HB3  | 17       | 0.28          |
| (1,592)  | 1:10:A:SER:H    | 1:10:A:SER:HB3  | 17       | 0.28          |
| (1,592)  | 1:10:A:SER:H    | 1:10:A:SER:HB3  | 18       | 0.28          |
| (1,489)  | 1:10:A:SER:HB3  | 1:75:A:ASN:HD22 | 10       | 0.28          |
| (1,304)  | 1:56:A:ARG:H    | 1:59:A:ASP:HB3  | 9        | 0.28          |
| (1,197)  | 1:23:A:HIS:H    | 1:23:A:HIS:HB3  | 7        | 0.28          |
| (1,180)  | 1:72:A:LYS:H    | 1:72:A:LYS:HG3  | 1        | 0.28          |
| (1,69)   | 1:69:A:LEU:HB2  | 1:70:A:LYS:H    | 15       | 0.28          |
| (1,15)   | 1:6:A:VAL:H     | 1:43:A:LEU:HB3  | 18       | 0.28          |
| (1,1309) | 1:55:A:GLN:HE21 | 1:58:A:MET:HE1  | 1        | 0.27          |
| (1,1309) | 1:55:A:GLN:HE21 | 1:58:A:MET:HE2  | 1        | 0.27          |
| (1,1309) | 1:55:A:GLN:HE21 | 1:58:A:MET:HE3  | 1        | 0.27          |
| (1,1163) | 1:4:A:PHE:HB2   | 1:78:A:LEU:HD21 | 9        | 0.27          |
| (1,1163) | 1:4:A:PHE:HB2   | 1:78:A:LEU:HD22 | 9        | 0.27          |
| (1,1163) | 1:4:A:PHE:HB2   | 1:78:A:LEU:HD23 | 9        | 0.27          |
| (1,1163) | 1:4:A:PHE:HB3   | 1:78:A:LEU:HD21 | 9        | 0.27          |
| (1,1163) | 1:4:A:PHE:HB3   | 1:78:A:LEU:HD22 | 9        | 0.27          |
| (1,1163) | 1:4:A:PHE:HB3   | 1:78:A:LEU:HD23 | 9        | 0.27          |
| (1,1160) | 1:78:A:LEU:HD21 | 1:79:A:THR:H    | 8        | 0.27          |
| (1,1160) | 1:78:A:LEU:HD22 | 1:79:A:THR:H    | 8        | 0.27          |
| (1,1160) | 1:78:A:LEU:HD23 | 1:79:A:THR:H    | 8        | 0.27          |
| (1,1132) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD11 | 4        | 0.27          |
| (1,1132) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD12 | 4        | 0.27          |
| (1,1132) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD13 | 4        | 0.27          |
| (1,1011) | 1:65:A:HIS:HB3  | 1:76:A:VAL:HB   | 7        | 0.27          |
| (1,789)  | 1:11:A:LEU:HB3  | 1:39:A:GLY:HA2  | 7        | 0.27          |
| (1,566)  | 1:59:A:ASP:HB2  | 1:60:A:ILE:HA   | 9        | 0.27          |
| (1,468)  | 1:64:A:GLN:H    | 1:65:A:HIS:HB3  | 13       | 0.27          |
| (1,440)  | 1:25:A:LYS:HB2  | 1:27:A:SER:H    | 17       | 0.27          |
| (1,343)  | 1:68:A:LEU:H    | 1:68:A:LEU:HB3  | 6        | 0.27          |
| (1,312)  | 1:58:A:MET:H    | 1:58:A:MET:HB3  | 13       | 0.27          |
| (1,180)  | 1:72:A:LYS:H    | 1:72:A:LYS:HG3  | 15       | 0.27          |
| (1,180)  | 1:72:A:LYS:H    | 1:72:A:LYS:HG3  | 20       | 0.27          |
| (1,15)   | 1:6:A:VAL:H     | 1:43:A:LEU:HB3  | 4        | 0.27          |
| (1,15)   | 1:6:A:VAL:H     | 1:43:A:LEU:HB3  | 12       | 0.27          |
| (1,15)   | 1:6:A:VAL:H     | 1:43:A:LEU:HB3  | 13       | 0.27          |
| (2,1)    | 1:76:A:VAL:N    | 1:65:A:HIS:HE2  | 2        | 0.26          |
| (2,1)    | 1:76:A:VAL:N    | 1:65:A:HIS:HE2  | 17       | 0.26          |
| (1,1163) | 1:4:A:PHE:HB2   | 1:78:A:LEU:HD21 | 15       | 0.26          |
| (1,1163) | 1:4:A:PHE:HB2   | 1:78:A:LEU:HD22 | 15       | 0.26          |
| (1,1163) | 1:4:A:PHE:HB2   | 1:78:A:LEU:HD23 | 15       | 0.26          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1163) | 1:4:A:PHE:HB3   | 1:78:A:LEU:HD21 | 15       | 0.26          |
| (1,1163) | 1:4:A:PHE:HB3   | 1:78:A:LEU:HD22 | 15       | 0.26          |
| (1,1163) | 1:4:A:PHE:HB3   | 1:78:A:LEU:HD23 | 15       | 0.26          |
| (1,1128) | 1:20:A:LEU:HD11 | 1:34:A:LEU:HB2  | 11       | 0.26          |
| (1,1128) | 1:20:A:LEU:HD12 | 1:34:A:LEU:HB2  | 11       | 0.26          |
| (1,1128) | 1:20:A:LEU:HD13 | 1:34:A:LEU:HB2  | 11       | 0.26          |
| (1,1121) | 1:40:A:ILE:HG12 | 1:42:A:PHE:HE1  | 7        | 0.26          |
| (1,1121) | 1:40:A:ILE:HG12 | 1:42:A:PHE:HE2  | 7        | 0.26          |
| (1,1084) | 1:33:A:ARG:H    | 1:33:A:ARG:HG2  | 4        | 0.26          |
| (1,1041) | 1:70:A:LYS:HB3  | 1:71:A:GLU:H    | 16       | 0.26          |
| (1,1040) | 1:12:A:PRO:HG2  | 1:70:A:LYS:HB3  | 13       | 0.26          |
| (1,1012) | 1:65:A:HIS:HB3  | 1:76:A:VAL:HG21 | 7        | 0.26          |
| (1,1012) | 1:65:A:HIS:HB3  | 1:76:A:VAL:HG22 | 7        | 0.26          |
| (1,1012) | 1:65:A:HIS:HB3  | 1:76:A:VAL:HG23 | 7        | 0.26          |
| (1,909)  | 1:59:A:ASP:HB3  | 1:60:A:ILE:HB   | 11       | 0.26          |
| (1,820)  | 1:68:A:LEU:HB2  | 1:71:A:GLU:H    | 10       | 0.26          |
| (1,808)  | 1:9:A:GLY:HA2   | 1:40:A:ILE:HG13 | 18       | 0.26          |
| (1,787)  | 1:11:A:LEU:HB2  | 1:12:A:PRO:HD2  | 10       | 0.26          |
| (1,787)  | 1:11:A:LEU:HB2  | 1:12:A:PRO:HD2  | 16       | 0.26          |
| (1,711)  | 1:68:A:LEU:HD11 | 1:73:A:LYS:HA   | 3        | 0.26          |
| (1,711)  | 1:68:A:LEU:HD12 | 1:73:A:LYS:HA   | 3        | 0.26          |
| (1,711)  | 1:68:A:LEU:HD13 | 1:73:A:LYS:HA   | 3        | 0.26          |
| (1,592)  | 1:10:A:SER:H    | 1:10:A:SER:HB3  | 14       | 0.26          |
| (1,592)  | 1:10:A:SER:H    | 1:10:A:SER:HB3  | 20       | 0.26          |
| (1,440)  | 1:25:A:LYS:HB2  | 1:27:A:SER:H    | 18       | 0.26          |
| (1,423)  | 1:55:A:GLN:HE22 | 1:59:A:ASP:HB3  | 6        | 0.26          |
| (1,312)  | 1:58:A:MET:H    | 1:58:A:MET:HB3  | 14       | 0.26          |
| (1,149)  | 1:23:A:HIS:HB2  | 1:25:A:LYS:H    | 18       | 0.26          |
| (1,15)   | 1:6:A:VAL:H     | 1:43:A:LEU:HB3  | 6        | 0.26          |
| (1,15)   | 1:6:A:VAL:H     | 1:43:A:LEU:HB3  | 16       | 0.26          |
| (2,2)    | 1:76:A:VAL:N    | 1:65:A:HIS:HD2  | 2        | 0.25          |
| (1,1232) | 1:6:A:VAL:HG11  | 1:7:A:PHE:HB2   | 3        | 0.25          |
| (1,1232) | 1:6:A:VAL:HG12  | 1:7:A:PHE:HB2   | 3        | 0.25          |
| (1,1232) | 1:6:A:VAL:HG13  | 1:7:A:PHE:HB2   | 3        | 0.25          |
| (1,1134) | 1:69:A:LEU:HD11 | 1:74:A:ILE:HD11 | 7        | 0.25          |
| (1,1134) | 1:69:A:LEU:HD11 | 1:74:A:ILE:HD12 | 7        | 0.25          |
| (1,1134) | 1:69:A:LEU:HD11 | 1:74:A:ILE:HD13 | 7        | 0.25          |
| (1,1134) | 1:69:A:LEU:HD12 | 1:74:A:ILE:HD11 | 7        | 0.25          |
| (1,1134) | 1:69:A:LEU:HD12 | 1:74:A:ILE:HD12 | 7        | 0.25          |
| (1,1134) | 1:69:A:LEU:HD12 | 1:74:A:ILE:HD13 | 7        | 0.25          |
| (1,1134) | 1:69:A:LEU:HD13 | 1:74:A:ILE:HD11 | 7        | 0.25          |
| (1,1134) | 1:69:A:LEU:HD13 | 1:74:A:ILE:HD12 | 7        | 0.25          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1134) | 1:69:A:LEU:HD13 | 1:74:A:ILE:HD13 | 7        | 0.25          |
| (1,1127) | 1:20:A:LEU:HD11 | 1:34:A:LEU:HG   | 6        | 0.25          |
| (1,1127) | 1:20:A:LEU:HD12 | 1:34:A:LEU:HG   | 6        | 0.25          |
| (1,1127) | 1:20:A:LEU:HD13 | 1:34:A:LEU:HG   | 6        | 0.25          |
| (1,1127) | 1:20:A:LEU:HD11 | 1:34:A:LEU:HG   | 15       | 0.25          |
| (1,1127) | 1:20:A:LEU:HD12 | 1:34:A:LEU:HG   | 15       | 0.25          |
| (1,1127) | 1:20:A:LEU:HD13 | 1:34:A:LEU:HG   | 15       | 0.25          |
| (1,1121) | 1:40:A:ILE:HG12 | 1:42:A:PHE:HE1  | 15       | 0.25          |
| (1,1121) | 1:40:A:ILE:HG12 | 1:42:A:PHE:HE2  | 15       | 0.25          |
| (1,1012) | 1:65:A:HIS:HB3  | 1:76:A:VAL:HG21 | 15       | 0.25          |
| (1,1012) | 1:65:A:HIS:HB3  | 1:76:A:VAL:HG22 | 15       | 0.25          |
| (1,1012) | 1:65:A:HIS:HB3  | 1:76:A:VAL:HG23 | 15       | 0.25          |
| (1,1011) | 1:65:A:HIS:HB3  | 1:76:A:VAL:HB   | 19       | 0.25          |
| (1,1003) | 1:55:A:GLN:HA   | 1:58:A:MET:HB3  | 4        | 0.25          |
| (1,909)  | 1:59:A:ASP:HB3  | 1:60:A:ILE:HB   | 6        | 0.25          |
| (1,892)  | 1:62:A:LEU:HB2  | 1:63:A:LEU:HA   | 20       | 0.25          |
| (1,592)  | 1:10:A:SER:H    | 1:10:A:SER:HB3  | 11       | 0.25          |
| (1,312)  | 1:58:A:MET:H    | 1:58:A:MET:HB3  | 2        | 0.25          |
| (1,312)  | 1:58:A:MET:H    | 1:58:A:MET:HB3  | 6        | 0.25          |
| (1,312)  | 1:58:A:MET:H    | 1:58:A:MET:HB3  | 8        | 0.25          |
| (1,181)  | 1:68:A:LEU:HB2  | 1:72:A:LYS:H    | 10       | 0.25          |
| (1,180)  | 1:72:A:LYS:H    | 1:72:A:LYS:HG3  | 9        | 0.25          |
| (1,88)   | 1:78:A:LEU:H    | 1:78:A:LEU:HD11 | 14       | 0.25          |
| (1,88)   | 1:78:A:LEU:H    | 1:78:A:LEU:HD12 | 14       | 0.25          |
| (1,88)   | 1:78:A:LEU:H    | 1:78:A:LEU:HD13 | 14       | 0.25          |
| (1,1313) | 1:58:A:MET:HB3  | 1:58:A:MET:HE1  | 9        | 0.24          |
| (1,1313) | 1:58:A:MET:HB3  | 1:58:A:MET:HE2  | 9        | 0.24          |
| (1,1313) | 1:58:A:MET:HB3  | 1:58:A:MET:HE3  | 9        | 0.24          |
| (1,1241) | 1:18:A:VAL:H    | 1:18:A:VAL:HG21 | 18       | 0.24          |
| (1,1241) | 1:18:A:VAL:H    | 1:18:A:VAL:HG22 | 18       | 0.24          |
| (1,1241) | 1:18:A:VAL:H    | 1:18:A:VAL:HG23 | 18       | 0.24          |
| (1,1012) | 1:65:A:HIS:HB3  | 1:76:A:VAL:HG21 | 11       | 0.24          |
| (1,1012) | 1:65:A:HIS:HB3  | 1:76:A:VAL:HG22 | 11       | 0.24          |
| (1,1012) | 1:65:A:HIS:HB3  | 1:76:A:VAL:HG23 | 11       | 0.24          |
| (1,1003) | 1:55:A:GLN:HA   | 1:58:A:MET:HB3  | 1        | 0.24          |
| (1,957)  | 1:6:A:VAL:HB    | 1:43:A:LEU:HB3  | 5        | 0.24          |
| (1,892)  | 1:62:A:LEU:HB2  | 1:63:A:LEU:HA   | 14       | 0.24          |
| (1,890)  | 1:59:A:ASP:HA   | 1:62:A:LEU:HB3  | 8        | 0.24          |
| (1,787)  | 1:11:A:LEU:HB2  | 1:12:A:PRO:HD2  | 6        | 0.24          |
| (1,468)  | 1:64:A:GLN:H    | 1:65:A:HIS:HB3  | 7        | 0.24          |
| (1,418)  | 1:80:A:VAL:HG21 | 1:82:A:GLY:H    | 12       | 0.24          |
| (1,418)  | 1:80:A:VAL:HG22 | 1:82:A:GLY:H    | 12       | 0.24          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,418)  | 1:80:A:VAL:HG23 | 1:82:A:GLY:H    | 12       | 0.24          |
| (1,378)  | 1:38:A:LYS:H    | 1:38:A:LYS:HG3  | 20       | 0.24          |
| (1,343)  | 1:68:A:LEU:H    | 1:68:A:LEU:HB3  | 1        | 0.24          |
| (1,312)  | 1:58:A:MET:H    | 1:58:A:MET:HB3  | 18       | 0.24          |
| (1,197)  | 1:23:A:HIS:H    | 1:23:A:HIS:HB3  | 17       | 0.24          |
| (1,135)  | 1:32:A:ILE:H    | 1:32:A:ILE:HG12 | 12       | 0.24          |
| (1,69)   | 1:69:A:LEU:HB2  | 1:70:A:LYS:H    | 10       | 0.24          |
| (1,69)   | 1:69:A:LEU:HB2  | 1:70:A:LYS:H    | 14       | 0.24          |
| (1,69)   | 1:69:A:LEU:HB2  | 1:70:A:LYS:H    | 17       | 0.24          |
| (1,53)   | 1:68:A:LEU:HB2  | 1:69:A:LEU:H    | 1        | 0.24          |
| (1,1309) | 1:55:A:GLN:HE21 | 1:58:A:MET:HE1  | 19       | 0.23          |
| (1,1309) | 1:55:A:GLN:HE21 | 1:58:A:MET:HE2  | 19       | 0.23          |
| (1,1309) | 1:55:A:GLN:HE21 | 1:58:A:MET:HE3  | 19       | 0.23          |
| (1,1241) | 1:18:A:VAL:H    | 1:18:A:VAL:HG21 | 2        | 0.23          |
| (1,1241) | 1:18:A:VAL:H    | 1:18:A:VAL:HG22 | 2        | 0.23          |
| (1,1241) | 1:18:A:VAL:H    | 1:18:A:VAL:HG23 | 2        | 0.23          |
| (1,1241) | 1:18:A:VAL:H    | 1:18:A:VAL:HG21 | 14       | 0.23          |
| (1,1241) | 1:18:A:VAL:H    | 1:18:A:VAL:HG22 | 14       | 0.23          |
| (1,1241) | 1:18:A:VAL:H    | 1:18:A:VAL:HG23 | 14       | 0.23          |
| (1,1226) | 1:8:A:VAL:HG21  | 1:11:A:LEU:HD21 | 14       | 0.23          |
| (1,1226) | 1:8:A:VAL:HG21  | 1:11:A:LEU:HD22 | 14       | 0.23          |
| (1,1226) | 1:8:A:VAL:HG21  | 1:11:A:LEU:HD23 | 14       | 0.23          |
| (1,1226) | 1:8:A:VAL:HG22  | 1:11:A:LEU:HD21 | 14       | 0.23          |
| (1,1226) | 1:8:A:VAL:HG22  | 1:11:A:LEU:HD22 | 14       | 0.23          |
| (1,1226) | 1:8:A:VAL:HG22  | 1:11:A:LEU:HD23 | 14       | 0.23          |
| (1,1226) | 1:8:A:VAL:HG23  | 1:11:A:LEU:HD21 | 14       | 0.23          |
| (1,1226) | 1:8:A:VAL:HG23  | 1:11:A:LEU:HD22 | 14       | 0.23          |
| (1,1226) | 1:8:A:VAL:HG23  | 1:11:A:LEU:HD23 | 14       | 0.23          |
| (1,1201) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD21 | 9        | 0.23          |
| (1,1201) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD22 | 9        | 0.23          |
| (1,1201) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD23 | 9        | 0.23          |
| (1,1163) | 1:4:A:PHE:HB2   | 1:78:A:LEU:HD21 | 6        | 0.23          |
| (1,1163) | 1:4:A:PHE:HB2   | 1:78:A:LEU:HD22 | 6        | 0.23          |
| (1,1163) | 1:4:A:PHE:HB2   | 1:78:A:LEU:HD23 | 6        | 0.23          |
| (1,1163) | 1:4:A:PHE:HB3   | 1:78:A:LEU:HD21 | 6        | 0.23          |
| (1,1163) | 1:4:A:PHE:HB3   | 1:78:A:LEU:HD22 | 6        | 0.23          |
| (1,1163) | 1:4:A:PHE:HB3   | 1:78:A:LEU:HD23 | 6        | 0.23          |
| (1,1160) | 1:78:A:LEU:HD21 | 1:79:A:THR:H    | 19       | 0.23          |
| (1,1160) | 1:78:A:LEU:HD22 | 1:79:A:THR:H    | 19       | 0.23          |
| (1,1160) | 1:78:A:LEU:HD23 | 1:79:A:THR:H    | 19       | 0.23          |
| (1,1084) | 1:33:A:ARG:H    | 1:33:A:ARG:HG2  | 18       | 0.23          |
| (1,1071) | 1:24:A:PHE:HE1  | 1:64:A:GLN:HB3  | 5        | 0.23          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1071) | 1:24:A:PHE:HE2  | 1:64:A:GLN:HB3  | 5        | 0.23          |
| (1,1053) | 1:12:A:PRO:HG2  | 1:70:A:LYS:HD2  | 5        | 0.23          |
| (1,1053) | 1:12:A:PRO:HG2  | 1:70:A:LYS:HD3  | 5        | 0.23          |
| (1,1041) | 1:70:A:LYS:HB3  | 1:71:A:GLU:H    | 5        | 0.23          |
| (1,1041) | 1:70:A:LYS:HB3  | 1:71:A:GLU:H    | 13       | 0.23          |
| (1,1030) | 1:29:A:PRO:HB2  | 1:43:A:LEU:HB2  | 13       | 0.23          |
| (1,1021) | 1:58:A:MET:HG2  | 1:78:A:LEU:HD11 | 12       | 0.23          |
| (1,1021) | 1:58:A:MET:HG2  | 1:78:A:LEU:HD12 | 12       | 0.23          |
| (1,1021) | 1:58:A:MET:HG2  | 1:78:A:LEU:HD13 | 12       | 0.23          |
| (1,808)  | 1:9:A:GLY:HA2   | 1:40:A:ILE:HG13 | 3        | 0.23          |
| (1,808)  | 1:9:A:GLY:HA2   | 1:40:A:ILE:HG13 | 7        | 0.23          |
| (1,808)  | 1:9:A:GLY:HA2   | 1:40:A:ILE:HG13 | 11       | 0.23          |
| (1,808)  | 1:9:A:GLY:HA2   | 1:40:A:ILE:HG13 | 20       | 0.23          |
| (1,789)  | 1:11:A:LEU:HB3  | 1:39:A:GLY:HA2  | 20       | 0.23          |
| (1,732)  | 1:31:A:GLN:HA   | 1:31:A:GLN:HG2  | 3        | 0.23          |
| (1,598)  | 1:12:A:PRO:HA   | 1:72:A:LYS:HG2  | 9        | 0.23          |
| (1,592)  | 1:10:A:SER:H    | 1:10:A:SER:HB3  | 13       | 0.23          |
| (1,461)  | 1:29:A:PRO:HB3  | 1:31:A:GLN:H    | 15       | 0.23          |
| (1,312)  | 1:58:A:MET:H    | 1:58:A:MET:HB3  | 3        | 0.23          |
| (1,197)  | 1:23:A:HIS:H    | 1:23:A:HIS:HB3  | 8        | 0.23          |
| (1,181)  | 1:68:A:LEU:HB2  | 1:72:A:LYS:H    | 19       | 0.23          |
| (1,149)  | 1:23:A:HIS:HB2  | 1:25:A:LYS:H    | 16       | 0.23          |
| (1,15)   | 1:6:A:VAL:H     | 1:43:A:LEU:HB3  | 10       | 0.23          |
| (2,2)    | 1:76:A:VAL:N    | 1:65:A:HIS:HD2  | 18       | 0.22          |
| (1,1255) | 1:18:A:VAL:HG11 | 1:22:A:ASN:HB2  | 16       | 0.22          |
| (1,1255) | 1:18:A:VAL:HG11 | 1:22:A:ASN:HB3  | 16       | 0.22          |
| (1,1255) | 1:18:A:VAL:HG12 | 1:22:A:ASN:HB2  | 16       | 0.22          |
| (1,1255) | 1:18:A:VAL:HG12 | 1:22:A:ASN:HB3  | 16       | 0.22          |
| (1,1255) | 1:18:A:VAL:HG13 | 1:22:A:ASN:HB2  | 16       | 0.22          |
| (1,1255) | 1:18:A:VAL:HG13 | 1:22:A:ASN:HB3  | 16       | 0.22          |
| (1,1255) | 1:18:A:VAL:HG11 | 1:22:A:ASN:HB2  | 20       | 0.22          |
| (1,1255) | 1:18:A:VAL:HG11 | 1:22:A:ASN:HB3  | 20       | 0.22          |
| (1,1255) | 1:18:A:VAL:HG12 | 1:22:A:ASN:HB2  | 20       | 0.22          |
| (1,1255) | 1:18:A:VAL:HG12 | 1:22:A:ASN:HB3  | 20       | 0.22          |
| (1,1255) | 1:18:A:VAL:HG13 | 1:22:A:ASN:HB2  | 20       | 0.22          |
| (1,1255) | 1:18:A:VAL:HG13 | 1:22:A:ASN:HB3  | 20       | 0.22          |
| (1,1241) | 1:18:A:VAL:H    | 1:18:A:VAL:HG21 | 3        | 0.22          |
| (1,1241) | 1:18:A:VAL:H    | 1:18:A:VAL:HG22 | 3        | 0.22          |
| (1,1241) | 1:18:A:VAL:H    | 1:18:A:VAL:HG23 | 3        | 0.22          |
| (1,1241) | 1:18:A:VAL:H    | 1:18:A:VAL:HG21 | 4        | 0.22          |
| (1,1241) | 1:18:A:VAL:H    | 1:18:A:VAL:HG22 | 4        | 0.22          |
| (1,1241) | 1:18:A:VAL:H    | 1:18:A:VAL:HG23 | 4        | 0.22          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1241) | 1:18:A:VAL:H    | 1:18:A:VAL:HG21 | 7        | 0.22          |
| (1,1241) | 1:18:A:VAL:H    | 1:18:A:VAL:HG22 | 7        | 0.22          |
| (1,1241) | 1:18:A:VAL:H    | 1:18:A:VAL:HG23 | 7        | 0.22          |
| (1,1084) | 1:33:A:ARG:H    | 1:33:A:ARG:HG2  | 1        | 0.22          |
| (1,1030) | 1:29:A:PRO:HB2  | 1:43:A:LEU:HB2  | 14       | 0.22          |
| (1,811)  | 1:7:A:PHE:HE1   | 1:9:A:GLY:HA2   | 9        | 0.22          |
| (1,811)  | 1:7:A:PHE:HE2   | 1:9:A:GLY:HA2   | 9        | 0.22          |
| (1,808)  | 1:9:A:GLY:HA2   | 1:40:A:ILE:HG13 | 15       | 0.22          |
| (1,806)  | 1:68:A:LEU:HA   | 1:69:A:LEU:HB3  | 14       | 0.22          |
| (1,789)  | 1:11:A:LEU:HB3  | 1:39:A:GLY:HA2  | 16       | 0.22          |
| (1,787)  | 1:11:A:LEU:HB2  | 1:12:A:PRO:HD2  | 3        | 0.22          |
| (1,787)  | 1:11:A:LEU:HB2  | 1:12:A:PRO:HD2  | 9        | 0.22          |
| (1,732)  | 1:31:A:GLN:HA   | 1:31:A:GLN:HG2  | 10       | 0.22          |
| (1,685)  | 1:13:A:ARG:HA   | 1:13:A:ARG:HB2  | 7        | 0.22          |
| (1,468)  | 1:64:A:GLN:H    | 1:65:A:HIS:HB3  | 5        | 0.22          |
| (1,418)  | 1:80:A:VAL:HG21 | 1:82:A:GLY:H    | 18       | 0.22          |
| (1,418)  | 1:80:A:VAL:HG22 | 1:82:A:GLY:H    | 18       | 0.22          |
| (1,418)  | 1:80:A:VAL:HG23 | 1:82:A:GLY:H    | 18       | 0.22          |
| (1,312)  | 1:58:A:MET:H    | 1:58:A:MET:HB3  | 4        | 0.22          |
| (1,312)  | 1:58:A:MET:H    | 1:58:A:MET:HB3  | 12       | 0.22          |
| (1,312)  | 1:58:A:MET:H    | 1:58:A:MET:HB3  | 17       | 0.22          |
| (1,222)  | 1:19:A:GLU:HB3  | 1:20:A:LEU:H    | 17       | 0.22          |
| (1,88)   | 1:78:A:LEU:H    | 1:78:A:LEU:HD11 | 19       | 0.22          |
| (1,88)   | 1:78:A:LEU:H    | 1:78:A:LEU:HD12 | 19       | 0.22          |
| (1,88)   | 1:78:A:LEU:H    | 1:78:A:LEU:HD13 | 19       | 0.22          |
| (1,15)   | 1:6:A:VAL:H     | 1:43:A:LEU:HB3  | 1        | 0.22          |
| (1,15)   | 1:6:A:VAL:H     | 1:43:A:LEU:HB3  | 20       | 0.22          |
| (2,2)    | 1:76:A:VAL:N    | 1:65:A:HIS:HD2  | 19       | 0.21          |
| (1,1241) | 1:18:A:VAL:H    | 1:18:A:VAL:HG21 | 5        | 0.21          |
| (1,1241) | 1:18:A:VAL:H    | 1:18:A:VAL:HG22 | 5        | 0.21          |
| (1,1241) | 1:18:A:VAL:H    | 1:18:A:VAL:HG23 | 5        | 0.21          |
| (1,1241) | 1:18:A:VAL:H    | 1:18:A:VAL:HG21 | 20       | 0.21          |
| (1,1241) | 1:18:A:VAL:H    | 1:18:A:VAL:HG22 | 20       | 0.21          |
| (1,1241) | 1:18:A:VAL:H    | 1:18:A:VAL:HG23 | 20       | 0.21          |
| (1,1232) | 1:6:A:VAL:HG11  | 1:7:A:PHE:HB2   | 1        | 0.21          |
| (1,1232) | 1:6:A:VAL:HG12  | 1:7:A:PHE:HB2   | 1        | 0.21          |
| (1,1232) | 1:6:A:VAL:HG13  | 1:7:A:PHE:HB2   | 1        | 0.21          |
| (1,1226) | 1:8:A:VAL:HG21  | 1:11:A:LEU:HD21 | 2        | 0.21          |
| (1,1226) | 1:8:A:VAL:HG21  | 1:11:A:LEU:HD22 | 2        | 0.21          |
| (1,1226) | 1:8:A:VAL:HG21  | 1:11:A:LEU:HD23 | 2        | 0.21          |
| (1,1226) | 1:8:A:VAL:HG22  | 1:11:A:LEU:HD21 | 2        | 0.21          |
| (1,1226) | 1:8:A:VAL:HG22  | 1:11:A:LEU:HD22 | 2        | 0.21          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1226) | 1:8:A:VAL:HG22  | 1:11:A:LEU:HD23 | 2        | 0.21          |
| (1,1226) | 1:8:A:VAL:HG23  | 1:11:A:LEU:HD21 | 2        | 0.21          |
| (1,1226) | 1:8:A:VAL:HG23  | 1:11:A:LEU:HD22 | 2        | 0.21          |
| (1,1226) | 1:8:A:VAL:HG23  | 1:11:A:LEU:HD23 | 2        | 0.21          |
| (1,1148) | 1:68:A:LEU:HD21 | 1:71:A:GLU:HA   | 9        | 0.21          |
| (1,1148) | 1:68:A:LEU:HD22 | 1:71:A:GLU:HA   | 9        | 0.21          |
| (1,1148) | 1:68:A:LEU:HD23 | 1:71:A:GLU:HA   | 9        | 0.21          |
| (1,1140) | 1:12:A:PRO:HG2  | 1:70:A:LYS:HG2  | 10       | 0.21          |
| (1,1140) | 1:12:A:PRO:HG2  | 1:70:A:LYS:HG3  | 10       | 0.21          |
| (1,1040) | 1:12:A:PRO:HG2  | 1:70:A:LYS:HB3  | 9        | 0.21          |
| (1,924)  | 1:37:A:ASP:HB2  | 1:38:A:LYS:HA   | 5        | 0.21          |
| (1,808)  | 1:9:A:GLY:HA2   | 1:40:A:ILE:HG13 | 13       | 0.21          |
| (1,808)  | 1:9:A:GLY:HA2   | 1:40:A:ILE:HG13 | 16       | 0.21          |
| (1,732)  | 1:31:A:GLN:HA   | 1:31:A:GLN:HG2  | 2        | 0.21          |
| (1,685)  | 1:13:A:ARG:HA   | 1:13:A:ARG:HB2  | 6        | 0.21          |
| (1,685)  | 1:13:A:ARG:HA   | 1:13:A:ARG:HB2  | 8        | 0.21          |
| (1,685)  | 1:13:A:ARG:HA   | 1:13:A:ARG:HB2  | 13       | 0.21          |
| (1,685)  | 1:13:A:ARG:HA   | 1:13:A:ARG:HB2  | 14       | 0.21          |
| (1,685)  | 1:13:A:ARG:HA   | 1:13:A:ARG:HB2  | 17       | 0.21          |
| (1,468)  | 1:64:A:GLN:H    | 1:65:A:HIS:HB3  | 10       | 0.21          |
| (1,440)  | 1:25:A:LYS:HB2  | 1:27:A:SER:H    | 7        | 0.21          |
| (1,440)  | 1:25:A:LYS:HB2  | 1:27:A:SER:H    | 10       | 0.21          |
| (1,304)  | 1:56:A:ARG:H    | 1:59:A:ASP:HB3  | 5        | 0.21          |
| (1,69)   | 1:69:A:LEU:HB2  | 1:70:A:LYS:H    | 8        | 0.21          |
| (1,15)   | 1:6:A:VAL:H     | 1:43:A:LEU:HB3  | 17       | 0.21          |
| (2,1)    | 1:76:A:VAL:N    | 1:65:A:HIS:HE2  | 18       | 0.2           |
| (1,1353) | 1:23:A:HIS:HB2  | 1:24:A:PHE:HD1  | 1        | 0.2           |
| (1,1353) | 1:23:A:HIS:HB2  | 1:24:A:PHE:HD2  | 1        | 0.2           |
| (1,1353) | 1:23:A:HIS:HB2  | 1:24:A:PHE:HD1  | 12       | 0.2           |
| (1,1353) | 1:23:A:HIS:HB2  | 1:24:A:PHE:HD2  | 12       | 0.2           |
| (1,1241) | 1:18:A:VAL:H    | 1:18:A:VAL:HG21 | 6        | 0.2           |
| (1,1241) | 1:18:A:VAL:H    | 1:18:A:VAL:HG22 | 6        | 0.2           |
| (1,1241) | 1:18:A:VAL:H    | 1:18:A:VAL:HG23 | 6        | 0.2           |
| (1,1241) | 1:18:A:VAL:H    | 1:18:A:VAL:HG21 | 19       | 0.2           |
| (1,1241) | 1:18:A:VAL:H    | 1:18:A:VAL:HG22 | 19       | 0.2           |
| (1,1241) | 1:18:A:VAL:H    | 1:18:A:VAL:HG23 | 19       | 0.2           |
| (1,1232) | 1:6:A:VAL:HG11  | 1:7:A:PHE:HB2   | 8        | 0.2           |
| (1,1232) | 1:6:A:VAL:HG12  | 1:7:A:PHE:HB2   | 8        | 0.2           |
| (1,1232) | 1:6:A:VAL:HG13  | 1:7:A:PHE:HB2   | 8        | 0.2           |
| (1,1226) | 1:8:A:VAL:HG21  | 1:11:A:LEU:HD21 | 20       | 0.2           |
| (1,1226) | 1:8:A:VAL:HG21  | 1:11:A:LEU:HD22 | 20       | 0.2           |
| (1,1226) | 1:8:A:VAL:HG21  | 1:11:A:LEU:HD23 | 20       | 0.2           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1226) | 1:8:A:VAL:HG22  | 1:11:A:LEU:HD21 | 20       | 0.2           |
| (1,1226) | 1:8:A:VAL:HG22  | 1:11:A:LEU:HD22 | 20       | 0.2           |
| (1,1226) | 1:8:A:VAL:HG22  | 1:11:A:LEU:HD23 | 20       | 0.2           |
| (1,1226) | 1:8:A:VAL:HG23  | 1:11:A:LEU:HD21 | 20       | 0.2           |
| (1,1226) | 1:8:A:VAL:HG23  | 1:11:A:LEU:HD22 | 20       | 0.2           |
| (1,1226) | 1:8:A:VAL:HG23  | 1:11:A:LEU:HD23 | 20       | 0.2           |
| (1,1196) | 1:34:A:LEU:HD21 | 1:36:A:ALA:H    | 4        | 0.2           |
| (1,1196) | 1:34:A:LEU:HD22 | 1:36:A:ALA:H    | 4        | 0.2           |
| (1,1196) | 1:34:A:LEU:HD23 | 1:36:A:ALA:H    | 4        | 0.2           |
| (1,1160) | 1:78:A:LEU:HD21 | 1:79:A:THR:H    | 18       | 0.2           |
| (1,1160) | 1:78:A:LEU:HD22 | 1:79:A:THR:H    | 18       | 0.2           |
| (1,1160) | 1:78:A:LEU:HD23 | 1:79:A:THR:H    | 18       | 0.2           |
| (1,1024) | 1:29:A:PRO:HB3  | 1:44:A:GLU:H    | 2        | 0.2           |
| (1,957)  | 1:6:A:VAL:HB    | 1:43:A:LEU:HB3  | 7        | 0.2           |
| (1,892)  | 1:62:A:LEU:HB2  | 1:63:A:LEU:HA   | 15       | 0.2           |
| (1,892)  | 1:62:A:LEU:HB2  | 1:63:A:LEU:HA   | 17       | 0.2           |
| (1,824)  | 1:56:A:ARG:HB2  | 1:56:A:ARG:HD2  | 16       | 0.2           |
| (1,824)  | 1:56:A:ARG:HB3  | 1:56:A:ARG:HD2  | 16       | 0.2           |
| (1,813)  | 1:33:A:ARG:HB2  | 1:33:A:ARG:HD2  | 16       | 0.2           |
| (1,811)  | 1:7:A:PHE:HE1   | 1:9:A:GLY:HA2   | 13       | 0.2           |
| (1,811)  | 1:7:A:PHE:HE2   | 1:9:A:GLY:HA2   | 13       | 0.2           |
| (1,808)  | 1:9:A:GLY:HA2   | 1:40:A:ILE:HG13 | 17       | 0.2           |
| (1,808)  | 1:9:A:GLY:HA2   | 1:40:A:ILE:HG13 | 19       | 0.2           |
| (1,789)  | 1:11:A:LEU:HB3  | 1:39:A:GLY:HA2  | 5        | 0.2           |
| (1,685)  | 1:13:A:ARG:HA   | 1:13:A:ARG:HB2  | 3        | 0.2           |
| (1,685)  | 1:13:A:ARG:HA   | 1:13:A:ARG:HB2  | 10       | 0.2           |
| (1,685)  | 1:13:A:ARG:HA   | 1:13:A:ARG:HB2  | 12       | 0.2           |
| (1,685)  | 1:13:A:ARG:HA   | 1:13:A:ARG:HB2  | 16       | 0.2           |
| (1,592)  | 1:10:A:SER:H    | 1:10:A:SER:HB3  | 12       | 0.2           |
| (1,555)  | 1:27:A:SER:HB2  | 1:60:A:ILE:HB   | 9        | 0.2           |
| (1,440)  | 1:25:A:LYS:HB2  | 1:27:A:SER:H    | 1        | 0.2           |
| (1,440)  | 1:25:A:LYS:HB2  | 1:27:A:SER:H    | 11       | 0.2           |
| (1,297)  | 1:53:A:GLY:HA3  | 1:56:A:ARG:H    | 6        | 0.2           |
| (1,290)  | 1:27:A:SER:HB2  | 1:60:A:ILE:H    | 2        | 0.2           |
| (1,290)  | 1:27:A:SER:HB2  | 1:60:A:ILE:H    | 3        | 0.2           |
| (1,222)  | 1:19:A:GLU:HB3  | 1:20:A:LEU:H    | 15       | 0.2           |
| (1,180)  | 1:72:A:LYS:H    | 1:72:A:LYS:HG3  | 3        | 0.2           |
| (1,149)  | 1:23:A:HIS:HB2  | 1:25:A:LYS:H    | 2        | 0.2           |
| (1,149)  | 1:23:A:HIS:HB2  | 1:25:A:LYS:H    | 12       | 0.2           |
| (1,69)   | 1:69:A:LEU:HB2  | 1:70:A:LYS:H    | 2        | 0.2           |
| (2,1)    | 1:76:A:VAL:N    | 1:65:A:HIS:HE2  | 16       | 0.19          |
| (1,1353) | 1:23:A:HIS:HB2  | 1:24:A:PHE:HD1  | 2        | 0.19          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1353) | 1:23:A:HIS:HB2  | 1:24:A:PHE:HD2  | 2        | 0.19          |
| (1,1353) | 1:23:A:HIS:HB2  | 1:24:A:PHE:HD1  | 8        | 0.19          |
| (1,1353) | 1:23:A:HIS:HB2  | 1:24:A:PHE:HD2  | 8        | 0.19          |
| (1,1241) | 1:18:A:VAL:H    | 1:18:A:VAL:HG21 | 16       | 0.19          |
| (1,1241) | 1:18:A:VAL:H    | 1:18:A:VAL:HG22 | 16       | 0.19          |
| (1,1241) | 1:18:A:VAL:H    | 1:18:A:VAL:HG23 | 16       | 0.19          |
| (1,1226) | 1:8:A:VAL:HG21  | 1:11:A:LEU:HD21 | 6        | 0.19          |
| (1,1226) | 1:8:A:VAL:HG21  | 1:11:A:LEU:HD22 | 6        | 0.19          |
| (1,1226) | 1:8:A:VAL:HG21  | 1:11:A:LEU:HD23 | 6        | 0.19          |
| (1,1226) | 1:8:A:VAL:HG22  | 1:11:A:LEU:HD21 | 6        | 0.19          |
| (1,1226) | 1:8:A:VAL:HG22  | 1:11:A:LEU:HD22 | 6        | 0.19          |
| (1,1226) | 1:8:A:VAL:HG22  | 1:11:A:LEU:HD23 | 6        | 0.19          |
| (1,1226) | 1:8:A:VAL:HG23  | 1:11:A:LEU:HD21 | 6        | 0.19          |
| (1,1226) | 1:8:A:VAL:HG23  | 1:11:A:LEU:HD22 | 6        | 0.19          |
| (1,1226) | 1:8:A:VAL:HG23  | 1:11:A:LEU:HD23 | 6        | 0.19          |
| (1,1120) | 1:40:A:ILE:HG12 | 1:41:A:ALA:H    | 12       | 0.19          |
| (1,1012) | 1:65:A:HIS:HB3  | 1:76:A:VAL:HG21 | 14       | 0.19          |
| (1,1012) | 1:65:A:HIS:HB3  | 1:76:A:VAL:HG22 | 14       | 0.19          |
| (1,1012) | 1:65:A:HIS:HB3  | 1:76:A:VAL:HG23 | 14       | 0.19          |
| (1,1004) | 1:54:A:ILE:HD11 | 1:58:A:MET:HB3  | 7        | 0.19          |
| (1,1004) | 1:54:A:ILE:HD12 | 1:58:A:MET:HB3  | 7        | 0.19          |
| (1,1004) | 1:54:A:ILE:HD13 | 1:58:A:MET:HB3  | 7        | 0.19          |
| (1,1004) | 1:54:A:ILE:HD11 | 1:58:A:MET:HB3  | 18       | 0.19          |
| (1,1004) | 1:54:A:ILE:HD12 | 1:58:A:MET:HB3  | 18       | 0.19          |
| (1,1004) | 1:54:A:ILE:HD13 | 1:58:A:MET:HB3  | 18       | 0.19          |
| (1,957)  | 1:6:A:VAL:HB    | 1:43:A:LEU:HB3  | 8        | 0.19          |
| (1,909)  | 1:59:A:ASP:HB3  | 1:60:A:ILE:HB   | 13       | 0.19          |
| (1,872)  | 1:30:A:ASP:HB3  | 1:46:A:ASP:H    | 20       | 0.19          |
| (1,789)  | 1:11:A:LEU:HB3  | 1:39:A:GLY:HA2  | 19       | 0.19          |
| (1,787)  | 1:11:A:LEU:HB2  | 1:12:A:PRO:HD2  | 5        | 0.19          |
| (1,787)  | 1:11:A:LEU:HB2  | 1:12:A:PRO:HD2  | 7        | 0.19          |
| (1,685)  | 1:13:A:ARG:HA   | 1:13:A:ARG:HB2  | 18       | 0.19          |
| (1,598)  | 1:12:A:PRO:HA   | 1:72:A:LYS:HG2  | 7        | 0.19          |
| (1,592)  | 1:10:A:SER:H    | 1:10:A:SER:HB3  | 8        | 0.19          |
| (1,566)  | 1:59:A:ASP:HB2  | 1:60:A:ILE:HA   | 17       | 0.19          |
| (1,468)  | 1:64:A:GLN:H    | 1:65:A:HIS:HB3  | 16       | 0.19          |
| (1,461)  | 1:29:A:PRO:HB3  | 1:31:A:GLN:H    | 11       | 0.19          |
| (1,461)  | 1:29:A:PRO:HB3  | 1:31:A:GLN:H    | 12       | 0.19          |
| (1,423)  | 1:55:A:GLN:HE22 | 1:59:A:ASP:HB3  | 19       | 0.19          |
| (1,180)  | 1:72:A:LYS:H    | 1:72:A:LYS:HG3  | 18       | 0.19          |
| (1,1226) | 1:8:A:VAL:HG21  | 1:11:A:LEU:HD21 | 15       | 0.18          |
| (1,1226) | 1:8:A:VAL:HG21  | 1:11:A:LEU:HD22 | 15       | 0.18          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1226) | 1:8:A:VAL:HG21  | 1:11:A:LEU:HD23 | 15       | 0.18          |
| (1,1226) | 1:8:A:VAL:HG22  | 1:11:A:LEU:HD21 | 15       | 0.18          |
| (1,1226) | 1:8:A:VAL:HG22  | 1:11:A:LEU:HD22 | 15       | 0.18          |
| (1,1226) | 1:8:A:VAL:HG22  | 1:11:A:LEU:HD23 | 15       | 0.18          |
| (1,1226) | 1:8:A:VAL:HG23  | 1:11:A:LEU:HD21 | 15       | 0.18          |
| (1,1226) | 1:8:A:VAL:HG23  | 1:11:A:LEU:HD22 | 15       | 0.18          |
| (1,1226) | 1:8:A:VAL:HG23  | 1:11:A:LEU:HD23 | 15       | 0.18          |
| (1,1120) | 1:40:A:ILE:HG12 | 1:41:A:ALA:H    | 3        | 0.18          |
| (1,1113) | 1:11:A:LEU:HD11 | 1:39:A:GLY:HA3  | 18       | 0.18          |
| (1,1113) | 1:11:A:LEU:HD12 | 1:39:A:GLY:HA3  | 18       | 0.18          |
| (1,1113) | 1:11:A:LEU:HD13 | 1:39:A:GLY:HA3  | 18       | 0.18          |
| (1,1071) | 1:24:A:PHE:HE1  | 1:64:A:GLN:HB3  | 4        | 0.18          |
| (1,1071) | 1:24:A:PHE:HE2  | 1:64:A:GLN:HB3  | 4        | 0.18          |
| (1,1041) | 1:70:A:LYS:HB3  | 1:71:A:GLU:H    | 3        | 0.18          |
| (1,1013) | 1:65:A:HIS:HB3  | 1:76:A:VAL:H    | 19       | 0.18          |
| (1,1012) | 1:65:A:HIS:HB3  | 1:76:A:VAL:HG21 | 20       | 0.18          |
| (1,1012) | 1:65:A:HIS:HB3  | 1:76:A:VAL:HG22 | 20       | 0.18          |
| (1,1012) | 1:65:A:HIS:HB3  | 1:76:A:VAL:HG23 | 20       | 0.18          |
| (1,949)  | 1:7:A:PHE:HB2   | 1:77:A:GLU:HG3  | 20       | 0.18          |
| (1,892)  | 1:62:A:LEU:HB2  | 1:63:A:LEU:HA   | 4        | 0.18          |
| (1,892)  | 1:62:A:LEU:HB2  | 1:63:A:LEU:HA   | 16       | 0.18          |
| (1,787)  | 1:11:A:LEU:HB2  | 1:12:A:PRO:HD2  | 11       | 0.18          |
| (1,732)  | 1:31:A:GLN:HA   | 1:31:A:GLN:HG2  | 20       | 0.18          |
| (1,685)  | 1:13:A:ARG:HA   | 1:13:A:ARG:HB2  | 20       | 0.18          |
| (1,621)  | 1:25:A:LYS:HA   | 1:25:A:LYS:HB3  | 17       | 0.18          |
| (1,592)  | 1:10:A:SER:H    | 1:10:A:SER:HB3  | 16       | 0.18          |
| (1,566)  | 1:59:A:ASP:HB2  | 1:60:A:ILE:HA   | 3        | 0.18          |
| (1,468)  | 1:64:A:GLN:H    | 1:65:A:HIS:HB3  | 1        | 0.18          |
| (1,304)  | 1:56:A:ARG:H    | 1:59:A:ASP:HB3  | 16       | 0.18          |
| (1,197)  | 1:23:A:HIS:H    | 1:23:A:HIS:HB3  | 11       | 0.18          |
| (1,180)  | 1:72:A:LYS:H    | 1:72:A:LYS:HG3  | 17       | 0.18          |
| (1,76)   | 1:68:A:LEU:HD11 | 1:73:A:LYS:H    | 14       | 0.18          |
| (1,76)   | 1:68:A:LEU:HD12 | 1:73:A:LYS:H    | 14       | 0.18          |
| (1,76)   | 1:68:A:LEU:HD13 | 1:73:A:LYS:H    | 14       | 0.18          |
| (1,69)   | 1:69:A:LEU:HB2  | 1:70:A:LYS:H    | 11       | 0.18          |
| (1,69)   | 1:69:A:LEU:HB2  | 1:70:A:LYS:H    | 20       | 0.18          |
| (1,15)   | 1:6:A:VAL:H     | 1:43:A:LEU:HB3  | 5        | 0.18          |
| (1,1370) | 1:27:A:SER:HB3  | 1:45:A:PHE:HZ   | 11       | 0.17          |
| (1,1353) | 1:23:A:HIS:HB2  | 1:24:A:PHE:HD1  | 3        | 0.17          |
| (1,1353) | 1:23:A:HIS:HB2  | 1:24:A:PHE:HD2  | 3        | 0.17          |
| (1,1313) | 1:58:A:MET:HB3  | 1:58:A:MET:HE1  | 3        | 0.17          |
| (1,1313) | 1:58:A:MET:HB3  | 1:58:A:MET:HE2  | 3        | 0.17          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1313) | 1:58:A:MET:HB3  | 1:58:A:MET:HE3  | 3        | 0.17          |
| (1,1309) | 1:55:A:GLN:HE21 | 1:58:A:MET:HE1  | 12       | 0.17          |
| (1,1309) | 1:55:A:GLN:HE21 | 1:58:A:MET:HE2  | 12       | 0.17          |
| (1,1309) | 1:55:A:GLN:HE21 | 1:58:A:MET:HE3  | 12       | 0.17          |
| (1,1241) | 1:18:A:VAL:H    | 1:18:A:VAL:HG21 | 9        | 0.17          |
| (1,1241) | 1:18:A:VAL:H    | 1:18:A:VAL:HG22 | 9        | 0.17          |
| (1,1241) | 1:18:A:VAL:H    | 1:18:A:VAL:HG23 | 9        | 0.17          |
| (1,1226) | 1:8:A:VAL:HG21  | 1:11:A:LEU:HD21 | 11       | 0.17          |
| (1,1226) | 1:8:A:VAL:HG21  | 1:11:A:LEU:HD22 | 11       | 0.17          |
| (1,1226) | 1:8:A:VAL:HG21  | 1:11:A:LEU:HD23 | 11       | 0.17          |
| (1,1226) | 1:8:A:VAL:HG22  | 1:11:A:LEU:HD21 | 11       | 0.17          |
| (1,1226) | 1:8:A:VAL:HG22  | 1:11:A:LEU:HD22 | 11       | 0.17          |
| (1,1226) | 1:8:A:VAL:HG22  | 1:11:A:LEU:HD23 | 11       | 0.17          |
| (1,1226) | 1:8:A:VAL:HG23  | 1:11:A:LEU:HD21 | 11       | 0.17          |
| (1,1226) | 1:8:A:VAL:HG23  | 1:11:A:LEU:HD22 | 11       | 0.17          |
| (1,1226) | 1:8:A:VAL:HG23  | 1:11:A:LEU:HD23 | 11       | 0.17          |
| (1,1132) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD11 | 6        | 0.17          |
| (1,1132) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD12 | 6        | 0.17          |
| (1,1132) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD13 | 6        | 0.17          |
| (1,1113) | 1:11:A:LEU:HD11 | 1:39:A:GLY:HA3  | 5        | 0.17          |
| (1,1113) | 1:11:A:LEU:HD12 | 1:39:A:GLY:HA3  | 5        | 0.17          |
| (1,1113) | 1:11:A:LEU:HD13 | 1:39:A:GLY:HA3  | 5        | 0.17          |
| (1,1041) | 1:70:A:LYS:HB3  | 1:71:A:GLU:H    | 6        | 0.17          |
| (1,1041) | 1:70:A:LYS:HB3  | 1:71:A:GLU:H    | 9        | 0.17          |
| (1,1041) | 1:70:A:LYS:HB3  | 1:71:A:GLU:H    | 17       | 0.17          |
| (1,787)  | 1:11:A:LEU:HB2  | 1:12:A:PRO:HD2  | 19       | 0.17          |
| (1,598)  | 1:12:A:PRO:HA   | 1:72:A:LYS:HG2  | 5        | 0.17          |
| (1,552)  | 1:27:A:SER:HB2  | 1:61:A:ALA:H    | 10       | 0.17          |
| (1,428)  | 1:9:A:GLY:HA3   | 1:11:A:LEU:H    | 4        | 0.17          |
| (1,312)  | 1:58:A:MET:H    | 1:58:A:MET:HB3  | 19       | 0.17          |
| (1,290)  | 1:27:A:SER:HB2  | 1:60:A:ILE:H    | 18       | 0.17          |
| (1,282)  | 1:59:A:ASP:H    | 1:59:A:ASP:HB3  | 13       | 0.17          |
| (1,222)  | 1:19:A:GLU:HB3  | 1:20:A:LEU:H    | 20       | 0.17          |
| (1,204)  | 1:43:A:LEU:HB2  | 1:44:A:GLU:H    | 16       | 0.17          |
| (1,1336) | 1:59:A:ASP:HB3  | 1:60:A:ILE:HD11 | 4        | 0.16          |
| (1,1336) | 1:59:A:ASP:HB3  | 1:60:A:ILE:HD12 | 4        | 0.16          |
| (1,1336) | 1:59:A:ASP:HB3  | 1:60:A:ILE:HD13 | 4        | 0.16          |
| (1,1232) | 1:6:A:VAL:HG11  | 1:7:A:PHE:HB2   | 7        | 0.16          |
| (1,1232) | 1:6:A:VAL:HG12  | 1:7:A:PHE:HB2   | 7        | 0.16          |
| (1,1232) | 1:6:A:VAL:HG13  | 1:7:A:PHE:HB2   | 7        | 0.16          |
| (1,1134) | 1:69:A:LEU:HD11 | 1:74:A:ILE:HD11 | 19       | 0.16          |
| (1,1134) | 1:69:A:LEU:HD11 | 1:74:A:ILE:HD12 | 19       | 0.16          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1134) | 1:69:A:LEU:HD11 | 1:74:A:ILE:HD13 | 19       | 0.16          |
| (1,1134) | 1:69:A:LEU:HD12 | 1:74:A:ILE:HD11 | 19       | 0.16          |
| (1,1134) | 1:69:A:LEU:HD12 | 1:74:A:ILE:HD12 | 19       | 0.16          |
| (1,1134) | 1:69:A:LEU:HD12 | 1:74:A:ILE:HD13 | 19       | 0.16          |
| (1,1134) | 1:69:A:LEU:HD13 | 1:74:A:ILE:HD11 | 19       | 0.16          |
| (1,1134) | 1:69:A:LEU:HD13 | 1:74:A:ILE:HD12 | 19       | 0.16          |
| (1,1134) | 1:69:A:LEU:HD13 | 1:74:A:ILE:HD13 | 19       | 0.16          |
| (1,1121) | 1:40:A:ILE:HG12 | 1:42:A:PHE:HE1  | 13       | 0.16          |
| (1,1121) | 1:40:A:ILE:HG12 | 1:42:A:PHE:HE2  | 13       | 0.16          |
| (1,1024) | 1:29:A:PRO:HB3  | 1:44:A:GLU:H    | 4        | 0.16          |
| (1,1018) | 1:33:A:ARG:HB3  | 1:42:A:PHE:HB3  | 20       | 0.16          |
| (1,1013) | 1:65:A:HIS:HB3  | 1:76:A:VAL:H    | 16       | 0.16          |
| (1,1013) | 1:65:A:HIS:HB3  | 1:76:A:VAL:H    | 17       | 0.16          |
| (1,1012) | 1:65:A:HIS:HB3  | 1:76:A:VAL:HG21 | 13       | 0.16          |
| (1,1012) | 1:65:A:HIS:HB3  | 1:76:A:VAL:HG22 | 13       | 0.16          |
| (1,1012) | 1:65:A:HIS:HB3  | 1:76:A:VAL:HG23 | 13       | 0.16          |
| (1,1001) | 1:22:A:ASN:HA   | 1:25:A:LYS:HB2  | 11       | 0.16          |
| (1,957)  | 1:6:A:VAL:HB    | 1:43:A:LEU:HB3  | 12       | 0.16          |
| (1,957)  | 1:6:A:VAL:HB    | 1:43:A:LEU:HB3  | 15       | 0.16          |
| (1,813)  | 1:33:A:ARG:HB2  | 1:33:A:ARG:HD2  | 10       | 0.16          |
| (1,811)  | 1:7:A:PHE:HE1   | 1:9:A:GLY:HA2   | 14       | 0.16          |
| (1,811)  | 1:7:A:PHE:HE2   | 1:9:A:GLY:HA2   | 14       | 0.16          |
| (1,808)  | 1:9:A:GLY:HA2   | 1:40:A:ILE:HG13 | 9        | 0.16          |
| (1,808)  | 1:9:A:GLY:HA2   | 1:40:A:ILE:HG13 | 14       | 0.16          |
| (1,787)  | 1:11:A:LEU:HB2  | 1:12:A:PRO:HD2  | 17       | 0.16          |
| (1,787)  | 1:11:A:LEU:HB2  | 1:12:A:PRO:HD2  | 18       | 0.16          |
| (1,673)  | 1:71:A:GLU:HA   | 1:71:A:GLU:HB2  | 2        | 0.16          |
| (1,673)  | 1:71:A:GLU:HA   | 1:71:A:GLU:HB2  | 5        | 0.16          |
| (1,673)  | 1:71:A:GLU:HA   | 1:71:A:GLU:HB2  | 7        | 0.16          |
| (1,673)  | 1:71:A:GLU:HA   | 1:71:A:GLU:HB2  | 12       | 0.16          |
| (1,673)  | 1:71:A:GLU:HA   | 1:71:A:GLU:HB2  | 13       | 0.16          |
| (1,673)  | 1:71:A:GLU:HA   | 1:71:A:GLU:HB2  | 15       | 0.16          |
| (1,673)  | 1:71:A:GLU:HA   | 1:71:A:GLU:HB2  | 16       | 0.16          |
| (1,621)  | 1:25:A:LYS:HA   | 1:25:A:LYS:HB3  | 4        | 0.16          |
| (1,489)  | 1:10:A:SER:HB3  | 1:75:A:ASN:HD22 | 17       | 0.16          |
| (1,482)  | 1:10:A:SER:HB3  | 1:75:A:ASN:HD21 | 4        | 0.16          |
| (1,423)  | 1:55:A:GLN:HE22 | 1:59:A:ASP:HB3  | 11       | 0.16          |
| (1,312)  | 1:58:A:MET:H    | 1:58:A:MET:HB3  | 20       | 0.16          |
| (1,304)  | 1:56:A:ARG:H    | 1:59:A:ASP:HB3  | 7        | 0.16          |
| (1,282)  | 1:59:A:ASP:H    | 1:59:A:ASP:HB3  | 1        | 0.16          |
| (1,197)  | 1:23:A:HIS:H    | 1:23:A:HIS:HB3  | 3        | 0.16          |
| (1,69)   | 1:69:A:LEU:HB2  | 1:70:A:LYS:H    | 12       | 0.16          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1373) | 1:23:A:HIS:HE1  | 1:69:A:LEU:HD21 | 19       | 0.15          |
| (1,1373) | 1:23:A:HIS:HE1  | 1:69:A:LEU:HD22 | 19       | 0.15          |
| (1,1373) | 1:23:A:HIS:HE1  | 1:69:A:LEU:HD23 | 19       | 0.15          |
| (1,1353) | 1:23:A:HIS:HB2  | 1:24:A:PHE:HD1  | 6        | 0.15          |
| (1,1353) | 1:23:A:HIS:HB2  | 1:24:A:PHE:HD2  | 6        | 0.15          |
| (1,1226) | 1:8:A:VAL:HG21  | 1:11:A:LEU:HD21 | 10       | 0.15          |
| (1,1226) | 1:8:A:VAL:HG21  | 1:11:A:LEU:HD22 | 10       | 0.15          |
| (1,1226) | 1:8:A:VAL:HG21  | 1:11:A:LEU:HD23 | 10       | 0.15          |
| (1,1226) | 1:8:A:VAL:HG22  | 1:11:A:LEU:HD21 | 10       | 0.15          |
| (1,1226) | 1:8:A:VAL:HG22  | 1:11:A:LEU:HD22 | 10       | 0.15          |
| (1,1226) | 1:8:A:VAL:HG22  | 1:11:A:LEU:HD23 | 10       | 0.15          |
| (1,1226) | 1:8:A:VAL:HG23  | 1:11:A:LEU:HD21 | 10       | 0.15          |
| (1,1226) | 1:8:A:VAL:HG23  | 1:11:A:LEU:HD22 | 10       | 0.15          |
| (1,1226) | 1:8:A:VAL:HG23  | 1:11:A:LEU:HD23 | 10       | 0.15          |
| (1,1163) | 1:4:A:PHE:HB2   | 1:78:A:LEU:HD21 | 13       | 0.15          |
| (1,1163) | 1:4:A:PHE:HB2   | 1:78:A:LEU:HD22 | 13       | 0.15          |
| (1,1163) | 1:4:A:PHE:HB2   | 1:78:A:LEU:HD23 | 13       | 0.15          |
| (1,1163) | 1:4:A:PHE:HB3   | 1:78:A:LEU:HD21 | 13       | 0.15          |
| (1,1163) | 1:4:A:PHE:HB3   | 1:78:A:LEU:HD22 | 13       | 0.15          |
| (1,1163) | 1:4:A:PHE:HB3   | 1:78:A:LEU:HD23 | 13       | 0.15          |
| (1,1127) | 1:20:A:LEU:HD11 | 1:34:A:LEU:HG   | 13       | 0.15          |
| (1,1127) | 1:20:A:LEU:HD12 | 1:34:A:LEU:HG   | 13       | 0.15          |
| (1,1127) | 1:20:A:LEU:HD13 | 1:34:A:LEU:HG   | 13       | 0.15          |
| (1,1120) | 1:40:A:ILE:HG12 | 1:41:A:ALA:H    | 8        | 0.15          |
| (1,1080) | 1:33:A:ARG:HG3  | 1:42:A:PHE:HD1  | 18       | 0.15          |
| (1,1080) | 1:33:A:ARG:HG3  | 1:42:A:PHE:HD2  | 18       | 0.15          |
| (1,1069) | 1:61:A:ALA:HA   | 1:64:A:GLN:HB3  | 11       | 0.15          |
| (1,1001) | 1:22:A:ASN:HA   | 1:25:A:LYS:HB2  | 10       | 0.15          |
| (1,1001) | 1:22:A:ASN:HA   | 1:25:A:LYS:HB2  | 14       | 0.15          |
| (1,1001) | 1:22:A:ASN:HA   | 1:25:A:LYS:HB2  | 15       | 0.15          |
| (1,896)  | 1:62:A:LEU:HB2  | 1:64:A:GLN:H    | 19       | 0.15          |
| (1,892)  | 1:62:A:LEU:HB2  | 1:63:A:LEU:HA   | 3        | 0.15          |
| (1,892)  | 1:62:A:LEU:HB2  | 1:63:A:LEU:HA   | 8        | 0.15          |
| (1,872)  | 1:30:A:ASP:HB3  | 1:46:A:ASP:H    | 10       | 0.15          |
| (1,820)  | 1:68:A:LEU:HB2  | 1:71:A:GLU:H    | 15       | 0.15          |
| (1,820)  | 1:68:A:LEU:HB2  | 1:71:A:GLU:H    | 19       | 0.15          |
| (1,808)  | 1:9:A:GLY:HA2   | 1:40:A:ILE:HG13 | 12       | 0.15          |
| (1,787)  | 1:11:A:LEU:HB2  | 1:12:A:PRO:HD2  | 4        | 0.15          |
| (1,787)  | 1:11:A:LEU:HB2  | 1:12:A:PRO:HD2  | 20       | 0.15          |
| (1,673)  | 1:71:A:GLU:HA   | 1:71:A:GLU:HB2  | 3        | 0.15          |
| (1,673)  | 1:71:A:GLU:HA   | 1:71:A:GLU:HB2  | 4        | 0.15          |
| (1,673)  | 1:71:A:GLU:HA   | 1:71:A:GLU:HB2  | 6        | 0.15          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,673)  | 1:71:A:GLU:HA   | 1:71:A:GLU:HB2  | 8        | 0.15          |
| (1,673)  | 1:71:A:GLU:HA   | 1:71:A:GLU:HB2  | 9        | 0.15          |
| (1,673)  | 1:71:A:GLU:HA   | 1:71:A:GLU:HB2  | 10       | 0.15          |
| (1,673)  | 1:71:A:GLU:HA   | 1:71:A:GLU:HB2  | 14       | 0.15          |
| (1,673)  | 1:71:A:GLU:HA   | 1:71:A:GLU:HB2  | 17       | 0.15          |
| (1,673)  | 1:71:A:GLU:HA   | 1:71:A:GLU:HB2  | 18       | 0.15          |
| (1,673)  | 1:71:A:GLU:HA   | 1:71:A:GLU:HB2  | 19       | 0.15          |
| (1,673)  | 1:71:A:GLU:HA   | 1:71:A:GLU:HB2  | 20       | 0.15          |
| (1,621)  | 1:25:A:LYS:HA   | 1:25:A:LYS:HB3  | 16       | 0.15          |
| (1,555)  | 1:27:A:SER:HB2  | 1:60:A:ILE:HB   | 10       | 0.15          |
| (1,440)  | 1:25:A:LYS:HB2  | 1:27:A:SER:H    | 3        | 0.15          |
| (1,440)  | 1:25:A:LYS:HB2  | 1:27:A:SER:H    | 12       | 0.15          |
| (1,428)  | 1:9:A:GLY:HA3   | 1:11:A:LEU:H    | 17       | 0.15          |
| (1,312)  | 1:58:A:MET:H    | 1:58:A:MET:HB3  | 10       | 0.15          |
| (1,282)  | 1:59:A:ASP:H    | 1:59:A:ASP:HB3  | 15       | 0.15          |
| (1,222)  | 1:19:A:GLU:HB3  | 1:20:A:LEU:H    | 11       | 0.15          |
| (1,197)  | 1:23:A:HIS:H    | 1:23:A:HIS:HB3  | 6        | 0.15          |
| (1,149)  | 1:23:A:HIS:HB2  | 1:25:A:LYS:H    | 14       | 0.15          |
| (1,149)  | 1:23:A:HIS:HB2  | 1:25:A:LYS:H    | 20       | 0.15          |
| (1,1241) | 1:18:A:VAL:H    | 1:18:A:VAL:HG21 | 12       | 0.14          |
| (1,1241) | 1:18:A:VAL:H    | 1:18:A:VAL:HG22 | 12       | 0.14          |
| (1,1241) | 1:18:A:VAL:H    | 1:18:A:VAL:HG23 | 12       | 0.14          |
| (1,1196) | 1:34:A:LEU:HD21 | 1:36:A:ALA:H    | 17       | 0.14          |
| (1,1196) | 1:34:A:LEU:HD22 | 1:36:A:ALA:H    | 17       | 0.14          |
| (1,1196) | 1:34:A:LEU:HD23 | 1:36:A:ALA:H    | 17       | 0.14          |
| (1,1041) | 1:70:A:LYS:HB3  | 1:71:A:GLU:H    | 20       | 0.14          |
| (1,1013) | 1:65:A:HIS:HB3  | 1:76:A:VAL:H    | 8        | 0.14          |
| (1,1012) | 1:65:A:HIS:HB3  | 1:76:A:VAL:HG21 | 4        | 0.14          |
| (1,1012) | 1:65:A:HIS:HB3  | 1:76:A:VAL:HG22 | 4        | 0.14          |
| (1,1012) | 1:65:A:HIS:HB3  | 1:76:A:VAL:HG23 | 4        | 0.14          |
| (1,1012) | 1:65:A:HIS:HB3  | 1:76:A:VAL:HG21 | 10       | 0.14          |
| (1,1012) | 1:65:A:HIS:HB3  | 1:76:A:VAL:HG22 | 10       | 0.14          |
| (1,1012) | 1:65:A:HIS:HB3  | 1:76:A:VAL:HG23 | 10       | 0.14          |
| (1,1012) | 1:65:A:HIS:HB3  | 1:76:A:VAL:HG21 | 17       | 0.14          |
| (1,1012) | 1:65:A:HIS:HB3  | 1:76:A:VAL:HG22 | 17       | 0.14          |
| (1,1012) | 1:65:A:HIS:HB3  | 1:76:A:VAL:HG23 | 17       | 0.14          |
| (1,1001) | 1:22:A:ASN:HA   | 1:25:A:LYS:HB2  | 7        | 0.14          |
| (1,909)  | 1:59:A:ASP:HB3  | 1:60:A:ILE:HB   | 12       | 0.14          |
| (1,892)  | 1:62:A:LEU:HB2  | 1:63:A:LEU:HA   | 13       | 0.14          |
| (1,808)  | 1:9:A:GLY:HA2   | 1:40:A:ILE:HG13 | 2        | 0.14          |
| (1,799)  | 1:57:A:ARG:H    | 1:57:A:ARG:HD3  | 13       | 0.14          |
| (1,799)  | 1:57:A:ARG:H    | 1:57:A:ARG:HD3  | 19       | 0.14          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,789)  | 1:11:A:LEU:HB3  | 1:39:A:GLY:HA2  | 2        | 0.14          |
| (1,789)  | 1:11:A:LEU:HB3  | 1:39:A:GLY:HA2  | 12       | 0.14          |
| (1,787)  | 1:11:A:LEU:HB2  | 1:12:A:PRO:HD2  | 12       | 0.14          |
| (1,673)  | 1:71:A:GLU:HA   | 1:71:A:GLU:HB2  | 1        | 0.14          |
| (1,592)  | 1:10:A:SER:H    | 1:10:A:SER:HB3  | 15       | 0.14          |
| (1,581)  | 1:10:A:SER:HB3  | 1:75:A:ASN:H    | 2        | 0.14          |
| (1,581)  | 1:10:A:SER:HB3  | 1:75:A:ASN:H    | 10       | 0.14          |
| (1,580)  | 1:10:A:SER:HB2  | 1:74:A:ILE:HB   | 18       | 0.14          |
| (1,555)  | 1:27:A:SER:HB2  | 1:60:A:ILE:HB   | 2        | 0.14          |
| (1,468)  | 1:64:A:GLN:H    | 1:65:A:HIS:HB3  | 15       | 0.14          |
| (1,461)  | 1:29:A:PRO:HB3  | 1:31:A:GLN:H    | 20       | 0.14          |
| (1,182)  | 1:68:A:LEU:HD11 | 1:72:A:LYS:H    | 10       | 0.14          |
| (1,182)  | 1:68:A:LEU:HD12 | 1:72:A:LYS:H    | 10       | 0.14          |
| (1,182)  | 1:68:A:LEU:HD13 | 1:72:A:LYS:H    | 10       | 0.14          |
| (1,182)  | 1:68:A:LEU:HD11 | 1:72:A:LYS:H    | 13       | 0.14          |
| (1,182)  | 1:68:A:LEU:HD12 | 1:72:A:LYS:H    | 13       | 0.14          |
| (1,182)  | 1:68:A:LEU:HD13 | 1:72:A:LYS:H    | 13       | 0.14          |
| (1,149)  | 1:23:A:HIS:HB2  | 1:25:A:LYS:H    | 4        | 0.14          |
| (1,149)  | 1:23:A:HIS:HB2  | 1:25:A:LYS:H    | 6        | 0.14          |
| (1,88)   | 1:78:A:LEU:H    | 1:78:A:LEU:HD11 | 11       | 0.14          |
| (1,88)   | 1:78:A:LEU:H    | 1:78:A:LEU:HD12 | 11       | 0.14          |
| (1,88)   | 1:78:A:LEU:H    | 1:78:A:LEU:HD13 | 11       | 0.14          |
| (1,69)   | 1:69:A:LEU:HB2  | 1:70:A:LYS:H    | 5        | 0.14          |
| (1,1258) | 1:79:A:THR:HG21 | 1:80:A:VAL:HG11 | 11       | 0.13          |
| (1,1258) | 1:79:A:THR:HG21 | 1:80:A:VAL:HG12 | 11       | 0.13          |
| (1,1258) | 1:79:A:THR:HG21 | 1:80:A:VAL:HG13 | 11       | 0.13          |
| (1,1258) | 1:79:A:THR:HG22 | 1:80:A:VAL:HG11 | 11       | 0.13          |
| (1,1258) | 1:79:A:THR:HG22 | 1:80:A:VAL:HG12 | 11       | 0.13          |
| (1,1258) | 1:79:A:THR:HG22 | 1:80:A:VAL:HG13 | 11       | 0.13          |
| (1,1258) | 1:79:A:THR:HG23 | 1:80:A:VAL:HG11 | 11       | 0.13          |
| (1,1258) | 1:79:A:THR:HG23 | 1:80:A:VAL:HG12 | 11       | 0.13          |
| (1,1258) | 1:79:A:THR:HG23 | 1:80:A:VAL:HG13 | 11       | 0.13          |
| (1,1196) | 1:34:A:LEU:HD21 | 1:36:A:ALA:H    | 12       | 0.13          |
| (1,1196) | 1:34:A:LEU:HD22 | 1:36:A:ALA:H    | 12       | 0.13          |
| (1,1196) | 1:34:A:LEU:HD23 | 1:36:A:ALA:H    | 12       | 0.13          |
| (1,1164) | 1:72:A:LYS:HA   | 1:72:A:LYS:HG3  | 7        | 0.13          |
| (1,1163) | 1:4:A:PHE:HB2   | 1:78:A:LEU:HD21 | 16       | 0.13          |
| (1,1163) | 1:4:A:PHE:HB2   | 1:78:A:LEU:HD22 | 16       | 0.13          |
| (1,1163) | 1:4:A:PHE:HB2   | 1:78:A:LEU:HD23 | 16       | 0.13          |
| (1,1163) | 1:4:A:PHE:HB3   | 1:78:A:LEU:HD21 | 16       | 0.13          |
| (1,1163) | 1:4:A:PHE:HB3   | 1:78:A:LEU:HD22 | 16       | 0.13          |
| (1,1163) | 1:4:A:PHE:HB3   | 1:78:A:LEU:HD23 | 16       | 0.13          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1121) | 1:40:A:ILE:HG12 | 1:42:A:PHE:HE1  | 11       | 0.13          |
| (1,1121) | 1:40:A:ILE:HG12 | 1:42:A:PHE:HE2  | 11       | 0.13          |
| (1,1041) | 1:70:A:LYS:HB3  | 1:71:A:GLU:H    | 1        | 0.13          |
| (1,1026) | 1:29:A:PRO:HB3  | 1:32:A:ILE:HD11 | 13       | 0.13          |
| (1,1026) | 1:29:A:PRO:HB3  | 1:32:A:ILE:HD12 | 13       | 0.13          |
| (1,1026) | 1:29:A:PRO:HB3  | 1:32:A:ILE:HD13 | 13       | 0.13          |
| (1,1024) | 1:29:A:PRO:HB3  | 1:44:A:GLU:H    | 20       | 0.13          |
| (1,1013) | 1:65:A:HIS:HB3  | 1:76:A:VAL:H    | 4        | 0.13          |
| (1,1004) | 1:54:A:ILE:HD11 | 1:58:A:MET:HB3  | 11       | 0.13          |
| (1,1004) | 1:54:A:ILE:HD12 | 1:58:A:MET:HB3  | 11       | 0.13          |
| (1,1004) | 1:54:A:ILE:HD13 | 1:58:A:MET:HB3  | 11       | 0.13          |
| (1,957)  | 1:6:A:VAL:HB    | 1:43:A:LEU:HB3  | 1        | 0.13          |
| (1,896)  | 1:62:A:LEU:HB2  | 1:64:A:GLN:H    | 17       | 0.13          |
| (1,813)  | 1:33:A:ARG:HB2  | 1:33:A:ARG:HD2  | 13       | 0.13          |
| (1,789)  | 1:11:A:LEU:HB3  | 1:39:A:GLY:HA2  | 14       | 0.13          |
| (1,787)  | 1:11:A:LEU:HB2  | 1:12:A:PRO:HD2  | 2        | 0.13          |
| (1,787)  | 1:11:A:LEU:HB2  | 1:12:A:PRO:HD2  | 8        | 0.13          |
| (1,732)  | 1:31:A:GLN:HA   | 1:31:A:GLN:HG2  | 13       | 0.13          |
| (1,721)  | 1:17:A:ALA:HA   | 1:20:A:LEU:HD11 | 11       | 0.13          |
| (1,721)  | 1:17:A:ALA:HA   | 1:20:A:LEU:HD12 | 11       | 0.13          |
| (1,721)  | 1:17:A:ALA:HA   | 1:20:A:LEU:HD13 | 11       | 0.13          |
| (1,670)  | 1:20:A:LEU:HA   | 1:23:A:HIS:HB3  | 16       | 0.13          |
| (1,621)  | 1:25:A:LYS:HA   | 1:25:A:LYS:HB3  | 1        | 0.13          |
| (1,621)  | 1:25:A:LYS:HA   | 1:25:A:LYS:HB3  | 2        | 0.13          |
| (1,621)  | 1:25:A:LYS:HA   | 1:25:A:LYS:HB3  | 9        | 0.13          |
| (1,592)  | 1:10:A:SER:H    | 1:10:A:SER:HB3  | 1        | 0.13          |
| (1,592)  | 1:10:A:SER:H    | 1:10:A:SER:HB3  | 6        | 0.13          |
| (1,581)  | 1:10:A:SER:HB3  | 1:75:A:ASN:H    | 3        | 0.13          |
| (1,581)  | 1:10:A:SER:HB3  | 1:75:A:ASN:H    | 9        | 0.13          |
| (1,503)  | 1:23:A:HIS:HB2  | 1:24:A:PHE:H    | 8        | 0.13          |
| (1,468)  | 1:64:A:GLN:H    | 1:65:A:HIS:HB3  | 8        | 0.13          |
| (1,468)  | 1:64:A:GLN:H    | 1:65:A:HIS:HB3  | 19       | 0.13          |
| (1,304)  | 1:56:A:ARG:H    | 1:59:A:ASP:HB3  | 8        | 0.13          |
| (1,304)  | 1:56:A:ARG:H    | 1:59:A:ASP:HB3  | 14       | 0.13          |
| (1,282)  | 1:59:A:ASP:H    | 1:59:A:ASP:HB3  | 6        | 0.13          |
| (1,204)  | 1:43:A:LEU:HB2  | 1:44:A:GLU:H    | 11       | 0.13          |
| (1,204)  | 1:43:A:LEU:HB2  | 1:44:A:GLU:H    | 20       | 0.13          |
| (1,182)  | 1:68:A:LEU:HD11 | 1:72:A:LYS:H    | 6        | 0.13          |
| (1,182)  | 1:68:A:LEU:HD12 | 1:72:A:LYS:H    | 6        | 0.13          |
| (1,182)  | 1:68:A:LEU:HD13 | 1:72:A:LYS:H    | 6        | 0.13          |
| (1,182)  | 1:68:A:LEU:HD11 | 1:72:A:LYS:H    | 9        | 0.13          |
| (1,182)  | 1:68:A:LEU:HD12 | 1:72:A:LYS:H    | 9        | 0.13          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,182)  | 1:68:A:LEU:HD13 | 1:72:A:LYS:H    | 9        | 0.13          |
| (1,182)  | 1:68:A:LEU:HD11 | 1:72:A:LYS:H    | 11       | 0.13          |
| (1,182)  | 1:68:A:LEU:HD12 | 1:72:A:LYS:H    | 11       | 0.13          |
| (1,182)  | 1:68:A:LEU:HD13 | 1:72:A:LYS:H    | 11       | 0.13          |
| (1,182)  | 1:68:A:LEU:HD11 | 1:72:A:LYS:H    | 12       | 0.13          |
| (1,182)  | 1:68:A:LEU:HD12 | 1:72:A:LYS:H    | 12       | 0.13          |
| (1,182)  | 1:68:A:LEU:HD13 | 1:72:A:LYS:H    | 12       | 0.13          |
| (1,182)  | 1:68:A:LEU:HD11 | 1:72:A:LYS:H    | 15       | 0.13          |
| (1,182)  | 1:68:A:LEU:HD12 | 1:72:A:LYS:H    | 15       | 0.13          |
| (1,182)  | 1:68:A:LEU:HD13 | 1:72:A:LYS:H    | 15       | 0.13          |
| (1,182)  | 1:68:A:LEU:HD11 | 1:72:A:LYS:H    | 16       | 0.13          |
| (1,182)  | 1:68:A:LEU:HD12 | 1:72:A:LYS:H    | 16       | 0.13          |
| (1,182)  | 1:68:A:LEU:HD13 | 1:72:A:LYS:H    | 16       | 0.13          |
| (1,182)  | 1:68:A:LEU:HD11 | 1:72:A:LYS:H    | 17       | 0.13          |
| (1,182)  | 1:68:A:LEU:HD12 | 1:72:A:LYS:H    | 17       | 0.13          |
| (1,182)  | 1:68:A:LEU:HD13 | 1:72:A:LYS:H    | 17       | 0.13          |
| (1,182)  | 1:68:A:LEU:HD11 | 1:72:A:LYS:H    | 19       | 0.13          |
| (1,182)  | 1:68:A:LEU:HD12 | 1:72:A:LYS:H    | 19       | 0.13          |
| (1,182)  | 1:68:A:LEU:HD13 | 1:72:A:LYS:H    | 19       | 0.13          |
| (1,88)   | 1:78:A:LEU:H    | 1:78:A:LEU:HD11 | 3        | 0.13          |
| (1,88)   | 1:78:A:LEU:H    | 1:78:A:LEU:HD12 | 3        | 0.13          |
| (1,88)   | 1:78:A:LEU:H    | 1:78:A:LEU:HD13 | 3        | 0.13          |
| (1,78)   | 1:59:A:ASP:HB3  | 1:61:A:ALA:H    | 13       | 0.13          |
| (1,1314) | 1:54:A:ILE:HD11 | 1:58:A:MET:HE1  | 20       | 0.12          |
| (1,1314) | 1:54:A:ILE:HD11 | 1:58:A:MET:HE2  | 20       | 0.12          |
| (1,1314) | 1:54:A:ILE:HD11 | 1:58:A:MET:HE3  | 20       | 0.12          |
| (1,1314) | 1:54:A:ILE:HD12 | 1:58:A:MET:HE1  | 20       | 0.12          |
| (1,1314) | 1:54:A:ILE:HD12 | 1:58:A:MET:HE2  | 20       | 0.12          |
| (1,1314) | 1:54:A:ILE:HD12 | 1:58:A:MET:HE3  | 20       | 0.12          |
| (1,1314) | 1:54:A:ILE:HD13 | 1:58:A:MET:HE1  | 20       | 0.12          |
| (1,1314) | 1:54:A:ILE:HD13 | 1:58:A:MET:HE2  | 20       | 0.12          |
| (1,1314) | 1:54:A:ILE:HD13 | 1:58:A:MET:HE3  | 20       | 0.12          |
| (1,1258) | 1:79:A:THR:HG21 | 1:80:A:VAL:HG11 | 1        | 0.12          |
| (1,1258) | 1:79:A:THR:HG21 | 1:80:A:VAL:HG12 | 1        | 0.12          |
| (1,1258) | 1:79:A:THR:HG21 | 1:80:A:VAL:HG13 | 1        | 0.12          |
| (1,1258) | 1:79:A:THR:HG22 | 1:80:A:VAL:HG11 | 1        | 0.12          |
| (1,1258) | 1:79:A:THR:HG22 | 1:80:A:VAL:HG12 | 1        | 0.12          |
| (1,1258) | 1:79:A:THR:HG22 | 1:80:A:VAL:HG13 | 1        | 0.12          |
| (1,1258) | 1:79:A:THR:HG23 | 1:80:A:VAL:HG11 | 1        | 0.12          |
| (1,1258) | 1:79:A:THR:HG23 | 1:80:A:VAL:HG12 | 1        | 0.12          |
| (1,1258) | 1:79:A:THR:HG23 | 1:80:A:VAL:HG13 | 1        | 0.12          |
| (1,1248) | 1:8:A:VAL:HG11  | 1:43:A:LEU:HD21 | 20       | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1248) | 1:8:A:VAL:HG11  | 1:43:A:LEU:HD22 | 20       | 0.12          |
| (1,1248) | 1:8:A:VAL:HG11  | 1:43:A:LEU:HD23 | 20       | 0.12          |
| (1,1248) | 1:8:A:VAL:HG12  | 1:43:A:LEU:HD21 | 20       | 0.12          |
| (1,1248) | 1:8:A:VAL:HG12  | 1:43:A:LEU:HD22 | 20       | 0.12          |
| (1,1248) | 1:8:A:VAL:HG12  | 1:43:A:LEU:HD23 | 20       | 0.12          |
| (1,1248) | 1:8:A:VAL:HG13  | 1:43:A:LEU:HD21 | 20       | 0.12          |
| (1,1248) | 1:8:A:VAL:HG13  | 1:43:A:LEU:HD22 | 20       | 0.12          |
| (1,1248) | 1:8:A:VAL:HG13  | 1:43:A:LEU:HD23 | 20       | 0.12          |
| (1,1232) | 1:6:A:VAL:HG11  | 1:7:A:PHE:HB2   | 13       | 0.12          |
| (1,1232) | 1:6:A:VAL:HG12  | 1:7:A:PHE:HB2   | 13       | 0.12          |
| (1,1232) | 1:6:A:VAL:HG13  | 1:7:A:PHE:HB2   | 13       | 0.12          |
| (1,1232) | 1:6:A:VAL:HG11  | 1:7:A:PHE:HB2   | 20       | 0.12          |
| (1,1232) | 1:6:A:VAL:HG12  | 1:7:A:PHE:HB2   | 20       | 0.12          |
| (1,1232) | 1:6:A:VAL:HG13  | 1:7:A:PHE:HB2   | 20       | 0.12          |
| (1,1226) | 1:8:A:VAL:HG21  | 1:11:A:LEU:HD21 | 4        | 0.12          |
| (1,1226) | 1:8:A:VAL:HG21  | 1:11:A:LEU:HD22 | 4        | 0.12          |
| (1,1226) | 1:8:A:VAL:HG21  | 1:11:A:LEU:HD23 | 4        | 0.12          |
| (1,1226) | 1:8:A:VAL:HG22  | 1:11:A:LEU:HD21 | 4        | 0.12          |
| (1,1226) | 1:8:A:VAL:HG22  | 1:11:A:LEU:HD22 | 4        | 0.12          |
| (1,1226) | 1:8:A:VAL:HG22  | 1:11:A:LEU:HD23 | 4        | 0.12          |
| (1,1226) | 1:8:A:VAL:HG23  | 1:11:A:LEU:HD21 | 4        | 0.12          |
| (1,1226) | 1:8:A:VAL:HG23  | 1:11:A:LEU:HD22 | 4        | 0.12          |
| (1,1226) | 1:8:A:VAL:HG23  | 1:11:A:LEU:HD23 | 4        | 0.12          |
| (1,1161) | 1:4:A:PHE:HD1   | 1:78:A:LEU:HD21 | 17       | 0.12          |
| (1,1161) | 1:4:A:PHE:HD1   | 1:78:A:LEU:HD22 | 17       | 0.12          |
| (1,1161) | 1:4:A:PHE:HD1   | 1:78:A:LEU:HD23 | 17       | 0.12          |
| (1,1161) | 1:4:A:PHE:HD2   | 1:78:A:LEU:HD21 | 17       | 0.12          |
| (1,1161) | 1:4:A:PHE:HD2   | 1:78:A:LEU:HD22 | 17       | 0.12          |
| (1,1161) | 1:4:A:PHE:HD2   | 1:78:A:LEU:HD23 | 17       | 0.12          |
| (1,1140) | 1:12:A:PRO:HG2  | 1:70:A:LYS:HG2  | 15       | 0.12          |
| (1,1140) | 1:12:A:PRO:HG2  | 1:70:A:LYS:HG3  | 15       | 0.12          |
| (1,1132) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD11 | 16       | 0.12          |
| (1,1132) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD12 | 16       | 0.12          |
| (1,1132) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD13 | 16       | 0.12          |
| (1,1121) | 1:40:A:ILE:HG12 | 1:42:A:PHE:HE1  | 19       | 0.12          |
| (1,1121) | 1:40:A:ILE:HG12 | 1:42:A:PHE:HE2  | 19       | 0.12          |
| (1,1041) | 1:70:A:LYS:HB3  | 1:71:A:GLU:H    | 10       | 0.12          |
| (1,1013) | 1:65:A:HIS:HB3  | 1:76:A:VAL:H    | 18       | 0.12          |
| (1,1001) | 1:22:A:ASN:HA   | 1:25:A:LYS:HB2  | 3        | 0.12          |
| (1,957)  | 1:6:A:VAL:HB    | 1:43:A:LEU:HB3  | 14       | 0.12          |
| (1,924)  | 1:37:A:ASP:HB2  | 1:38:A:LYS:HA   | 7        | 0.12          |
| (1,892)  | 1:62:A:LEU:HB2  | 1:63:A:LEU:HA   | 5        | 0.12          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,892)  | 1:62:A:LEU:HB2  | 1:63:A:LEU:HA  | 18       | 0.12          |
| (1,823)  | 1:33:A:ARG:HA   | 1:33:A:ARG:HD3 | 14       | 0.12          |
| (1,822)  | 1:56:A:ARG:H    | 1:56:A:ARG:HD2 | 1        | 0.12          |
| (1,811)  | 1:7:A:PHE:HE1   | 1:9:A:GLY:HA2  | 17       | 0.12          |
| (1,811)  | 1:7:A:PHE:HE2   | 1:9:A:GLY:HA2  | 17       | 0.12          |
| (1,787)  | 1:11:A:LEU:HB2  | 1:12:A:PRO:HD2 | 14       | 0.12          |
| (1,621)  | 1:25:A:LYS:HA   | 1:25:A:LYS:HB3 | 12       | 0.12          |
| (1,595)  | 1:28:A:SER:HB2  | 1:45:A:PHE:HE1 | 3        | 0.12          |
| (1,595)  | 1:28:A:SER:HB2  | 1:45:A:PHE:HE2 | 3        | 0.12          |
| (1,581)  | 1:10:A:SER:HB3  | 1:75:A:ASN:H   | 7        | 0.12          |
| (1,290)  | 1:27:A:SER:HB2  | 1:60:A:ILE:H   | 4        | 0.12          |
| (1,282)  | 1:59:A:ASP:H    | 1:59:A:ASP:HB3 | 10       | 0.12          |
| (1,222)  | 1:19:A:GLU:HB3  | 1:20:A:LEU:H   | 16       | 0.12          |
| (1,182)  | 1:68:A:LEU:HD11 | 1:72:A:LYS:H   | 1        | 0.12          |
| (1,182)  | 1:68:A:LEU:HD12 | 1:72:A:LYS:H   | 1        | 0.12          |
| (1,182)  | 1:68:A:LEU:HD13 | 1:72:A:LYS:H   | 1        | 0.12          |
| (1,182)  | 1:68:A:LEU:HD11 | 1:72:A:LYS:H   | 2        | 0.12          |
| (1,182)  | 1:68:A:LEU:HD12 | 1:72:A:LYS:H   | 2        | 0.12          |
| (1,182)  | 1:68:A:LEU:HD13 | 1:72:A:LYS:H   | 2        | 0.12          |
| (1,182)  | 1:68:A:LEU:HD11 | 1:72:A:LYS:H   | 3        | 0.12          |
| (1,182)  | 1:68:A:LEU:HD12 | 1:72:A:LYS:H   | 3        | 0.12          |
| (1,182)  | 1:68:A:LEU:HD13 | 1:72:A:LYS:H   | 3        | 0.12          |
| (1,182)  | 1:68:A:LEU:HD11 | 1:72:A:LYS:H   | 4        | 0.12          |
| (1,182)  | 1:68:A:LEU:HD12 | 1:72:A:LYS:H   | 4        | 0.12          |
| (1,182)  | 1:68:A:LEU:HD13 | 1:72:A:LYS:H   | 4        | 0.12          |
| (1,182)  | 1:68:A:LEU:HD11 | 1:72:A:LYS:H   | 7        | 0.12          |
| (1,182)  | 1:68:A:LEU:HD12 | 1:72:A:LYS:H   | 7        | 0.12          |
| (1,182)  | 1:68:A:LEU:HD13 | 1:72:A:LYS:H   | 7        | 0.12          |
| (1,182)  | 1:68:A:LEU:HD11 | 1:72:A:LYS:H   | 8        | 0.12          |
| (1,182)  | 1:68:A:LEU:HD12 | 1:72:A:LYS:H   | 8        | 0.12          |
| (1,182)  | 1:68:A:LEU:HD13 | 1:72:A:LYS:H   | 8        | 0.12          |
| (1,182)  | 1:68:A:LEU:HD11 | 1:72:A:LYS:H   | 18       | 0.12          |
| (1,182)  | 1:68:A:LEU:HD12 | 1:72:A:LYS:H   | 18       | 0.12          |
| (1,182)  | 1:68:A:LEU:HD13 | 1:72:A:LYS:H   | 18       | 0.12          |
| (1,182)  | 1:68:A:LEU:HD11 | 1:72:A:LYS:H   | 20       | 0.12          |
| (1,182)  | 1:68:A:LEU:HD12 | 1:72:A:LYS:H   | 20       | 0.12          |
| (1,182)  | 1:68:A:LEU:HD13 | 1:72:A:LYS:H   | 20       | 0.12          |
| (1,149)  | 1:23:A:HIS:HB2  | 1:25:A:LYS:H   | 9        | 0.12          |
| (1,15)   | 1:6:A:VAL:H     | 1:43:A:LEU:HB3 | 19       | 0.12          |
| (1,1313) | 1:58:A:MET:HB3  | 1:58:A:MET:HE1 | 8        | 0.11          |
| (1,1313) | 1:58:A:MET:HB3  | 1:58:A:MET:HE2 | 8        | 0.11          |
| (1,1313) | 1:58:A:MET:HB3  | 1:58:A:MET:HE3 | 8        | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1248) | 1:8:A:VAL:HG11  | 1:43:A:LEU:HD21 | 2        | 0.11          |
| (1,1248) | 1:8:A:VAL:HG11  | 1:43:A:LEU:HD22 | 2        | 0.11          |
| (1,1248) | 1:8:A:VAL:HG11  | 1:43:A:LEU:HD23 | 2        | 0.11          |
| (1,1248) | 1:8:A:VAL:HG12  | 1:43:A:LEU:HD21 | 2        | 0.11          |
| (1,1248) | 1:8:A:VAL:HG12  | 1:43:A:LEU:HD22 | 2        | 0.11          |
| (1,1248) | 1:8:A:VAL:HG12  | 1:43:A:LEU:HD23 | 2        | 0.11          |
| (1,1248) | 1:8:A:VAL:HG13  | 1:43:A:LEU:HD21 | 2        | 0.11          |
| (1,1248) | 1:8:A:VAL:HG13  | 1:43:A:LEU:HD22 | 2        | 0.11          |
| (1,1248) | 1:8:A:VAL:HG13  | 1:43:A:LEU:HD23 | 2        | 0.11          |
| (1,1226) | 1:8:A:VAL:HG21  | 1:11:A:LEU:HD21 | 13       | 0.11          |
| (1,1226) | 1:8:A:VAL:HG21  | 1:11:A:LEU:HD22 | 13       | 0.11          |
| (1,1226) | 1:8:A:VAL:HG21  | 1:11:A:LEU:HD23 | 13       | 0.11          |
| (1,1226) | 1:8:A:VAL:HG22  | 1:11:A:LEU:HD21 | 13       | 0.11          |
| (1,1226) | 1:8:A:VAL:HG22  | 1:11:A:LEU:HD22 | 13       | 0.11          |
| (1,1226) | 1:8:A:VAL:HG22  | 1:11:A:LEU:HD23 | 13       | 0.11          |
| (1,1226) | 1:8:A:VAL:HG23  | 1:11:A:LEU:HD21 | 13       | 0.11          |
| (1,1226) | 1:8:A:VAL:HG23  | 1:11:A:LEU:HD22 | 13       | 0.11          |
| (1,1226) | 1:8:A:VAL:HG23  | 1:11:A:LEU:HD23 | 13       | 0.11          |
| (1,1132) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD11 | 19       | 0.11          |
| (1,1132) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD12 | 19       | 0.11          |
| (1,1132) | 1:23:A:HIS:HB3  | 1:69:A:LEU:HD13 | 19       | 0.11          |
| (1,1049) | 1:15:A:ILE:HG13 | 1:70:A:LYS:HE2  | 4        | 0.11          |
| (1,1049) | 1:15:A:ILE:HG13 | 1:70:A:LYS:HE3  | 4        | 0.11          |
| (1,1041) | 1:70:A:LYS:HB3  | 1:71:A:GLU:H    | 4        | 0.11          |
| (1,989)  | 1:24:A:PHE:HE1  | 1:64:A:GLN:HG2  | 10       | 0.11          |
| (1,989)  | 1:24:A:PHE:HE2  | 1:64:A:GLN:HG2  | 10       | 0.11          |
| (1,987)  | 1:24:A:PHE:HD1  | 1:64:A:GLN:HG2  | 8        | 0.11          |
| (1,987)  | 1:24:A:PHE:HD2  | 1:64:A:GLN:HG2  | 8        | 0.11          |
| (1,896)  | 1:62:A:LEU:HB2  | 1:64:A:GLN:H    | 14       | 0.11          |
| (1,892)  | 1:62:A:LEU:HB2  | 1:63:A:LEU:HA   | 6        | 0.11          |
| (1,892)  | 1:62:A:LEU:HB2  | 1:63:A:LEU:HA   | 11       | 0.11          |
| (1,892)  | 1:62:A:LEU:HB2  | 1:63:A:LEU:HA   | 12       | 0.11          |
| (1,873)  | 1:75:A:ASN:H    | 1:75:A:ASN:HB2  | 11       | 0.11          |
| (1,873)  | 1:75:A:ASN:H    | 1:75:A:ASN:HB2  | 12       | 0.11          |
| (1,873)  | 1:75:A:ASN:H    | 1:75:A:ASN:HB2  | 19       | 0.11          |
| (1,873)  | 1:75:A:ASN:H    | 1:75:A:ASN:HB2  | 20       | 0.11          |
| (1,789)  | 1:11:A:LEU:HB3  | 1:39:A:GLY:HA2  | 1        | 0.11          |
| (1,789)  | 1:11:A:LEU:HB3  | 1:39:A:GLY:HA2  | 10       | 0.11          |
| (1,581)  | 1:10:A:SER:HB3  | 1:75:A:ASN:H    | 19       | 0.11          |
| (1,440)  | 1:25:A:LYS:HB2  | 1:27:A:SER:H    | 14       | 0.11          |
| (1,428)  | 1:9:A:GLY:HA3   | 1:11:A:LEU:H    | 2        | 0.11          |
| (1,416)  | 1:55:A:GLN:HE22 | 1:59:A:ASP:HA   | 11       | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,312)  | 1:58:A:MET:H    | 1:58:A:MET:HB3  | 5        | 0.11          |
| (1,312)  | 1:58:A:MET:H    | 1:58:A:MET:HB3  | 11       | 0.11          |
| (1,180)  | 1:72:A:LYS:H    | 1:72:A:LYS:HG3  | 7        | 0.11          |
| (1,78)   | 1:59:A:ASP:HB3  | 1:61:A:ALA:H    | 6        | 0.11          |
| (1,1360) | 1:23:A:HIS:HB2  | 1:23:A:HIS:HD2  | 12       | 0.1           |
| (1,1334) | 1:4:A:PHE:HD1   | 1:54:A:ILE:HD11 | 11       | 0.1           |
| (1,1334) | 1:4:A:PHE:HD1   | 1:54:A:ILE:HD12 | 11       | 0.1           |
| (1,1334) | 1:4:A:PHE:HD1   | 1:54:A:ILE:HD13 | 11       | 0.1           |
| (1,1334) | 1:4:A:PHE:HD2   | 1:54:A:ILE:HD11 | 11       | 0.1           |
| (1,1334) | 1:4:A:PHE:HD2   | 1:54:A:ILE:HD12 | 11       | 0.1           |
| (1,1334) | 1:4:A:PHE:HD2   | 1:54:A:ILE:HD13 | 11       | 0.1           |
| (1,1279) | 1:5:A:ILE:HG21  | 1:79:A:THR:HG21 | 6        | 0.1           |
| (1,1279) | 1:5:A:ILE:HG21  | 1:79:A:THR:HG22 | 6        | 0.1           |
| (1,1279) | 1:5:A:ILE:HG21  | 1:79:A:THR:HG23 | 6        | 0.1           |
| (1,1279) | 1:5:A:ILE:HG22  | 1:79:A:THR:HG21 | 6        | 0.1           |
| (1,1279) | 1:5:A:ILE:HG22  | 1:79:A:THR:HG22 | 6        | 0.1           |
| (1,1279) | 1:5:A:ILE:HG22  | 1:79:A:THR:HG23 | 6        | 0.1           |
| (1,1279) | 1:5:A:ILE:HG23  | 1:79:A:THR:HG21 | 6        | 0.1           |
| (1,1279) | 1:5:A:ILE:HG23  | 1:79:A:THR:HG22 | 6        | 0.1           |
| (1,1279) | 1:5:A:ILE:HG23  | 1:79:A:THR:HG23 | 6        | 0.1           |
| (1,1248) | 1:8:A:VAL:HG11  | 1:43:A:LEU:HD21 | 6        | 0.1           |
| (1,1248) | 1:8:A:VAL:HG11  | 1:43:A:LEU:HD22 | 6        | 0.1           |
| (1,1248) | 1:8:A:VAL:HG11  | 1:43:A:LEU:HD23 | 6        | 0.1           |
| (1,1248) | 1:8:A:VAL:HG12  | 1:43:A:LEU:HD21 | 6        | 0.1           |
| (1,1248) | 1:8:A:VAL:HG12  | 1:43:A:LEU:HD22 | 6        | 0.1           |
| (1,1248) | 1:8:A:VAL:HG12  | 1:43:A:LEU:HD23 | 6        | 0.1           |
| (1,1248) | 1:8:A:VAL:HG13  | 1:43:A:LEU:HD21 | 6        | 0.1           |
| (1,1248) | 1:8:A:VAL:HG13  | 1:43:A:LEU:HD22 | 6        | 0.1           |
| (1,1248) | 1:8:A:VAL:HG13  | 1:43:A:LEU:HD23 | 6        | 0.1           |
| (1,1222) | 1:16:A:THR:HG21 | 1:18:A:VAL:HG21 | 1        | 0.1           |
| (1,1222) | 1:16:A:THR:HG21 | 1:18:A:VAL:HG22 | 1        | 0.1           |
| (1,1222) | 1:16:A:THR:HG21 | 1:18:A:VAL:HG23 | 1        | 0.1           |
| (1,1222) | 1:16:A:THR:HG22 | 1:18:A:VAL:HG21 | 1        | 0.1           |
| (1,1222) | 1:16:A:THR:HG22 | 1:18:A:VAL:HG22 | 1        | 0.1           |
| (1,1222) | 1:16:A:THR:HG22 | 1:18:A:VAL:HG23 | 1        | 0.1           |
| (1,1222) | 1:16:A:THR:HG23 | 1:18:A:VAL:HG21 | 1        | 0.1           |
| (1,1222) | 1:16:A:THR:HG23 | 1:18:A:VAL:HG22 | 1        | 0.1           |
| (1,1222) | 1:16:A:THR:HG23 | 1:18:A:VAL:HG23 | 1        | 0.1           |
| (1,1123) | 1:20:A:LEU:HD11 | 1:24:A:PHE:HE1  | 18       | 0.1           |
| (1,1123) | 1:20:A:LEU:HD11 | 1:24:A:PHE:HE2  | 18       | 0.1           |
| (1,1123) | 1:20:A:LEU:HD12 | 1:24:A:PHE:HE1  | 18       | 0.1           |
| (1,1123) | 1:20:A:LEU:HD12 | 1:24:A:PHE:HE2  | 18       | 0.1           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1123) | 1:20:A:LEU:HD13 | 1:24:A:PHE:HE1  | 18       | 0.1           |
| (1,1123) | 1:20:A:LEU:HD13 | 1:24:A:PHE:HE2  | 18       | 0.1           |
| (1,1069) | 1:61:A:ALA:HA   | 1:64:A:GLN:HB3  | 18       | 0.1           |
| (1,1049) | 1:15:A:ILE:HG13 | 1:70:A:LYS:HE2  | 1        | 0.1           |
| (1,1049) | 1:15:A:ILE:HG13 | 1:70:A:LYS:HE3  | 1        | 0.1           |
| (1,1049) | 1:15:A:ILE:HG13 | 1:70:A:LYS:HE2  | 5        | 0.1           |
| (1,1049) | 1:15:A:ILE:HG13 | 1:70:A:LYS:HE3  | 5        | 0.1           |
| (1,1013) | 1:65:A:HIS:HB3  | 1:76:A:VAL:H    | 11       | 0.1           |
| (1,1013) | 1:65:A:HIS:HB3  | 1:76:A:VAL:H    | 12       | 0.1           |
| (1,989)  | 1:24:A:PHE:HE1  | 1:64:A:GLN:HG2  | 15       | 0.1           |
| (1,989)  | 1:24:A:PHE:HE2  | 1:64:A:GLN:HG2  | 15       | 0.1           |
| (1,979)  | 1:54:A:ILE:HG21 | 1:55:A:GLN:HG2  | 6        | 0.1           |
| (1,979)  | 1:54:A:ILE:HG21 | 1:55:A:GLN:HG3  | 6        | 0.1           |
| (1,979)  | 1:54:A:ILE:HG22 | 1:55:A:GLN:HG2  | 6        | 0.1           |
| (1,979)  | 1:54:A:ILE:HG22 | 1:55:A:GLN:HG3  | 6        | 0.1           |
| (1,979)  | 1:54:A:ILE:HG23 | 1:55:A:GLN:HG2  | 6        | 0.1           |
| (1,979)  | 1:54:A:ILE:HG23 | 1:55:A:GLN:HG3  | 6        | 0.1           |
| (1,979)  | 1:54:A:ILE:HG21 | 1:55:A:GLN:HG2  | 11       | 0.1           |
| (1,979)  | 1:54:A:ILE:HG21 | 1:55:A:GLN:HG3  | 11       | 0.1           |
| (1,979)  | 1:54:A:ILE:HG22 | 1:55:A:GLN:HG2  | 11       | 0.1           |
| (1,979)  | 1:54:A:ILE:HG22 | 1:55:A:GLN:HG3  | 11       | 0.1           |
| (1,979)  | 1:54:A:ILE:HG23 | 1:55:A:GLN:HG2  | 11       | 0.1           |
| (1,979)  | 1:54:A:ILE:HG23 | 1:55:A:GLN:HG3  | 11       | 0.1           |
| (1,979)  | 1:54:A:ILE:HG21 | 1:55:A:GLN:HG2  | 19       | 0.1           |
| (1,979)  | 1:54:A:ILE:HG21 | 1:55:A:GLN:HG3  | 19       | 0.1           |
| (1,979)  | 1:54:A:ILE:HG22 | 1:55:A:GLN:HG2  | 19       | 0.1           |
| (1,979)  | 1:54:A:ILE:HG22 | 1:55:A:GLN:HG3  | 19       | 0.1           |
| (1,979)  | 1:54:A:ILE:HG23 | 1:55:A:GLN:HG2  | 19       | 0.1           |
| (1,979)  | 1:54:A:ILE:HG23 | 1:55:A:GLN:HG3  | 19       | 0.1           |
| (1,957)  | 1:6:A:VAL:HB    | 1:43:A:LEU:HB3  | 16       | 0.1           |
| (1,902)  | 1:50:A:ASP:HB2  | 1:54:A:ILE:HG21 | 20       | 0.1           |
| (1,902)  | 1:50:A:ASP:HB2  | 1:54:A:ILE:HG22 | 20       | 0.1           |
| (1,902)  | 1:50:A:ASP:HB2  | 1:54:A:ILE:HG23 | 20       | 0.1           |
| (1,902)  | 1:50:A:ASP:HB3  | 1:54:A:ILE:HG21 | 20       | 0.1           |
| (1,902)  | 1:50:A:ASP:HB3  | 1:54:A:ILE:HG22 | 20       | 0.1           |
| (1,902)  | 1:50:A:ASP:HB3  | 1:54:A:ILE:HG23 | 20       | 0.1           |
| (1,873)  | 1:75:A:ASN:H    | 1:75:A:ASN:HB2  | 2        | 0.1           |
| (1,873)  | 1:75:A:ASN:H    | 1:75:A:ASN:HB2  | 9        | 0.1           |
| (1,872)  | 1:30:A:ASP:HB3  | 1:46:A:ASP:H    | 14       | 0.1           |
| (1,811)  | 1:7:A:PHE:HE1   | 1:9:A:GLY:HA2   | 2        | 0.1           |
| (1,811)  | 1:7:A:PHE:HE2   | 1:9:A:GLY:HA2   | 2        | 0.1           |
| (1,799)  | 1:57:A:ARG:H    | 1:57:A:ARG:HD3  | 7        | 0.1           |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,650) | 1:51:A:ARG:HA  | 1:52:A:THR:HG21 | 2        | 0.1           |
| (1,650) | 1:51:A:ARG:HA  | 1:52:A:THR:HG22 | 2        | 0.1           |
| (1,650) | 1:51:A:ARG:HA  | 1:52:A:THR:HG23 | 2        | 0.1           |
| (1,650) | 1:51:A:ARG:HA  | 1:52:A:THR:HG21 | 15       | 0.1           |
| (1,650) | 1:51:A:ARG:HA  | 1:52:A:THR:HG22 | 15       | 0.1           |
| (1,650) | 1:51:A:ARG:HA  | 1:52:A:THR:HG23 | 15       | 0.1           |
| (1,621) | 1:25:A:LYS:HA  | 1:25:A:LYS:HB3  | 6        | 0.1           |
| (1,461) | 1:29:A:PRO:HB3 | 1:31:A:GLN:H    | 7        | 0.1           |
| (1,312) | 1:58:A:MET:H   | 1:58:A:MET:HB3  | 9        | 0.1           |
| (1,282) | 1:59:A:ASP:H   | 1:59:A:ASP:HB3  | 19       | 0.1           |
| (1,222) | 1:19:A:GLU:HB3 | 1:20:A:LEU:H    | 7        | 0.1           |
| (1,204) | 1:43:A:LEU:HB2 | 1:44:A:GLU:H    | 2        | 0.1           |

## 10 Dihedral-angle violation analysis [i](#)

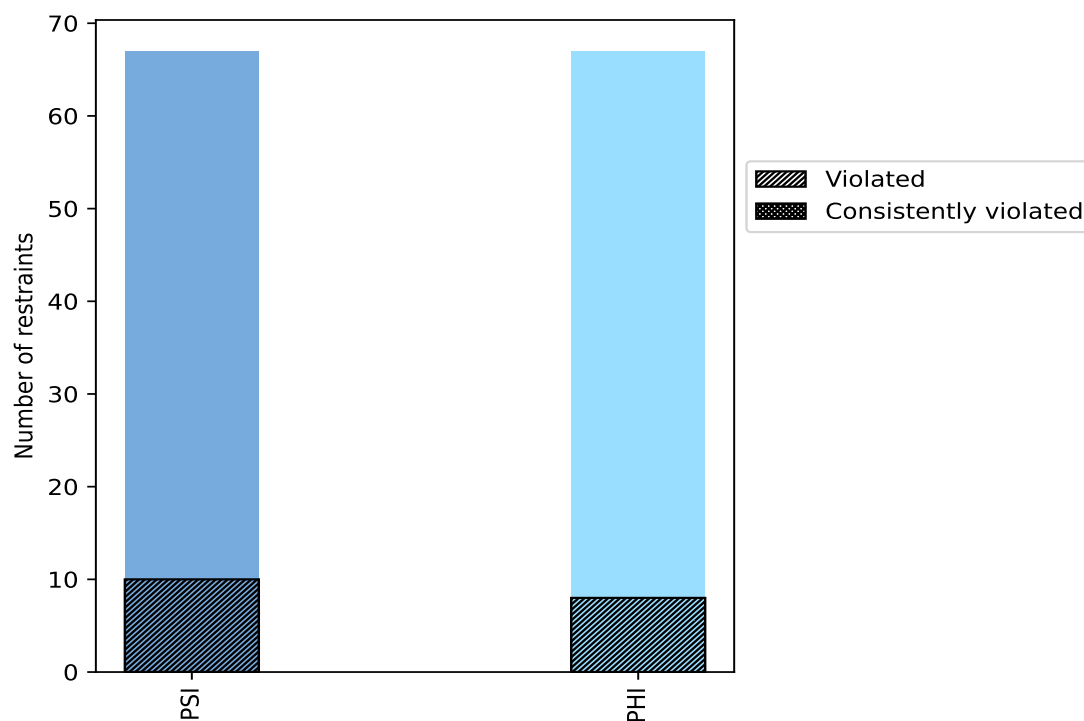
### 10.1 Summary of dihedral-angle violations [i](#)

The following table provides the summary of dihedral-angle violations in different dihedral-angle types. Violations less than 1° are not included in the calculation.

| Angle 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> |
| PSI        | 67    | 50.0           | 10                    | 14.9           | 7.5            | 0                                  | 0.0            | 0.0            |
| PHI        | 67    | 50.0           | 8                     | 11.9           | 6.0            | 0                                  | 0.0            | 0.0            |
| Total      | 134   | 100.0          | 18                    | 13.4           | 13.4           | 0                                  | 0.0            | 0.0            |

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

#### 10.1.1 Bar chart : Distribution of dihedral-angles and violations [i](#)



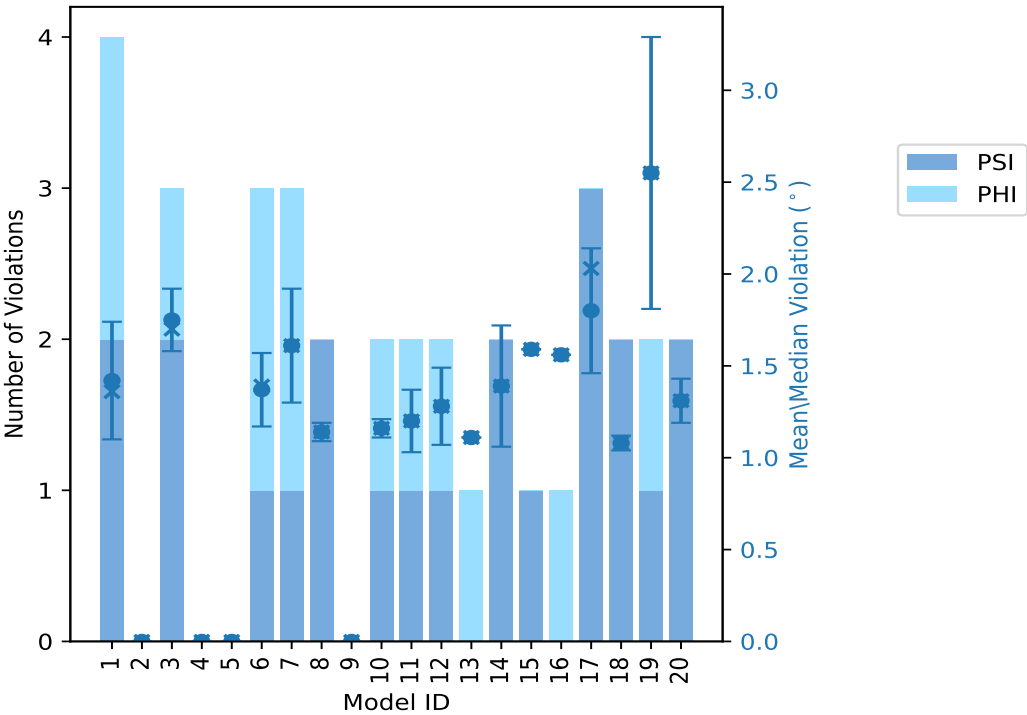
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

## 10.2 Dihedral-angle violation statistics for each model ⓘ

The following table provides the dihedral-angle violation statistics for each model in the ensemble. Violations less than 1° are not included in the statistics.

| Model ID | Number of violations |     |       | Mean (°) | Max (°) | SD (°) | Median (°) |
|----------|----------------------|-----|-------|----------|---------|--------|------------|
|          | PSI                  | PHI | Total |          |         |        |            |
| 1        | 2                    | 2   | 4     | 1.42     | 1.91    | 0.32   | 1.36       |
| 2        | 0                    | 0   | 0     | 0.0      | 0.0     | 0.0    | 0.0        |
| 3        | 2                    | 1   | 3     | 1.75     | 1.98    | 0.17   | 1.7        |
| 4        | 0                    | 0   | 0     | 0.0      | 0.0     | 0.0    | 0.0        |
| 5        | 0                    | 0   | 0     | 0.0      | 0.0     | 0.0    | 0.0        |
| 6        | 1                    | 2   | 3     | 1.37     | 1.61    | 0.2    | 1.39       |
| 7        | 1                    | 2   | 3     | 1.61     | 1.99    | 0.31   | 1.61       |
| 8        | 2                    | 0   | 2     | 1.14     | 1.2     | 0.05   | 1.14       |
| 9        | 0                    | 0   | 0     | 0.0      | 0.0     | 0.0    | 0.0        |
| 10       | 1                    | 1   | 2     | 1.16     | 1.21    | 0.05   | 1.16       |
| 11       | 1                    | 1   | 2     | 1.2      | 1.37    | 0.17   | 1.2        |
| 12       | 1                    | 1   | 2     | 1.28     | 1.5     | 0.21   | 1.28       |
| 13       | 0                    | 1   | 1     | 1.11     | 1.11    | 0.0    | 1.11       |
| 14       | 2                    | 0   | 2     | 1.39     | 1.72    | 0.33   | 1.39       |
| 15       | 1                    | 0   | 1     | 1.59     | 1.59    | 0.0    | 1.59       |
| 16       | 0                    | 1   | 1     | 1.56     | 1.56    | 0.0    | 1.56       |
| 17       | 3                    | 0   | 3     | 1.8      | 2.05    | 0.34   | 2.03       |
| 18       | 2                    | 0   | 2     | 1.08     | 1.11    | 0.04   | 1.08       |
| 19       | 1                    | 1   | 2     | 2.55     | 3.3     | 0.74   | 2.55       |
| 20       | 2                    | 0   | 2     | 1.31     | 1.43    | 0.12   | 1.31       |

10.2.1 Bar graph : Dihedral violation statistics for each model ⓘ



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

10.3 Dihedral-angle violation statistics for the ensemble ⓘ

Violation analysis may find that some restraints are violated in very 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 ensemble.

| Number of violated restraints |     |       | Fraction of the ensemble |      |
|-------------------------------|-----|-------|--------------------------|------|
| PSI                           | PHI | Total | Count <sup>1</sup>       | %    |
| 4                             | 5   | 9     | 1                        | 5.0  |
| 4                             | 1   | 5     | 2                        | 10.0 |
| 0                             | 2   | 2     | 3                        | 15.0 |
| 1                             | 0   | 1     | 4                        | 20.0 |
| 0                             | 0   | 0     | 5                        | 25.0 |
| 1                             | 0   | 1     | 6                        | 30.0 |
| 0                             | 0   | 0     | 7                        | 35.0 |
| 0                             | 0   | 0     | 8                        | 40.0 |
| 0                             | 0   | 0     | 9                        | 45.0 |
| 0                             | 0   | 0     | 10                       | 50.0 |
| 0                             | 0   | 0     | 11                       | 55.0 |

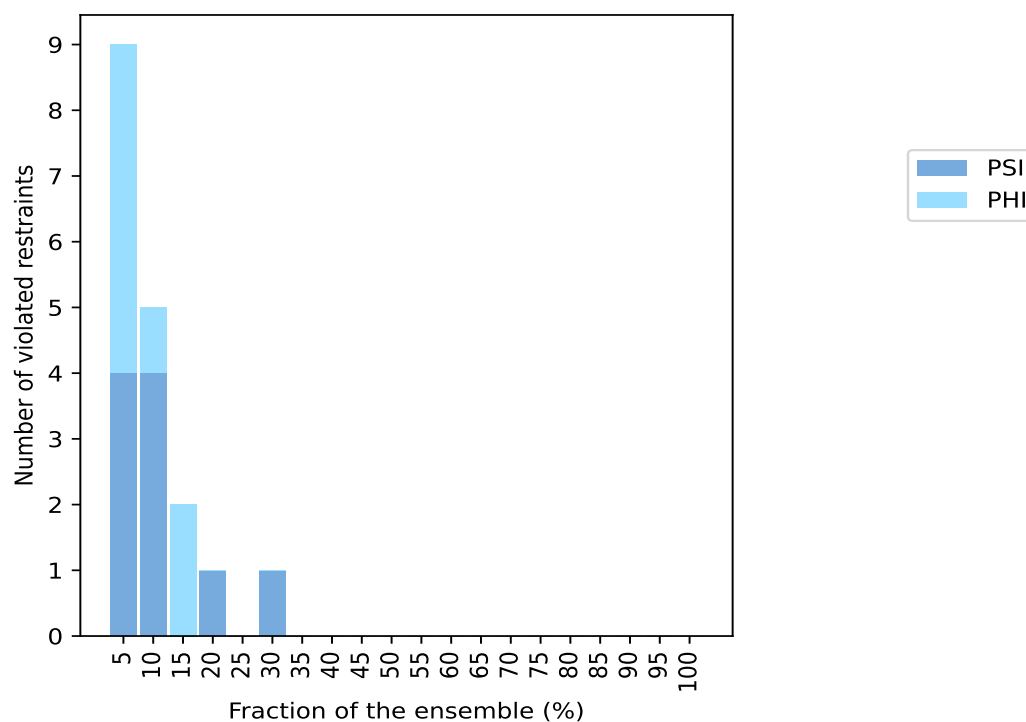
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| Number of violated restraints |     |       | Fraction of the ensemble |       |
|-------------------------------|-----|-------|--------------------------|-------|
| PSI                           | PHI | Total | Count <sup>1</sup>       | %     |
| 0                             | 0   | 0     | 12                       | 60.0  |
| 0                             | 0   | 0     | 13                       | 65.0  |
| 0                             | 0   | 0     | 14                       | 70.0  |
| 0                             | 0   | 0     | 15                       | 75.0  |
| 0                             | 0   | 0     | 16                       | 80.0  |
| 0                             | 0   | 0     | 17                       | 85.0  |
| 0                             | 0   | 0     | 18                       | 90.0  |
| 0                             | 0   | 0     | 19                       | 95.0  |
| 0                             | 0   | 0     | 20                       | 100.0 |

<sup>1</sup> Number of models with violations

### 10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)

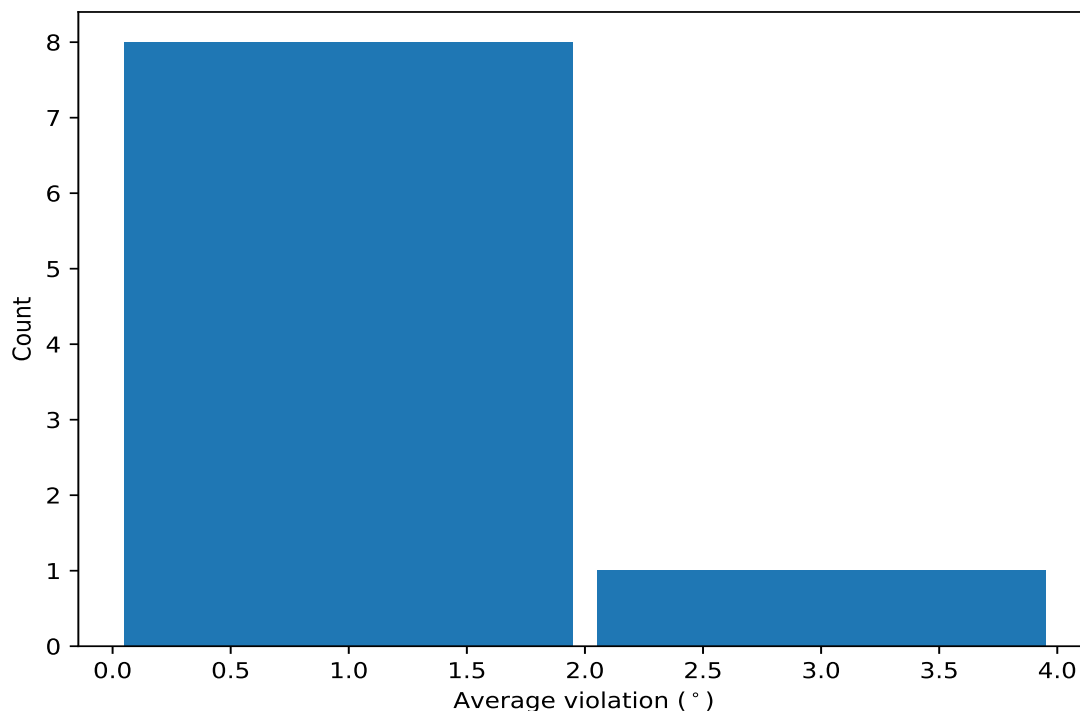


## 10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

### 10.4.1 Histogram : Distribution of mean dihedral-angle violations [i](#)

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

in the ensemble



#### 10.4.2 Table: Most violated dihedral-angle 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.

| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Models <sup>1</sup> | Mean | SD <sup>2</sup> | Median |
|---------|--------------|---------------|---------------|--------------|---------------------|------|-----------------|--------|
| (1,50)  | 1:33:A:ARG:N | 1:33:A:ARG:CA | 1:33:A:ARG:C  | 1:34:A:LEU:N | 6                   | 1.34 | 0.37            | 1.14   |
| (1,124) | 1:74:A:ILE:N | 1:74:A:ILE:CA | 1:74:A:ILE:C  | 1:75:A:ASN:N | 4                   | 2.03 | 0.79            | 1.81   |
| (1,107) | 1:63:A:LEU:C | 1:64:A:GLN:N  | 1:64:A:GLN:CA | 1:64:A:GLN:C | 3                   | 1.64 | 0.38            | 1.81   |
| (1,79)  | 1:48:A:ASP:C | 1:49:A:LYS:N  | 1:49:A:LYS:CA | 1:49:A:LYS:C | 3                   | 1.43 | 0.15            | 1.5    |
| (1,5)   | 1:4:A:PHE:C  | 1:5:A:ILE:N   | 1:5:A:ILE:CA  | 1:5:A:ILE:C  | 2                   | 1.6  | 0.38            | 1.6    |
| (1,132) | 1:78:A:LEU:N | 1:78:A:LEU:CA | 1:78:A:LEU:C  | 1:79:A:THR:N | 2                   | 1.4  | 0.31            | 1.4    |
| (1,6)   | 1:5:A:ILE:N  | 1:5:A:ILE:CA  | 1:5:A:ILE:C   | 1:6:A:VAL:N  | 2                   | 1.35 | 0.08            | 1.35   |
| (1,86)  | 1:52:A:THR:N | 1:52:A:THR:CA | 1:52:A:THR:C  | 1:53:A:GLY:N | 2                   | 1.21 | 0.18            | 1.21   |
| (1,114) | 1:68:A:LEU:N | 1:68:A:LEU:CA | 1:68:A:LEU:C  | 1:69:A:LEU:N | 2                   | 1.21 | 0.11            | 1.21   |

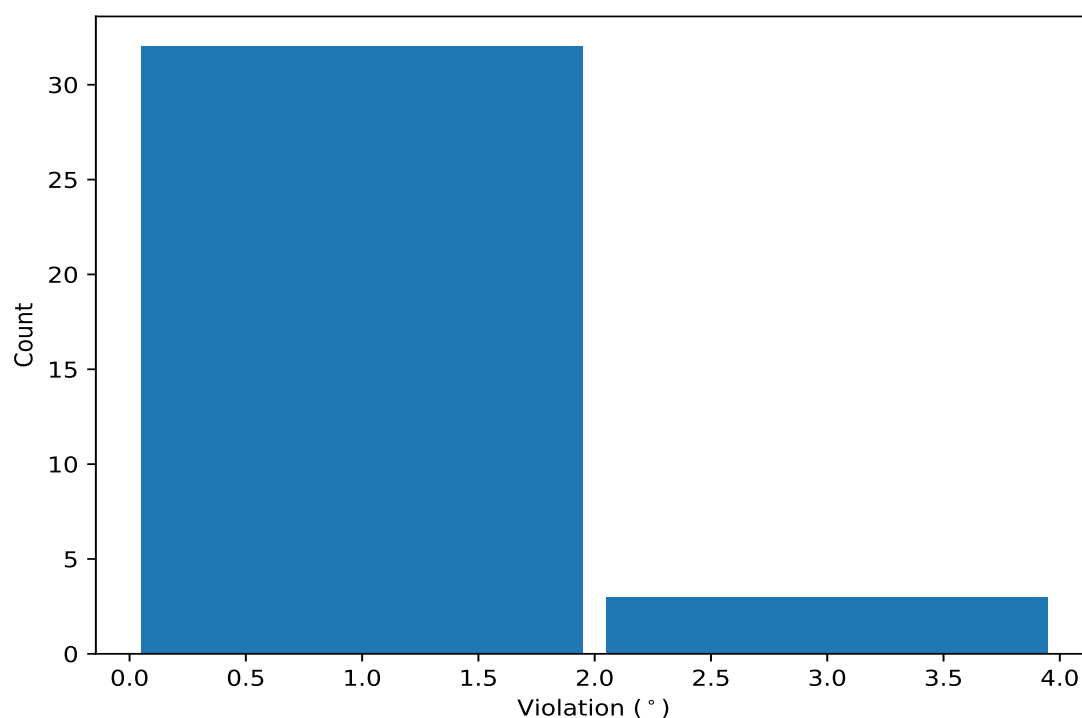
<sup>1</sup> Number of violated models, <sup>2</sup>Standard deviation, All angle values are in degree (°)

## 10.5 All violated dihedral-angle restraints [i](#)

### 10.5.1 Histogram : Distribution of violations [i](#)

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





### 10.5.2 Table: All violated dihedral-angle restraints [i](#)

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,124) | 1:74:A:ILE:N | 1:74:A:ILE:CA | 1:74:A:ILE:C  | 1:75:A:ASN:N | 19       | 3.3           |
| (1,50)  | 1:33:A:ARG:N | 1:33:A:ARG:CA | 1:33:A:ARG:C  | 1:34:A:LEU:N | 17       | 2.05          |
| (1,124) | 1:74:A:ILE:N | 1:74:A:ILE:CA | 1:74:A:ILE:C  | 1:75:A:ASN:N | 17       | 2.03          |
| (1,107) | 1:63:A:LEU:C | 1:64:A:GLN:N  | 1:64:A:GLN:CA | 1:64:A:GLN:C | 7        | 1.99          |
| (1,5)   | 1:4:A:PHE:C  | 1:5:A:ILE:N   | 1:5:A:ILE:CA  | 1:5:A:ILE:C  | 3        | 1.98          |
| (1,26)  | 1:19:A:GLU:N | 1:19:A:GLU:CA | 1:19:A:GLU:C  | 1:20:A:LEU:N | 1        | 1.91          |
| (1,107) | 1:63:A:LEU:C | 1:64:A:GLN:N  | 1:64:A:GLN:CA | 1:64:A:GLN:C | 19       | 1.81          |
| (1,132) | 1:78:A:LEU:N | 1:78:A:LEU:CA | 1:78:A:LEU:C  | 1:79:A:THR:N | 14       | 1.72          |
| (1,134) | 1:79:A:THR:N | 1:79:A:THR:CA | 1:79:A:THR:C  | 1:80:A:VAL:N | 3        | 1.7           |
| (1,113) | 1:67:A:THR:C | 1:68:A:LEU:N  | 1:68:A:LEU:CA | 1:68:A:LEU:C | 6        | 1.61          |
| (1,50)  | 1:33:A:ARG:N | 1:33:A:ARG:CA | 1:33:A:ARG:C  | 1:34:A:LEU:N | 7        | 1.61          |
| (1,124) | 1:74:A:ILE:N | 1:74:A:ILE:CA | 1:74:A:ILE:C  | 1:75:A:ASN:N | 15       | 1.59          |
| (1,130) | 1:77:A:GLU:N | 1:77:A:GLU:CA | 1:77:A:GLU:C  | 1:78:A:LEU:N | 3        | 1.56          |
| (1,79)  | 1:48:A:ASP:C | 1:49:A:LYS:N  | 1:49:A:LYS:CA | 1:49:A:LYS:C | 16       | 1.56          |
| (1,79)  | 1:48:A:ASP:C | 1:49:A:LYS:N  | 1:49:A:LYS:CA | 1:49:A:LYS:C | 12       | 1.5           |
| (1,27)  | 1:19:A:GLU:C | 1:20:A:LEU:N  | 1:20:A:LEU:CA | 1:20:A:LEU:C | 1        | 1.45          |
| (1,6)   | 1:5:A:ILE:N  | 1:5:A:ILE:CA  | 1:5:A:ILE:C   | 1:6:A:VAL:N  | 20       | 1.43          |
| (1,86)  | 1:52:A:THR:N | 1:52:A:THR:CA | 1:52:A:THR:C  | 1:53:A:GLY:N | 6        | 1.39          |
| (1,49)  | 1:32:A:ILE:C | 1:33:A:ARG:N  | 1:33:A:ARG:CA | 1:33:A:ARG:C | 11       | 1.37          |
| (1,114) | 1:68:A:LEU:N | 1:68:A:LEU:CA | 1:68:A:LEU:C  | 1:69:A:LEU:N | 17       | 1.32          |
| (1,6)   | 1:5:A:ILE:N  | 1:5:A:ILE:CA  | 1:5:A:ILE:C   | 1:6:A:VAL:N  | 1        | 1.27          |

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| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,79)  | 1:48:A:ASP:C | 1:49:A:LYS:N  | 1:49:A:LYS:CA | 1:49:A:LYS:C | 7        | 1.22          |
| (1,5)   | 1:4:A:PHE:C  | 1:5:A:ILE:N   | 1:5:A:ILE:CA  | 1:5:A:ILE:C  | 10       | 1.21          |
| (1,50)  | 1:33:A:ARG:N | 1:33:A:ARG:CA | 1:33:A:ARG:C  | 1:34:A:LEU:N | 8        | 1.2           |
| (1,124) | 1:74:A:ILE:N | 1:74:A:ILE:CA | 1:74:A:ILE:C  | 1:75:A:ASN:N | 20       | 1.19          |
| (1,57)  | 1:36:A:ALA:C | 1:37:A:ASP:N  | 1:37:A:ASP:CA | 1:37:A:ASP:C | 6        | 1.12          |
| (1,107) | 1:63:A:LEU:C | 1:64:A:GLN:N  | 1:64:A:GLN:CA | 1:64:A:GLN:C | 13       | 1.11          |
| (1,10)  | 1:7:A:PHE:N  | 1:7:A:PHE:CA  | 1:7:A:PHE:C   | 1:8:A:VAL:N  | 18       | 1.11          |
| (1,114) | 1:68:A:LEU:N | 1:68:A:LEU:CA | 1:68:A:LEU:C  | 1:69:A:LEU:N | 10       | 1.1           |
| (1,132) | 1:78:A:LEU:N | 1:78:A:LEU:CA | 1:78:A:LEU:C  | 1:79:A:THR:N | 8        | 1.09          |
| (1,50)  | 1:33:A:ARG:N | 1:33:A:ARG:CA | 1:33:A:ARG:C  | 1:34:A:LEU:N | 12       | 1.07          |
| (1,50)  | 1:33:A:ARG:N | 1:33:A:ARG:CA | 1:33:A:ARG:C  | 1:34:A:LEU:N | 14       | 1.06          |
| (1,59)  | 1:37:A:ASP:C | 1:38:A:LYS:N  | 1:38:A:LYS:CA | 1:38:A:LYS:C | 1        | 1.04          |
| (1,50)  | 1:33:A:ARG:N | 1:33:A:ARG:CA | 1:33:A:ARG:C  | 1:34:A:LEU:N | 18       | 1.04          |
| (1,86)  | 1:52:A:THR:N | 1:52:A:THR:CA | 1:52:A:THR:C  | 1:53:A:GLY:N | 11       | 1.03          |